Multidisciplinary modeling for sustainable engineering design and assessment

Dissertation

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Abstract

Design and assessment activities have traditionally been performed with respect to a relatively narrow analysis boundary and without accounting for influences from or on the world outside the boundary. This “all other things being equal” mindset results in tractable, generally solvable problems, but it precludes the detection of externalities, consequences that manifest outside the analysis boundary. From a sustainability perspective, externalities - whether they affect the environment, society, the economy, or other systems - cannot be ignored. Moreover, many externalities lead in turn to feedback effects, often negative, on the system of interest. Failing to account for these effects can result in decisions that appear economically, environmentally, or otherwise optimal within a narrow analysis boundary but are sub-optimal or simply incorrect when a larger perspective is taken.

To anticipate externalities and avoid the unpleasant surprises they lead to, it is critical to use a holistic perspective for sustainable design and assessment. While this is not a novel concept, to date most efforts towards sustainable design and assessment have been made within single fields of study, including engineering, economic analysis and life cycle assessment. The models used within each discipline are well-suited to the traditional, narrow analysis boundary but frequently capture systems outside that boundary in a simplistic and even unrealistic fashion. This dissertation posits that for sustainability applications, a holistic perspective is best accomplished
by combining modeling techniques and other methods from a variety of previously
disparate disciplines. These various techniques each have shortcomings and advan-
tages that are often complementary. Combining models from multiple disciplines thus
offers an opportunity to create a widely applicable, integrated method with all of the
advantages and relatively few of the shortcomings of each individual approach.

This dissertation addresses the need for multidisciplinary modeling in sustainabil-
ity applications. Two methods for sustainable assessment, both of which combine
mathematical and statistical modeling with life cycle assessment, are developed. Re-
gression streamlining applies linear regression and model cross-validation techniques
to streamlined life cycle assessment, resulting in a simple and intuitive way to generate
streamlined life cycle inventories as well as estimates of the error in the streamlined
inventories relative to a full inventory. The Comprehensive Allocation Investigation
Strategy (CAIS) is a calculation procedure for modeling life cycle inventories as func-
tions of allocation decisions. The results can be used to detect situations in which
one life cycle appears environmentally superior to another due to allocation decisions
rather than differences in the inventories.

The final contribution of this dissertation is the process-to-planet (P2P) modeling
framework for sustainable engineering applications. Several applications of the P2P
framework to engineering design are presented, with the conclusion that the P2P
framework results in environmentally superior designs compared to conventional sus-
tainable design methods. The P2P modeling approach also offers an opportunity to
integrate fundamental engineering models with macro-economic equilibrium models,
allowing engineering and economic policy design problems to be addressed within the
same framework. As a first step towards this integration, a methodology and case
study for modeling the effects of an environmental tax policy on a P2P system is presented. Extensions of the existing framework to include partial, general and hybrid equilibrium models are also discussed.
For Dad.
Acknowledgments

This dissertation happened because a large number of things amazingly failed to go wrong.\(^1\) Many thanks to my family, the Hanes Twig & Associates, for providing copious amounts of (in decreasing order of importance) love, support, sympathetic ears and food, both in times when things inevitably did go wrong and when things were going swimmingly. Thanks related to the actual research are due to Dr. Nathan Cruze and Prof. Prem Goel, who contributed much of the math behind Chapter 5 and provided extensive guidance on the path to publication, to John Davenport who laid the groundwork for Chapter 4, and to Varsha Gopalakrishnan who contributed greatly to Chapter 3 and to the renewable energy production case study. To my fellow researchers in the PSE Group, it has been a joy to work and commiserate with all of you. Thank you for patiently listening to me explain matrix after matrix after matrix, and for helping me to realize that, perhaps, six slides of equations is a few too many and maybe a figure is in order. Finally, infinite thanks to my advisor Dr. Bhavik Bakshi, who is to be relied upon to ask the difficult (and interesting) questions and provide excellent advice.

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Chapter 1: Introduction

1.1 Motivation

Problems are traditionally solved by drawing a line or analysis boundary around the problem and stating either explicitly or implicitly that the world outside the boundary is unaffected by the problem inside the boundary, and vice versa: a ceteris paribus or “all other things being equal” assumption. Engineers draw their boundaries around a process, a supply chain, a material, etc.; economists draw their boundaries around flows of goods and money; and life cycle assessment (LCA) practitioners draw their boundary around flows of energy, materials and pollutants.

Ceteris paribus yields a tractable, understandable problem that can generally be solved if a solution exists. However, the approach has a significant blind spot when it comes to capturing externalities, the effects of actions taken or decisions made inside the analysis boundary that manifest outside the boundary. Externalities are frequently problematic in and of themselves. For instance, land use change and the associated carbon debt is an indirect externality of biofuels production. [254] Moreover, externalities cause feedback effects on the system within the boundary which are rarely positive in nature. For many years industries ignored environmental externalities, leading eventually to public outcry and to government regulations (feedback)
on waste treatment, toxic pollutants and various emissions. Industries were forced to retrofit existing processes and to develop and implement new technology to remain in compliance, leading to increased production costs (negative feedback).

These are two examples of the ceteris paribus approach failing to deal with sustainability issues, which by definition require that the world outside the traditional boundary be accounted for in finding a solution to the problem inside the boundary. A holistic approach that explicitly accounts for externalities of various types (not only environmental and ecological) is therefore necessary, if negative feedback effects are to be avoided.

That sustainability must be addressed with a holistic approach is not a new idea; many of the current state-of-the-art methods for assessing and designing for sustainability were developed with a holistic approach in mind. Engineers deal with sustainability by combining LCA with design and optimization, thereby accounting for the environmental impacts caused by the engineering system. [154, 231, 294] Sustainability economics (more commonly called energy or environmental economics) examine the interplay between economic systems, technology and the environment. [184, 207] LCA is inherently a holistic approach [78], and has been made more so through the development of hybrid LCA [171] and consequential LCA approaches [94], both of which link life cycles to the surrounding economy. Figure 1.1 diagrams several approaches that address sustainability issues, showing how each approach is related to four separate disciplines.

Current efforts towards designing and assessing sustainability do rely on a holistic approach. However, for the most part engineering, economic, life cycle and environmental systems are studied in isolation from one another, or at best systems outside
Figure 1.1: Methods and models currently used to address sustainability issues. Dotted lines indicate one contribution of this dissertation.

that of interest are modeled in such a simplified manner that the models are only poor representations of the actual systems. [130] Sustainable engineering expands the analysis boundary of traditional engineering through LCA, but still treats life cycle processes as fixed and in particular models life cycle environmental interventions using constant emissions factors. [168] Any influence that the surrounding economy has on the engineering system is likewise neglected, or modeled in a simplistic manner that ignores the underlying complexity of the economic system. [115] Life cycle methods consider ever-larger boundaries through the use of global scale multi-regional input-output models, [65] but rely on empirical data, treat the constituent processes as fixed and linearly scalable, and do not benefit from the availability of engineering process models. Conversely, the ability of LCA and of economic models to consider...
scales all the way from the value chain to the planet has not been extended to sustainable engineering.

Addressing sustainability requires that models from previously disparate disciplines be brought together and applied to the same problem, for two reasons. First, combining multidisciplinary methods allows for different components of the same system, interactions within the system and with the world outside the system to be modeled: engineering systems with economic, ecological systems with societal and industrial, and so on. This allows the aforementioned externalities and feedback effects to be modeled explicitly and to be anticipated, rather than having feedback effects turn into unpleasant surprises. Second, because sustainability is fundamentally multi-objective [102], methods from different disciplines must be applied in order to quantify the various objectives. It is possible to define, for instance, a societal objective from an engineering perspective. [314] But because there are not likely to be any solutions that represent the best-case scenario for all objectives being considered in a sustainability-related problem, it is critical that trade-offs between the objectives and interactions between the different systems considered are captured as accurately and realistically as is feasible. This is accomplished by using the most relevant method to quantify each objective being considered, and by ensuring that the applied methods are mathematically and theoretically sound.

Multidisciplinarity is therefore a requirement and not merely an option when dealing with sustainability. It is impossible to think about sustainability in terms of a single approach or a single discipline: engineering and technology alone, economics alone, environment and ecology alone, and social aspects alone. The multiple objectives of sustainability are not separate problems to be solved but are rather several
aspects among many others of a large, complex and wicked problem. Methods and models from separate disciplines are complementary in that each provides insight unobtainable from the others, and while each method has its shortcomings, each method also has some advantage(s) over the others. [56] However, because “all models are wrong, but some are useful” ([57], p. 424), care must be taken that models used are just wrong (simplified) enough to be tractable, but not so wrong that they lose their accuracy and utility.

1.2 Objectives

The primary objective of this dissertation is to develop general and systematic methods for sustainability assessment and sustainable engineering that integrate techniques from previously disparate fields of study. The secondary objectives are the application of proposed methods to case studies and, where possible, quantitative demonstrations of the proposed method’s superiority over analogous state-of-the-art methods.

Specific objectives relating to sustainability assessment are as follows.

• Develop and demonstrate the use of an approach for streamlined life cycle assessment that allows for the calculation of streamlining error.

• Develop and demonstrate the use of a procedure for (a) modeling a life cycle inventory as a function of allocation decisions and (b) extracting information relevant to decision support from the resulting inventory functions.

Further specific objectives that relate to sustainable engineering are as follows.
• Develop and demonstrate several uses of a modeling framework for sustainable engineering applications that expands the analysis boundary of the design problem relative to conventional methods.

• Discuss methods for linking the aforementioned framework to economic modeling tools.

1.3 Contributions

This dissertation contributes to the field of sustainability assessment by developing quantitative and theoretically rigorous methods for performing streamlined LCAs and for dealing with allocation in life cycle inventories. This dissertation further contributes to the field of sustainable engineering by integrating models from engineering, life cycle assessment and economic input-output into a general multi-scale framework with a variety of design and assessment applications. Specific contributions are as follows.

• A statistical modeling and cross-validation method for streamlined life cycle assessment

• The Comprehensive Allocation Investigation Strategy for examining a life cycle inventory over all possible allocation decisions

• The process-to-planet (P2P) modeling framework for sustainable engineering applications
1.4 Organization

Chapter 2 presents background on methodologies currently used in sustainability assessment and design as well as relevant literature. Following the background, Chapter 3 presents a process based and tiered hybrid life cycle assessment of an integrated anaerobic digestion plant, with inventories given in Appendix A. Chapter 4 develops an approach to streamlined life cycle assessment that utilizes statistical modeling and applies this approach to two case studies. Appendix B contains raw data and R code for the two case studies of Chapter 4. Chapter 5 focuses on a strategy for dealing with multi-functionality and allocation in life cycle inventories, and presents two case studies. Appendix C contains inventory data, MATLAB code, complete results for both case studies and other relevant information for the work in Chapter 5.

The remainder of the dissertation focuses on a techno-economic modeling framework for sustainable engineering applications, the “process to planet” framework. This framework is developed in Chapter 6, with supporting information given in Appendix D. Chapter 7 discusses the application of the P2P framework to sustainable engineering design. A toy example is presented as a demonstration in this chapter as well as two case studies. Data and code for the case studies and demonstration is given in Appendix E. Several economic modeling extensions to the P2P framework, including prospective applications, are discussed in Chapter 8. Chapter 9 summarizes the contributions of this dissertation and discusses ongoing and future work.
Chapter 2: Background

2.1 Life cycle assessment

The life cycle of a product or service includes all of the activities and processes involved in production, use and end-of-life processing. Life cycle assessment (LCA) is a systematic method of accounting for the materials, fuels and other inputs used throughout the life cycle, as well as the environmental interventions involved in the life cycle. [104, 208, 293] Environmental interventions are life cycle inputs and outputs that come from or return to the environment, and include pollutant production and natural resource use.

There are four stages in a typical LCA study: goal and scope definition, inventory analysis, [127] impact assessment, and interpretation and improvement analysis. [126] These stages are usually performed in an iterative rather than a linear fashion, because the results of one stage may indicate the need to revisit a previous stage. Figure 2.1 shows the structure of a generic LCA study.

In the goal and scope definition stage, the objective of the study is determined; this in turn determines whether the study is attributional or consequential in nature (see section 2.1.1 for details). The functional unit is also specified in this stage. A functional unit is some measure of the function provided by the product or service
being assessed, such as kilometers driven for a fuel life cycle study. Functional units are specified based on the product function rather than some product characteristic such as mass to facilitate comparison between dissimilar products that provide the same function, such as ethanol and gasoline, and to allow comparison between the results of different LCA studies. Finally, the scope of the study, which represents an initial life cycle boundary, is defined. The scope refers to which life cycle stages are to be included in the study. Common scopes include gate-to-gate, cradle-to-gate and cradle-to-grave; in fuel life cycle studies, cradle-to-gate and cradle-to-grave are frequently referred to as well-to-pump and well-to-wheels respectively. Life cycle stages and processes outside of the scope may interact with life cycle processes but are not considered to be part of the life cycle itself. [61, 270] Figure 2.2 illustrates the differences between several common life cycle scopes.

After goal and scope definition, the study proceeds to inventory analysis. This stage involves gathering data on processes involved in each stage of the life cycle. The
inventory data consists of technological inputs and outputs such as materials, chemical feedstocks and energy, as well as environmental interventions including natural resource use and pollutant production. During this stage, the life cycle boundary is refined and revised. After inventory analysis, a set of intermediate results is produced that quantifies life cycle environmental interventions generated by production of the functional unit. These results consist of physical environmental flows to and from the life cycle, such as crude oil consumed and carbon dioxide emitted.

The next stage is impact assessment, in which the intermediate results of the inventory analysis stage are weighted and normalized according to each particular intervention’s contribution to an environmental or human impact. For instance, the total amount of each type of greenhouse gas produced by the life cycle is calculated during inventory analysis; these quantities are used to calculate global warming potential during impact assessment.

The final stage of a life cycle assessment study is interpretation and improvement analysis. In this stage, results and insight obtained from the previous stages are used to identify potential areas for environmental improvement in the life cycle, sometimes
called “hot spots.” Recommendations can then be made for changes to the life cycle that are expected to improve the functional unit’s environmental performance.

2.1.1 Attributional and consequential LCA

Attributional and consequential are two types of LCA studies that differ in the modeling approach and in the overall objective. The objective of attributional LCA is to assess and quantify all technological and environmental inputs and outputs associated with the production of a functional unit. For instance, if a LCA is performed to calculate the carbon footprint of a consumer product currently on shelves, attributional LCA would be used. The objective of consequential LCA is to predict and quantify the consequences of changes, either exogenous or endogenous, to an existing life cycle.

Attributional LCA describes a static, status quo system, while consequential LCA describes the response of a system to a disturbance [96, 98]; different types of models must therefore be utilized in attributional and consequential LCA. Attributional LCA relies on models of the physical flows within a life cycle and does not capture cause-effect relationships. The system boundary of an attributional LCA includes all life cycle stages that contribute significant and quantifiable environmental interventions to the life cycle inventory. In contrast, consequential LCA frequently combines physical and economic models in an attempt to capture causal relationships between the life cycle, demand for the functional unit and market forces. [94, 97] The system boundary of a consequential LCA includes all life cycle stages that are affected by whatever exogenous change is being modeled for the study; life cycle stages that are
not affected by the change can be excluded from the system boundary even though they may contribute environmental interventions to the inventory.

### 2.1.2 Process based life cycle assessment

Process based LCA is the method of choice for most LCA studies and other life cycle-oriented applications. The majority of existing inventory databases, including the commercial ecoinvent database [275] and the U.S. NREL and USDA databases [219, 288] contain data and models specifically for process based LCA. LCA softwares that rely on these databases such as SimaPro [232] and openLCA [120] use this method to model life cycles and generate results. The widely used Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) fuel and vehicle life cycle models [29, 30] also rely on process based LCA.

A process based life cycle inventory (LCI) is assembled from the bottom up: processes are added to the inventory individually, based on the importance of each process’ contribution to the life cycle environmental impacts, until including more processes in the life cycle is determined to have a negligible effect on the inventory. [50, 137, 205] This approach allows the LCI to be tailored very specifically to a product or process and to the desired level of detail. However, process based LCA excludes many relevant processes from the life cycle boundary, by necessity. The level of interconnectedness in the modern economy means that every life cycle is essentially infinite, and building a LCI process by process becomes impractical beyond a certain point. [66] As a result, process based LCAs under-estimate life cycle impacts, often by a significant amount. This under-estimation is called truncation error, and is estimated to be between 20 – 50% for many process based studies. [189, 270]
Systematic methods of drawing the life cycle boundary have been developed, but even among similar functional units, similar boundaries do not guarantee the same accuracy in results or the same level of truncation error. [236, 237]

2.1.3 Matrix notation for inventory data

The matrix notation for process based inventory data provides an efficient and systematic way to represent the life cycle. [136, 138] A process based inventory contains data on the exchange of \( p \) distinct products among the \( n \) processes in the life cycle. Using the matrix notation, these exchanges are represented in the \( p \times n \) technology matrix \( \mathbf{X} \). Each column in \( \mathbf{X} \) represents a single process in the life cycle, and each row represents the production and consumption of a single product. Negative entries indicate process inputs and positive entries indicate process outputs. The data in \( \mathbf{X} \) is in mixed physical units, normalized to some unit of time chosen such that all processes can be assumed to operate at steady state. [267] Data on \( r \) environmental interventions is organized in the \( r \times n \) interventions matrix \( \mathbf{B} \). Each column in \( \mathbf{B} \) contains intervention data for a single process. Data in the \( \mathbf{B} \) matrix is normalized to each process’ level of output given in \( \mathbf{X} \). The functional unit of the LCA study is represented as a \( p \times 1 \) vector \( \mathbf{f} \). Each element of \( \mathbf{f} \) corresponds to one of the \( p \) products. \( \mathbf{X} \) and \( \mathbf{f} \) determine an \( n \times 1 \) scaling vector \( \mathbf{s} \) such that the following holds:

\[
\mathbf{Xs} = \mathbf{f}
\]  

(2.1)

Equation (2.1) imposes mass and energy balances on the products in the life cycle. The scaling vector \( \mathbf{s} \) represents the level of production required from each life cycle process such that the functional unit is delivered.
Figure 2.3: Widget life cycle diagram (square system, no multi-functional processes)

The intervention data in $\mathbf{B}$ is scaled by $\mathbf{s}$ to calculate the $r \times 1$ inventory vector $\mathbf{g}$. Assuming that the life cycle contains only mono-functional processes that provide a single product or function, $p = n$ and $\mathbf{X}$ is a square matrix. Further assuming that $\mathbf{X}$ is nonsingular, [73] $\mathbf{g}$ is calculated via matrix inversion: [138]

$$\mathbf{g} = \mathbf{BX}^{-1}\mathbf{f}$$  \hspace{1cm} (2.2)

**Illustrative example**

A toy life cycle for widget production is used to demonstrate the matrix notation for inventory data. In the life cycle shown in Figure 2.3, widgets are manufactured from electricity, steel and plastic. Electricity is consumed by the steel production, plastic production and widget manufacturing processes, while steel and plastic are consumed only by widget manufacturing. One widget is produced from 15 kWh electricity, 2 kg steel and 1.5 kg expanded (exp.) plastic. Four environmental interventions are considered: CO$_2$ (kg), CH$_4$ (kg), PM10 (kg), and water use (L).

Table 2.1 contains inventory data for the widget life cycle in the form of a technology matrix. This inventory data is also shown in Figure 2.3. Table 2.2 contains the intervention matrix $\mathbf{B}$. The data in Table 2.2 is read as intervention amounts per total process output: the electricity generation process produces 3 kg CO$_2$ per
Table 2.1: Widget technology matrix (square system)

<table>
<thead>
<tr>
<th></th>
<th>Electricity generation</th>
<th>Steel production</th>
<th>Plastic production</th>
<th>Widget manufacturing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity (kWh)</td>
<td>15</td>
<td>-7</td>
<td>-2</td>
<td>-6</td>
</tr>
<tr>
<td>Steel (kg)</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-2</td>
</tr>
<tr>
<td>Plastic (kg)</td>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>-1.5</td>
</tr>
<tr>
<td>Widget (units)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2.2: Widget intervention matrix (square system)

<table>
<thead>
<tr>
<th></th>
<th>Electricity generation</th>
<th>Steel production</th>
<th>Plastic production</th>
<th>Widget manufacturing</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ (kg)</td>
<td>3</td>
<td>5</td>
<td>2.5</td>
<td>1.2</td>
</tr>
<tr>
<td>CH₄ (kg)</td>
<td>0.8</td>
<td>1.3</td>
<td>1.5</td>
<td>0.4</td>
</tr>
<tr>
<td>PM10 (kg)</td>
<td>4.1</td>
<td>6.2</td>
<td>1.9</td>
<td>0.7</td>
</tr>
<tr>
<td>Water use (L)</td>
<td>15</td>
<td>8.7</td>
<td>4</td>
<td>0.5</td>
</tr>
</tbody>
</table>

15 kWh electricity, and steel production consumes 8.7 L water per 2 kg steel. The functional unit of one widget is expressed in vector form as

\[
f = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}
\]  

(2.3)

Equations (2.1) and (2.2) are then applied to calculate the inventory vector for the production of one widget:

\[
g = \begin{bmatrix} 3 & 5 & 2.5 & 1.2 \\ 0.8 & 1.3 & 1.5 & 0.4 \\ 4.1 & 6.2 & 1.9 & 0.7 \\ 15 & 8.7 & 4 & 0.5 \end{bmatrix} \begin{bmatrix} 15 & -7 & -2 & -6 \\ 0 & 2 & 0 & -2 \\ 0 & 0 & 1.5 & -1.5 \\ 0 & 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}
\]  

(2.4)

\[
= \begin{bmatrix} 11.7 & 12.9 & 28.2 \\ 4.0 & 4.0 & 12.9 \\ 0 & 0 & 0 \end{bmatrix}
\]  

kg CO₂, kg CH₄, kg PM10, L water
2.1.4 Economic input-output life cycle assessment

Process based LCA relies on a somewhat subjective and limited life cycle boundary. In contrast, economic input-output model based LCA (EIO-LCA), a top down inventory method, includes a macro-economic system, usually at the national scale, in the life cycle boundary. [119, 188, 268] (Economic input-output models are discussed in more detail in Section 2.3.) Intervention data at the sector level, given in physical amounts per dollar of sector output, is used to calculate economy-wide interventions generated as a result of the economic activity required to produce the functional unit. [60, 193] Given a direct requirements matrix $A$, an intervention matrix $B$, and a final demand vector $f$ that corresponds to the functional unit, the inventory vector $g$ is calculated as

$$g = B(I - A)^{-1}f$$

in which $I$ is the identity matrix of the same dimensions as $A$.

EIO-LCA produces a more comprehensive inventory than the process based method and can lead to more accurate results for some studies. [45, 139, 140, 192] However, EIO models tend to be highly aggregated, meaning it can be difficult to distinguish between products with similar material and energy requirements and products that are produced by the same sector. [171, 189] In addition, EIO models and therefore EIO-LCA results tend to have a higher level of uncertainty compared to the models used in process LCA.

2.1.5 Hybrid life cycle assessment

Hybrid LCA methods combine the comprehensive life cycle boundary of EIO-LCA with the specific process data used in process based LCA. These methods therefore
address many of the boundary issues and other shortcomings of EIO-LCA and process LCA. [129, 213, 269] The basic concept of hybrid LCA is that the production of some life cycle inputs is modeled in the process based inventory, and the production of other inputs called cutoff flows is modeled in the EIO-LCA inventory. Differences between hybrid methods lie in the degree of integration of the process based and EIO life cycle models and in the representation of the hybrid model.

To stay in keeping with the terminology used throughout Chapters 6 - 8, processes modeled in detail in a hybrid life cycle model are referred to throughout this section as value chain activities.

**Tiered hybrid**

The tiered hybrid method, the simplest of the hybrid methods, develops an inventory for the value chain activities and quantifies the upstream cutoffs for these activities in monetary units. The upstream cutoffs form the final demand on the EIO model, allowing the remainder of the inventory to be calculated and added to the value chain inventory. [61, 290] The calculation of the tiered hybrid inventory vector \( \mathbf{g}_t \) is as follows:

\[
\mathbf{g}_t = \mathbf{g} + \mathbf{g}
\]

\[
= \mathbf{B} (\mathbf{I} - \mathbf{A})^{-1} \mathbf{f} + \mathbf{g}
\]

In Equation (3.4), \( \mathbf{A} \), \( \mathbf{B} \), \( \mathbf{f} \) and \( \mathbf{g} \) are as defined for Equation (2.5). \( \mathbf{g} \) is the inventory vector for the value chain, calculated from Equation (2.2).

**Integrated hybrid**

The value chain and economy models used in the tiered hybrid method remain essentially separate, connected only by the vector \( \mathbf{f} \). In contrast, the integrated hybrid
method [267] disaggregates key sectors in the EIO models into value chain activities and the remainder of the sector. The value chain activities are modeled in detail using the matrix notation discussed in Section 2.1.3, and flows both upstream and downstream (i.e. flows from the value chain back to the economy) of the value chain are captured. The disaggregated EIO model, value chain activities, and upstream and downstream cutoff flows are represented in a single, hybrid technology matrix:

\[
\mathbf{X}_{\text{int}} = \begin{bmatrix}
\mathbf{I} - \mathbf{A}^* \\
-\mathbf{A}_d \\
-\mathbf{X}_u \\
\mathbf{X}
\end{bmatrix}
\]  

(2.7)

in which \(\mathbf{A}^*\) is the disaggregated direct requirements matrix (economy scale), \(\mathbf{X}\) is the value chain technology matrix, and \(\mathbf{A}_d\) and \(\mathbf{X}_u\) are the downstream and upstream cutoff matrices, respectively. The hybrid interventions matrix is similarly constructed from the economy and value chain interventions matrices:

\[
\mathbf{B}_{\text{int}} = \begin{bmatrix}
\mathbf{B}^* \\
\mathbf{B}
\end{bmatrix}
\]

(2.8)

Note that the economy environmental interventions matrix has been disaggregated as well (\(\mathbf{B}^*\)), indicating that interventions produced by the value chain activities have been removed.

Calculation of the integrated hybrid inventory vector is analogous to the process based inventory vector:

\[
\mathbf{g}_{\text{int}} = \mathbf{B}_{\text{int}} \mathbf{X}_{\text{int}}^{-1} \mathbf{f}_{\text{int}}
\]

(2.9)

### 2.1.6 Streamlined life cycle assessment

Streamlining refers to any method that reduces the time, effort or data required to obtain LCA results. [81, 306, 307] In its most basic form, streamlining involves restricting the life cycle boundary to processes and inputs that are considered the most important. [118, 278]
Several forms of streamlined LCA use qualitative data in place of quantitative, for example ranking impact magnitude on a continuous scale instead of using impact quantities. Average impact data for a group of similar products can be used in place of data on individual products. Proxy indicators such as carbon footprint are also used in place of more detailed results. Several streamlining methods use the fact that many environmental impacts tend to be highly correlated with each other. The purpose of these methods is to predict a large set of environmental impacts given either product parameters or a small set of easily calculated environmental impacts. Table 2.3 summarizes these common approaches to streamlined LCA and lists examples of studies that have applied these methods.

2.2 Multi-functionality in life cycle assessment

In Section 2.1.2, the technology matrix $X$ was assumed to be square. This will only be the case when the life cycle does not contain any multi-functional processes, which provide more than one useful product or service. Multi-functional processes provide primary products that are consumed elsewhere in the life cycle, and by-products that are consumed outside the life cycle boundary. Because a life cycle inventory should include only the materials and energy embodied in the functional unit – that is, consumed within the life cycle – the inputs and interventions attributable to the production of by-products must be removed from the inventory before proceeding to impact assessment and interpretation.

There are two types of multi-functionality: joint production and combined production. [302] In joint production, primary and by-products cannot be produced independently of one another: varying the amount of primary product produced will affect
Table 2.3: Summary of common streamlining approaches and studies. List of approaches adapted from [278].

<table>
<thead>
<tr>
<th>Type</th>
<th>Approach</th>
<th>Applied in . . .</th>
</tr>
</thead>
<tbody>
<tr>
<td>Restricting system boundary</td>
<td>Removing upstream components</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Partially removing upstream components</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Removing downstream components</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Removing up- and downstream components</td>
<td>[163]</td>
</tr>
<tr>
<td></td>
<td>Limiting raw materials</td>
<td>-</td>
</tr>
<tr>
<td>Using proxy indicators</td>
<td>Using specific entries to represent or predict impacts</td>
<td>[28, 142, 158, 159, 243]</td>
</tr>
<tr>
<td></td>
<td>Using non-inventory data to predict impacts</td>
<td>[204, 212, 220, 224, 262, 292]</td>
</tr>
<tr>
<td></td>
<td>Using specific entries to represent LCI</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Using “knockout criteria”</td>
<td>-</td>
</tr>
<tr>
<td>Using lower quality data</td>
<td>Using qualitative or less accurate data</td>
<td>[105, 146, 160, 310]</td>
</tr>
<tr>
<td></td>
<td>Using surrogate process data</td>
<td>[83, 152, 241, 272]</td>
</tr>
<tr>
<td>Other</td>
<td></td>
<td>[215, 223]</td>
</tr>
</tbody>
</table>
the amount of by-product, and vice versa. Corn farming and oil refining are both multi-functional processes that exhibit joint production. Processes that exhibit combined production produce co-products in independently variable proportions. A pharmaceuticals plant that produces several products in alternating batches exhibits combined production. Combined production multi-functionality is simpler to deal with in LCA, as the components of the multi-functional process that produce each product can be modeled as separate, independently variable mono-functional sub-processes. The sub-processes that produce by-products are then removed from $X$, leaving the sub-processes that produce primary products.

Choosing a method for dealing with multi-functional joint production processes is one of the most controversial aspects of LCA methodology, because the choice of method generally has a significant effect on results of the impact assessment and interpretation phases. Two popular methods are system expansion, also called displacement, and partitioning allocation.

### 2.2.1 System expansion

System expansion relies on the assumption that the production of functionally equivalent products involves the same environmental interventions regardless of how the products are produced. This assumption implies that by-products of multi-functional processes have the same environmental interventions as equivalent products produced by other, ideally mono-functional, processes. By-products that are consumed outside the life cycle are assumed to displace functionally equivalent products, avoiding the production of equivalent products and the associated environmental interventions. Credit for the avoided environmental interventions is assigned to
the life cycle functional unit, reducing the life cycle inventory by the amount of the avoided environmental interventions. Prior to performing system expansion, the life cycle inventory represents production of both the functional unit and any by-products. After system expansion is performed for all by-products, and provided that none of the displaced products are themselves products of multi-functional processes, the inventory represents production of only the functional unit.

A limitation of system expansion is that it is not generally feasible for agricultural or other biologically-based processes such as fishing and hunting. Agricultural by-products often (1) cannot be produced by mono-functional processes and (2) cannot be produced by multiple different processes. Examples of non-separable agricultural products include corn stover and corn grain, cow milk and beef, and fish and fish by-products. [63, 274, 299]

Performing system expansion entails gathering inventory data on processes external to the original life cycle that produce the by-products. [302, 304] The inventory for the external processes is subtracted from the original inventory, leaving only the material and energy inputs embodied in the functional unit. When the matrix notation is used, the external processes are added to the original inventory as an extra column in the technology matrix. However, the external processes are represented as running in reverse, that is, the negative of the inventory data for the external processes is added to the inventory such that inputs become outputs and vice versa. The entire inventory, consisting of the original inventory plus the external processes, then captures the production of the functional unit along with its by-products and the avoided production of those by-products by the external processes. This process is illustrated in Section 2.2.3.
System expansion has several further downsides related to choosing external processes. Gathering inventory data for the external processes adds time and effort to life cycle studies. More problematically, external processes that produce the correct by-products may themselves be multi-functional, requiring more and more external processes to account for the extra by-products. This is known as the endless regression problem. [303, 305]

2.2.2 Partitioning allocation

In partitioning allocation, multi-functional processes are divided into several mono-functional sub-processes, each of which provide a single product. [138] The sub-processes that produce by-products are removed from the life cycle inventory, leaving only the part of the original multi-functional process that provides the primary products. Partitioning into sub-processes is done according to the relative amounts of each product measured in a particular unit such as mass, energetic content or cost. [271] The unit used in the partitioning is called the partitioning criterion.

2.2.3 Illustrative example: System expansion and partitioning allocation

The widget life cycle is used to demonstrate the application of partitioning allocation and system expansion. While the life cycle used previously contained no multi-functional processes, the life cycle shown in Figure 2.4 now contains a multi-functional plastic production process that provides both expanded (exp.) and thermoformed (thm.) plastic. Only expanded plastic is required to manufacture widgets, thus expanded plastic is the primary product and thermoformed plastic is the by-product.
Figure 2.4: Widget life cycle (rectangular system).

Table 2.4: Widget technology matrix (rectangular system)

<table>
<thead>
<tr>
<th></th>
<th>Electricity generation</th>
<th>Steel production</th>
<th>Plastic production</th>
<th>Widget manufacturing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity (kWh)</td>
<td>15</td>
<td>-7</td>
<td>-2</td>
<td>-6</td>
</tr>
<tr>
<td>Steel (kg)</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-2</td>
</tr>
<tr>
<td>Exp. Plastic (kg)</td>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>-1.5</td>
</tr>
<tr>
<td>Thm. Plastic (kg)</td>
<td>0</td>
<td>0</td>
<td>0.85</td>
<td>0</td>
</tr>
<tr>
<td>Widget (units)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

The rectangular technology matrix for the life cycle in Figure 2.4 is given in Table 2.4, and the interventions matrix in Table 2.5. Note that in Table 2.4, there are no negative entries in the Thm. Plastic row, indicating that thermoformed plastic is not consumed within the life cycle.

It is of interest to calculate the total environmental interventions attributable to the production of 1 widget by the life cycle in Figure 2.4. Inventory vectors will be via both partitioning allocation and system expansion.
Table 2.5: Widget intervention matrix (rectangular system)

<table>
<thead>
<tr>
<th></th>
<th>Electricity production</th>
<th>Steel generation</th>
<th>Plastic production</th>
<th>Widget manufacturing</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ (kg)</td>
<td>3</td>
<td>5</td>
<td>2.5</td>
<td>1.2</td>
</tr>
<tr>
<td>CH₄ (kg)</td>
<td>0.8</td>
<td>1.3</td>
<td>1.5</td>
<td>0.4</td>
</tr>
<tr>
<td>PM10 (kg)</td>
<td>4.1</td>
<td>6.2</td>
<td>1.9</td>
<td>0.7</td>
</tr>
<tr>
<td>Water use (L)</td>
<td>15</td>
<td>8.7</td>
<td>4</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Partitioning allocation

Let \( w \) be the fraction of plastic production inputs and interventions allocated to expanded plastic, and \( 1 - w \) the fraction allocated to thermoformed plastic. \( w \) is called an allocation weight. \( w \) is used to re-write the rectangular technology matrix of Table 2.4 as a square technology matrix with some elements dependent on the value of \( w \). This is done by separating the column of \( X \) that corresponds to the multi-functional process into as many new columns (processes) as there are co-products. In this case, the single column for plastic production becomes two columns, one for expanded plastic production and one for thermoformed plastic production. Input elements in these new processes are written as functions of \( w \), and each new process produces all of one co-product. Table 2.6 shows this expanded technology matrix \( X_\star(w) \). The intervention matrix is similarly expanded to \( B_\star(w) \) shown in Table 2.7.

Note that Tables 2.6 and 2.7 contain columns labeled “Exp. plastic production” and “Thm. plastic production.” These are the artificial mono-functional processes created by dividing the original multi-functional process “Plastic production” into two sub-processes. If the columns for expanded plastic and thermoformed plastic
production are added, the result is the original column of data for the multi-functional plastic production process.

\( \mathbf{x}_* (w) \) is square and, given some value of \( w \), \( \mathbf{g}_* \) can now be calculated. The exact value of \( w \) is calculated from the relative amounts of expanded and thermoformed plastic being produced, measured in some choice of units called the partitioning criterion. Suppose mass is chosen as the partitioning criterion. \( w_{\text{mass}} \) is calculated as

\[
w_{\text{mass}} = \frac{1.5 \text{ kg}}{0.85 \text{ kg} + 1.5 \text{ kg}} = 0.638
\]  

(2.10)

1.5 kg, the mass of expanded plastic produced, is in the numerator because according to the definition of \( w \) given above, \( w_{\text{mass}} \) must represent the fraction of plastic production inputs and interventions allocated to expanded plastic. The value of \( w \)
Figure 2.5: Widget life cycle after mass allocation

from Equation (2.10) is used to obtain the allocated technology matrix \( X_{\text{mass}} \) and the allocated intervention matrix \( B_{\text{mass}} \), which are used in Equation (2.2) to calculate the product inventory vector \( g_{\text{mass}} \):

\[
g_{\text{mass}} = B \cdot X_{\text{mass}} \cdot f \tag{2.11}
\]

\[
\begin{bmatrix}
3 & 5 & 1.595 & 0.905 & 1.27 \\
0.8 & 1.3 & 0.957 & 0.543 & 0.4 \\
4.1 & 6.2 & 1.2065 & 0.6878 & 0.7 \\
15 & 8.7 & 2.552 & 1.448 & 0.5
\end{bmatrix}
\begin{bmatrix}
15 & -7 & -1.276 & -0.724 & -6 \\
0 & 2 & 0 & 0 & -2 \\
0 & 0 & 1.5 & 0 & -1.5 \\
0 & 0 & 0 & 0.85 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}^{-1}
\begin{bmatrix}
0 \\
0 \\
0 \\
1
\end{bmatrix}
\]

\[
= \begin{bmatrix}
10.65 \\
3.42 \\
12.00 \\
26.03
\end{bmatrix} \text{ kg CO}_2 \\
= \begin{bmatrix}
0 \\
0 \\
0 \\
1
\end{bmatrix} \text{ kg CH}_4 \\
= \begin{bmatrix}
0 \\
0 \\
0 \\
1
\end{bmatrix} \text{ kg PM10} \\
= \begin{bmatrix}
0 \\
0 \\
0 \\
1
\end{bmatrix} \text{ L water}
\]

Figure 2.5 shows how flows in the widget life cycle are affected by applying mass allocation.

**System expansion (displacement)**

Suppose there exists a mono-functional thermoformed plastic production process external to the life cycle in Figure 2.4. Inventory data for this process is given in Tables 2.8 and 2.9. System expansion is performed by adding this external process to the original life cycle. The external process is represented as running backwards,
Table 2.8: Inventory data for a thermoformed plastic production process

<table>
<thead>
<tr>
<th></th>
<th>Thm. Plastic Production</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity (kWh)</td>
<td>-0.76</td>
</tr>
<tr>
<td>Steel (kg)</td>
<td>0</td>
</tr>
<tr>
<td>Exp. Plastic (kg)</td>
<td>0</td>
</tr>
<tr>
<td>Thm. Plastic (kg)</td>
<td>0.83</td>
</tr>
<tr>
<td>Widget (units)</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2.9: Environmental interventions data for a thermoformed plastic production process

<table>
<thead>
<tr>
<th></th>
<th>Thm. Plastic Production</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ (kg)</td>
<td>0.82</td>
</tr>
<tr>
<td>CH₄ (kg)</td>
<td>0.56</td>
</tr>
<tr>
<td>PM10 (kg)</td>
<td>0.71</td>
</tr>
<tr>
<td>Water use (L)</td>
<td>1.32</td>
</tr>
</tbody>
</table>

indicating avoided production of thermoformed plastic as a primary product. To represent the process as running backwards, the inventory data for that process is multiplied by -1 such that the process is “consuming” thermoformed plastic and “producing” electricity.

The widget technology matrix and environmental interventions matrix after system expansion, \( \mathbf{X}_d \) and \( \mathbf{B}_d \), are given in Table 2.10 and 2.11. Note that \( \mathbf{X}_d \) is now square and invertible, thus Equation (2.2) can be applied to calculate the inventory
Figure 2.6: Widget life cycle after system expansion, showing avoided production of thermoformed plastic.

vector:

\[
g_d = \begin{bmatrix}
3 & 5 & 2.5 & -0.85 & 1.2 \\
0.8 & 1.3 & 1.5 & -0.56 & 0.4 \\
4.1 & 6.2 & 1.9 & -0.71 & 0.7 \\
15 & 8.7 & 4 & -1.32 & 0.5
\end{bmatrix}
\begin{bmatrix}
15 & -7 & -2 & 0.76 & -6 \\
0 & 2 & 0 & 0 & -2 \\
0 & 0 & 1.5 & 0 & -1.5 \\
0 & 0 & 0.85 & -0.83 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}^{-1}
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
1
\end{bmatrix}
\]

\[= \begin{bmatrix}
10.67 \\
3.38 \\
11.96 \\
26.07
\end{bmatrix}
\begin{bmatrix}
\text{kg CO}_2 \\
\text{kg CH}_4 \\
\text{kg PM10} \\
\text{L water}
\end{bmatrix}
\]

2.2.4 Duality between system expansion and partitioning allocation

System expansion is widely called a method for avoiding partitioning allocation. However, if inputs and interventions are allocated independently with different allocation weights for each flow, then system expansion data can be used to derive partitioning allocation weights. The following discussion follows that in Cherubini et al [69].
Table 2.10: Expanded widget technology matrix after system expansion. The column for the external thermoformed plastic production process has been multiplied by -1 to indicate avoided production.

<table>
<thead>
<tr>
<th></th>
<th>Electricity gen.</th>
<th>Steel prodn.</th>
<th>Plastic production</th>
<th>Thm. plastic production</th>
<th>Widget manuf.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity (kWh)</td>
<td>15</td>
<td>-7</td>
<td>-2</td>
<td>0.76</td>
<td>-6</td>
</tr>
<tr>
<td>Steel (kg)</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>-2</td>
</tr>
<tr>
<td>Exp. Plastic (kg)</td>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>0</td>
<td>-1.5</td>
</tr>
<tr>
<td>Thm. Plastic (kg)</td>
<td>0</td>
<td>0</td>
<td>0.85</td>
<td>-0.83</td>
<td>0</td>
</tr>
<tr>
<td>Widget (units)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 2.11: Expanded widget intervention matrix after system expansion.

<table>
<thead>
<tr>
<th></th>
<th>Electricity gen.</th>
<th>Steel prodn.</th>
<th>Plastic production</th>
<th>Thm. plastic production</th>
<th>Widget manuf.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ (kg)</td>
<td>3</td>
<td>5</td>
<td>2.5</td>
<td>-0.85</td>
<td>1.2</td>
</tr>
<tr>
<td>CH₄ (kg)</td>
<td>0.8</td>
<td>1.3</td>
<td>1.5</td>
<td>-0.56</td>
<td>0.4</td>
</tr>
<tr>
<td>PM10 (kg)</td>
<td>4.1</td>
<td>6.2</td>
<td>1.9</td>
<td>-0.71</td>
<td>0.7</td>
</tr>
<tr>
<td>Water use (L)</td>
<td>15</td>
<td>8.7</td>
<td>4</td>
<td>-1.32</td>
<td>0.5</td>
</tr>
</tbody>
</table>
A multi-functional life cycle process \( i \),

\[
\begin{bmatrix}
-a_{1i} \\
a_{2i} \\
a_{3i} \\
-a_{4i}
\end{bmatrix}
\]

(2.13)

\[
\begin{bmatrix}
b_{1i} \\
b_{2i} \\
b_{3i}
\end{bmatrix}
\]

(2.14)

is partitioned into two mono-functional processes using weights \( w_1, \ldots, w_5 \) as follows:

\[
\begin{bmatrix}
-w_1a_{1i} \\
a_{2i} \\
0 \\
-w_2a_{4i}
\end{bmatrix}
+ 
\begin{bmatrix}
-(1 - w_1)a_{1i} \\
0 \\
a_{3i} \\
-(1 - w_2)a_{4i}
\end{bmatrix}
\]

(2.15)

\[
\begin{bmatrix}
w_3b_{1i} \\
w_4b_{2i} \\
w_5b_{3i}
\end{bmatrix}
+ 
\begin{bmatrix}
(1 - w_3)b_{1i} \\
(1 - w_4)b_{2i} \\
(1 - w_5)b_{3i}
\end{bmatrix}
\]

(2.16)

in which \( w_1, \ldots, w_5 \) may have the same value or different values between 0 and 1.

Suppose there is also data available for an external process \( \tilde{i} \) that produces product 3 but not product 2, like so:

\[
\begin{bmatrix}
-\tilde{a}_{1i} \\
0 \\
\tilde{a}_{3i} \\
-\tilde{a}_{4i}
\end{bmatrix}
\]

(2.17)

\[
\begin{bmatrix}
\tilde{b}_{1i} \\
\tilde{b}_{2i} \\
\tilde{b}_{3i}
\end{bmatrix}
\]

(2.18)

Then \( w_1, \ldots w_5 \) can be calculated by equating input and intervention flows for the partitioned and external process, as follows:

\[-(1 - w_1)a_{1i} = -\tilde{a}_{1i}\]

(2.19)

\[
w_1 = \frac{\tilde{a}_{1i}}{a_{1i}}
\]

and so on for all inputs and interventions.
2.3 Input-output analysis

Economic input-output (EIO) models represent the exchange of commodities between sectors in an economic system. The data required to construct a basic economic input-output model consists of a transactions matrix $X$, a vector of value added $v$ and a vector of final demand $f$. The transactions matrix contains in monetary units the exchange of commodities between sectors. Value added are inputs to production such as labor that do not come from a producing sector. Final demand refers to commodities that are sold to consumers of final demand, which are purchasers that are not consuming sectors. A diagram of a two-sector EIO model is shown in Figure 2.3, and a transactions table showing the transactions matrix, value added and final demand is given in Table 2.12.

2.3.1 The sector-sector approach

The following two sections follow the material in Chapters 2 and 5 of [209]. To simplify the discussion, the number of sectors and the number of commodities in the economy are assumed to be equal throughout.
Table 2.12: Transactions, value added, final demand and environmental interventions for a two-sector economic system.

<table>
<thead>
<tr>
<th>Producing Sectors ($)</th>
<th>Final Demand ($)</th>
<th>Total Output ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sector 1</td>
<td>$x_{11}$</td>
<td>$f_{1}$</td>
</tr>
<tr>
<td>Sector 2</td>
<td>$x_{21}$</td>
<td>$f_{2}$</td>
</tr>
<tr>
<td></td>
<td>$x_{12}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$x_{22}$</td>
<td></td>
</tr>
</tbody>
</table>

Value Added ($v$)

<table>
<thead>
<tr>
<th>Consuming Sectors ($)</th>
<th>Final Demand ($)</th>
<th>Total Input ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sector 1</td>
<td>$v_{1}$</td>
<td>$x_{11} + x_{12} + f_{1}$</td>
</tr>
<tr>
<td>Sector 2</td>
<td>$v_{2}$</td>
<td>$x_{21} + x_{22} + f_{2}$</td>
</tr>
</tbody>
</table>

Environmental Interventions

<table>
<thead>
<tr>
<th>Environmental Interventions</th>
<th>$b_{11}$</th>
<th>$b_{12}$</th>
<th>$b_{13}$</th>
<th>$\vdots$</th>
<th>$b_{1r}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$b_{21}$</td>
<td>$b_{22}$</td>
<td>$b_{23}$</td>
<td>$\vdots$</td>
<td>$b_{2r}$</td>
</tr>
</tbody>
</table>

Note: $x_{ij}$ represents the exchange between sector i and sector j, $f_i$ represents the final demand for sector i, $v_i$ represents the value added in sector i, and $b_{ir}$ represents the environmental intervention in sector i for intervention r.
From the information in Table 2.12, a direct requirements matrix $\overline{A}$ can be calculated by normalizing the elements of $\overline{Z}$ by the total output of each sector $\overline{x}$, as follows.

$$\overline{A} = \overline{Z}\overline{x}^{-1}$$  \hspace{1cm} (2.20)

A hat over a vector denotes diagonalization: the elements of the vector are placed on the diagonal of a square matrix with off-diagonal elements equal to zero.

The elements of $\overline{A}$ are called technical coefficients. $a_{ij}$ represents the amount of commodity inputs required from the $i$th producing sector per dollar output of the $j$th 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 inputs required by a sector is directly proportional to the amount of output produced and (2) sectors consume commodities in fixed proportions regardless of the amount of output produced.

The total output of each sector is equal to the amount of commodities consumed within the economy plus commodities sold as final demand. This relationship, equivalent to an economy-wide balance on monetary flows, is shown in Equation (2.21).

$$\overline{x} = \overline{A}\overline{x} + \overline{f}$$  \hspace{1cm} (2.21)

Equation (2.21) can be solved for $\overline{x}$ by rearranging as shown in Equations (2.22) - (2.24).

$$\overline{x} - \overline{A}\overline{x} = \overline{f}$$  \hspace{1cm} (2.22)

$$(\mathbf{I} - \overline{A}) \overline{x} = \overline{f}$$  \hspace{1cm} (2.23)

$$\overline{x} = (\mathbf{I} - \overline{A})^{-1}\overline{f}$$  \hspace{1cm} (2.24)
The matrix \((\mathbf{I} - \mathbf{A})^{-1}\) is the total requirements matrix, also called the Leontief inverse. With the assumption of fixed \(\sigma_{ij}\), \(\mathbf{x}\) can be calculated for an arbitrary \(\mathbf{f}\) using Equation (2.24).

### 2.3.2 The commodity-sector approach

Another way to represent an EIO model is using make and use matrices. In the EIO model derived from the transactions matrix, flows from sector \(i\) to sector \(j\) are assumed to consist of sector \(i\)'s primary commodity product. This model, known as the sector-sector approach, does not account for sectors that produce more than one commodity. The make-use approach to EIO, also known as the commodity-sector approach, offers greater flexibility when dealing with such cases of secondary production.

The use matrix \(\mathbf{U}\) describes the consumption of commodities by economic sectors. In contrast to the transactions matrix \(\mathbf{Z}\), in which both rows and columns corresponded to sectors, the rows of \(\mathbf{U}\) correspond to commodities and the columns correspond to sectors. The make matrix \(\mathbf{V}\) describes the production of commodities by sectors; its rows correspond to sectors and its columns to commodities.

When secondary production exists in the economic system, the sector-sector and commodity-sector EIO models are not equivalent. In contrast to the single direct requirements matrix of the sector-sector approach, under the commodity-sector approach there are several direct requirements matrices that can be derived from \(\mathbf{U}\) and \(\mathbf{V}\). These matrices differ in their dimensions – commodities-by-commodities or sectors-by-commodities – and in the technology assumption used in the derivation. 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, while the sector-technology assumption states that all commodity outputs from a sector are produced from the same combination of commodity inputs regardless of the commodity type. For the purposes of Chapter 6, only the commodity-commodity direct requirements matrix under the commodity-technology assumption will be derived here.

The commodity-technology assumption defines a relationship between $\mathbf{U}$ and $\mathbf{V}$ that is used to derive the total requirements matrix. Consider the matrix $\mathbf{U}^{-1}$, the columns of which give the mix of commodity inputs to each sector per dollar sector output. As in Equations (2.20) - (2.24), $\mathbf{x}$ is a vector of total sector outputs. The mix of commodity outputs produced by each sector are given by the columns of $\mathbf{C}$, defined in Equation (2.25).

$$\mathbf{C} = \mathbf{V}^{\top} \mathbf{x}^{-1}$$ (2.25)

Let $\mathbf{A}_c$ be the commodity-commodity direct requirements matrix under the commodity-technology assumption. The $j$th column of $\mathbf{A}_c$ gives the combination of commodity inputs required to produce a dollar’s worth of commodity $j$. Under the commodity-technology assumption, the $j$th column of $\mathbf{U}^{-1}$ can be written as a linear combination of the columns of $\mathbf{A}_c$ weighted by the elements in the $j$th column of $\mathbf{C}$. In other words, the 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 shown in Equation (2.26).

$$\mathbf{U}^{-1} = \mathbf{A}_c \mathbf{C}$$ (2.26)
Equation (2.26) can be solved to yield the commodity-commodity direct requirements matrix as follows.

\[ \tilde{A}_c \tilde{V} \tilde{x}^{-1} = U \tilde{x}^{-1} \]  
\[ (2.27) \]

\[ \tilde{A}_c = U \tilde{x}^{-1} \left( \tilde{V}^T \tilde{x}^{-1} \right)^{-1} \]  
\[ (2.28) \]

\[ \tilde{A}_c = U \tilde{x}^{-1} \tilde{x} \left( \tilde{V}^T \right)^{-1} \]  
\[ (2.29) \]

\[ \tilde{A}_c = U \left( \tilde{V}^T \right)^{-1} \]  
\[ (2.30) \]

Because the number of sectors and the number of commodities are assumed to be equal, \( \tilde{A}_c \) has the same dimensions as the sector-sector direct requirements matrix \( \tilde{A} \). However, the elements of \( \tilde{A}_c \) are in general not equal to the elements of \( \tilde{A} \).

The commodity-commodity EIO model is directly analogous to the sector-sector model in Equation (2.24). Writing a commodity balance over the entire economy gives the following.

\[ \bar{q} = \tilde{A}_c \bar{q} + \bar{e} \]  
\[ (2.31) \]

In Equation (2.31), \( \bar{q} \) is a vector of total commodity outputs (different from \( \bar{x} \), a vector of total sector outputs) and \( \bar{e} \) is the final commodity demand. The assumption of fixed technical coefficients applies here as well, thus the calculation of \( \bar{q} \) for an arbitrary final demand \( \bar{e} \) is as follows.

\[ \bar{q} = (\bar{I} - \tilde{A}_c)^{-1} \bar{e} \]  
\[ (2.32) \]

### 2.3.3 Environmentally extended input-output analysis

The original purpose of EIO models was to examine interdependencies between economic sectors. Another application, environmentally extended input-output (EEIO) analysis, calculates the economy-wide environmental interventions caused by producing \( \tilde{f} \) or \( \bar{e} \). [193, 194] In addition to the information in Table 2.12, an EEIO
sector-sector model requires an intervention matrix $\mathbf{B}$ that contains environmental intervention amounts for each sector per dollar of output. The inventory vector of economy-wide interventions $\mathbf{g}$ caused by producing $\mathbf{f}$ is calculated by post-multiplying $\mathbf{B}$ with the vector of total sector outputs $\mathbf{x}$:

$$\mathbf{g} = \mathbf{B} (\mathbf{I} - \mathbf{A})^{-1} \mathbf{f} = \mathbf{B} \mathbf{x} \quad (2.33)$$

2.4 Equilibrium modeling

Equilibrium models are economic models used to simulate and analyze the impact of shocks, including taxes, subsidies, changes in final demand and international trade regulations, on markets within the economy and other connected systems. Input-output and equilibrium models have essentially the same objective: that of modeling activity within an economy and how that activity changes over time and in response to exogenous (imposed externally) changes. However, the assumptions underlying the two modeling approaches are quite different. [308] EIO models rely on the assumption of fixed, exogenously determined prices for all commodities for the time period represented by the EIO model. Another EIO assumption is that all sectors in the economy are adequately modeled with Leontief production functions in which inputs and outputs are related by fixed proportions (hence the technical coefficients $\bar{a}_{ij}$ are fixed). This assumption implies that (1) there are no economies of scale for any technology within the economy, (2) the production capacity of each sector is unlimited and (3) there are no additional capital or other costs for a sector that expands its production capacity.

Applying an EIO model involves an implicit optimization problem in which the throughput vector $\mathbf{x}$ is the decision variable. The problem of finding $\mathbf{x}$ for an arbitrary
\(\bar{f}\), stated in linear algebra form in Equation (2.24), is re-stated here as an optimization problem:

\[
\begin{align*}
\text{minimize} & \quad \sum_j \bar{x}_j \\
\text{subject to} & \quad (\mathbf{I} - \mathbf{A}) \mathbf{x} = \bar{f} \\
& \quad \mathbf{x} \geq 0
\end{align*}
\] (2.34)

Equation (2.34) is interpreted as minimizing total economic activity, which is equivalent to total commodity production. Because the final demand \(\bar{f}\) is fixed, revenue to the economy is also fixed although revenue does not appear explicitly in Equation (2.34). Minimizing total economic activity also minimizes costs and maximizes total profit, subject to the final demand being provided. Producers in the economy can therefore be said to have “profit maximizing” behavior, an assumption that is also used in equilibrium modeling. Although Equation (2.34) results in the same \(\mathbf{x}\) as does Equation (2.24) for the same \(\mathbf{A}\) and \(\bar{f}\), it is rarely applied in practice and EIO models are only occasionally used in an optimization context. (See for instance [91], [92] and [295].)

Within an equilibrium model, both producer and consumer behavior is captured; in contrast, consumer behavior is specified exogenously to an EIO model via the final demand vector \(\bar{f}\). Producers and consumers are assumed to behave such that their own well-being, measured in monetary units, is maximized. This corresponds to profit-maximizing behavior for producers and surplus- or welfare-maximizing behavior for consumers. Consumer surplus can be interpreted as profit to consumers. Many of the remaining assumptions used in equilibrium modeling deal with the existence and properties of the “equilibrium point,” a set of production quantities and commodity
prices. Some properties of the equilibrium point are as follows. The supply of each commodity is exactly equal to the demand; producer profits and consumer surplus are simultaneously maximized; the profit or surplus of a single producer or consumer cannot be increased without an equivalent decrease in profit or surplus elsewhere (that is, the equilibrium point is a Pareto optimum); and unprofitable economic activities do not take place. [183, 258]

Production in an equilibrium model is captured with a non-linear production function that relates units of output to units of capital, labor and other inputs. One common form of the production function is the Cobb-Douglas function, stated for an arbitrary number of inputs as [258]

\[ X = \prod_i Y_i^{\alpha_i} \] (2.35)

and for capital and labor only as [89]

\[ X = AC^{\alpha_C} L^{\alpha_L} \] (2.36)

in which \( C \) represents capital input and \( L \) labor input, both measured in monetary units. The \( \alpha_i \) parameters represent the share of total expenditures for production of commodity \( X \) spent on input \( i \), and in general sum to 1. \( \alpha_i \) describes the responsiveness of the amount of \( X \) produced to the amount of commodity \( i \) purchased. \( A \) in Equation (2.36) is total factor productivity, an empirical parameter that represents the effects of all non-capital and non-labor inputs.

Another common production function is the constant elasticity of substitution (CES) function, which for an arbitrary number of inputs is [258]

\[ X = \left[ \sum_i \alpha_i^{1/\sigma} Y_i^{(\sigma-1)/\sigma} \right]^{\sigma/(\sigma-1)} \] (2.37)

40
In Equation (2.37), the \( \alpha_i^{1/\sigma} \) parameters sum to 1. For only capital and labor inputs, the CES function reduces to \[ \text{(2.38)} \]

\[
X = F \left( \alpha C^{(\sigma-1)/\sigma} + (1 - \alpha) L^{(\sigma-1)/\sigma} \right)^{\sigma/(\sigma-1)}
\]

The \( \sigma \) parameters in Equations (2.37) and (2.38) are the aforementioned elasticities of substitution, which in this production function are equal for all possible pairs of inputs. \( F \) in Equation (2.38) is a parameter called factor productivity, which similar to \( A \) in Equation (2.36) represents the effects on output of \( X \) due to inputs other than capital and labor. The non-linear production functions used in equilibrium modeling allow for both economies and diseconomies of scale for a particular production technology, as well as some flexibility in inputs utilized by each production technology. This is in contrast to EIO models which assume constant returns to scale and fixed input proportions for all technologies.

The different models and assumptions used in equilibrium and EIO modeling does not imply that one approach is objectively better than the other. While assuming all prices to be fixed and neglecting the cost of capital in EIO analysis is clearly unrealistic, so too is the equilibrium assumption that all economic decision makers act to maximize their own profits, and that no unprofitable economic activity takes place. \[ \text{[244]} \] Table 2.13 summarizes a few key differences between input-output, partial equilibrium and general equilibrium models.

### 2.4.1 Partial equilibrium modeling

A partial equilibrium model is an explicit optimization problem similar to Equation (2.34), in which commodity prices and production quantities are the decision
Table 2.13: Summary of key differences between economic input-output models, partial equilibrium and general equilibrium models.

<table>
<thead>
<tr>
<th></th>
<th>Economic input-output</th>
<th>Partial equilibrium</th>
<th>General equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>Entire economy</td>
<td>Key markets (≠ economy)</td>
<td>Entire economy</td>
</tr>
<tr>
<td>Prices</td>
<td>Fixed (exogenous)</td>
<td>Variable (endogenous)</td>
<td>Variable (endogenous)</td>
</tr>
<tr>
<td>Quantities</td>
<td>Variable</td>
<td>Variable</td>
<td>Variable</td>
</tr>
<tr>
<td>Elasticities</td>
<td>None</td>
<td>Supply and demand</td>
<td>Supply, demand and substitution</td>
</tr>
<tr>
<td>Producers</td>
<td>Act to maximize profit</td>
<td>Act to maximize profit</td>
<td>Act to maximize profit</td>
</tr>
<tr>
<td>Consumers</td>
<td>Do not act</td>
<td>Act to maximize surplus</td>
<td>Act to maximize surplus</td>
</tr>
<tr>
<td>Model</td>
<td>Implicit optimization</td>
<td>Explicit optimization</td>
<td>Implicit optimization</td>
</tr>
<tr>
<td></td>
<td>(system of linear equations)</td>
<td></td>
<td>(system of non-linear equations)</td>
</tr>
</tbody>
</table>
Figure 2.8: A partial equilibrium model involves optimization over commodity prices and quantities (red lines) such that the sum of producer surplus (green area) and consumer surplus (blue area) is maximized.

Partial equilibrium models include only a few key markets in an economy and therefore rely on the assumption that the portion of the economy not captured in the PE model is fixed and unaffected by the markets captured by the PE model. As a result, PE models tend to be applied to smaller scale problems than input-output
or general equilibrium models. Recently, partial equilibrium has been applied extensively to supply chain analysis and particularly to analysis of biomass and biofuels supply chains. [247, 284] The general approach is to use a partial equilibrium model to simulate how the different markets (resource extraction, intermediate production and final production) involved in a particular supply chain will interact in order to supply the demand of the final product(s). [296] The well-known 2008 *Science* article discussing the effects of corn ethanol production on land use change used a partial equilibrium model as part of the analysis. [254] Similar models have been applied to analyzing how demand for biofuel affects food supply in the U.S. [170] and in Europe. [164] Other applications focus on how a change in demand for biomass-based products will affect the resource extraction stages and production technologies used within the supply chain. [173, 245, 273]

Partial equilibrium analysis of supply chains differs from engineering analysis because of the focus on micro-economic decision making (supply and demand) rather than technological decision making (unit operation and plant design variables). Hybrid general equilibrium models, discussed in the next section, are a step towards integrating economic and technological decisions in the same model. [153]

### 2.4.2 General and hybrid equilibrium modeling

General equilibrium models, also called computable general equilibrium (CGE) models, capture the entire national or global economy rather than the few markets captured by PE models. [141] A CGE model is formulated as a system of non-linear equations rather than an optimization problem. The system of equations is derived from the assumption that produces and consumers act to maximize their own surplus,
thus the solution to the system of equations is also the equilibrium point, with the same characteristics as in a partial equilibrium model.

Hybrid equilibrium models, similar to hybrid life cycle assessment, combine the macro-economic comprehensiveness of CGE models with greater technological detail than is achievable in standard CGE models. \cite{51, 52} Such details include the specification of production technologies as discrete type modeled with Leontief production functions, rather than the more standard technology “continuum” modeled with Cobb-Douglas and CES production functions. \cite{233, 252} This allows the hybrid model to be used to model economy-wide technology shifts and associated capacity expansion. \cite{217, 253, 266}

### 2.5 Sustainable engineering design

Increasing environmental regulations have driven a shift in engineering design from traditional economics-oriented methods towards sustainable engineering design (SED) methods that consider environmental and social impacts in addition to economic criteria. The goal of SED is not necessarily to design the most profitable or efficient system, but rather to find the design that offers the best compromise between economic benefits, environmental impacts and in some methods, social impacts.

A fundamental difference between SED and traditional engineering design is the expanded analysis boundary. A SED problem includes the system of interest as well as relevant connected systems, often industrial processes in the supply and demand networks. \cite{36} In contrast, the boundary of a traditional engineering design problem includes only the system of interest. The profitability of processing stages upstream and downstream of the system of interest is of no concern, as it has no effect on
Figure 2.9: Sustainable engineering design expands the analysis boundary of traditional engineering, within the dotted rectangle, to the life cycle scale.

the primary system’s profitability except indirectly through input prices. However, the environmental performance of upstream and downstream stages has a large effect on the primary system’s environmental performance. When inputs are purchased from upstream processes and outputs are sold to downstream processes, the system of interest is assigned responsibility for the environmental impacts incurred in the production of inputs and the further processing of its outputs. [256] SED therefore relies on the system boundary shown in Figure 2.9, which includes the system of interest within the dotted rectangle as well as its life cycle (circles).

Most methods for sustainable engineering design use life cycle assessment to quantify environmental interventions, including pollutant production and natural resource consumption, attributable to the system of interest. 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 earliest design methods that considered both process economics and environmental impacts strongly resembled traditional, process economics-oriented design methods. A single process was considered and optimized for efficiency, thereby reducing resource consumption and waste production. Such methods include procedures for increasing process efficiency through process integration [99, 108, 198] and designing for waste reduction [88, 148].

The narrow analysis boundary of process integration, intensification and waste reduction methods makes for a tractable design problem but neglects many relevant systems connected to the process of interest, including upstream stages such as feedstock processing and downstream stages such as wastewater treatment. Because these connected systems are neglected, design decisions that appear optimal when only the process of interest is considered may in fact be sub-optimal or incorrect, due to the effects of those decisions on systems outside the process of interest. [103, 121, 176] For instance, a plant design that includes several processing stages located off-site will appear to have lower environmental impacts due to the smaller energy and resource consumption, but in reality the net environmental impacts caused by the plant have not necessarily decreased and may have increased.

Environmentally conscious process design methods developed after the design-for-process-efficiency methods considered upstream and downstream processing stages as well as the process of interest in the analysis boundary. The waste reduction (WAR) algorithm designed for pollutant and waste reduction, considering both the physical amount of waste produced [143, 316] and the environmental impacts, particularly toxicity, of the waste. [144] Various applications of the WAR algorithm considered, in addition to the process of interest, processes such as raw materials extraction,
power generation [231, 264], production of intermediate inputs and waste treatment. [169, 242]

Life cycle assessment (LCA) was developed and standardized roughly in parallel with early environmentally conscious process design methodologies. [126, 127] LCA offered a standardized and rigorous methodology for further expanding the analysis boundary of process design, and was formally integrated with process design in the Method for Environmental Impact Minimization (MEIM). [181, 265] The MEIM applied LCA to quantify environmental impacts attributable to the process of interest throughout its life cycle. This and subsequent sustainable process design (SPD) methods designed for reduced environmental impacts at the life cycle scale rather than at the process of interest alone. The existence of trade-offs between process economics and life cycle impacts led to the widespread use of multi-objective optimization techniques. [31, 156]

Recent developments in SPD methods have relied on advances in process systems engineering (PSE), particularly the ability to formulate and solve large optimization problems, and on the increased availability and reliability of life cycle inventory data. [122] SPD methods now account for uncertainties in life cycle data [110, 125, 279], consider the “triple bottom line” by combining economic, environmental and social objective functions [38, 319], and account for spatial and temporal variables. [180, 315] Advancements in sustainable supply chain design include techniques for making planning and logistics decisions [117, 201] and designing for risk management. [116]

SPD problems are typically formulated as optimization problems with at least two objective functions, one economic and one environmental. [62, 122] 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 (GWP) [44, 298] or Eco-Indicator 99 [123, 250] based on the system of interest and its life cycle.

Given the system shown in Figure 2.9, a generic sustainable process design problem consists of optimizing the system within the dotted rectangle with respect to both economic and environmental objectives: [62]

\[
\begin{align*}
\text{maximize} & \quad Z_1; \quad \text{minimize} \quad Z_2 \\
\text{subject to} & \quad f(z) \geq 0; \quad Z_1 = Pg(z); \quad Z_2 = Bh(z)
\end{align*}
\]

\( f(z) \) represents process models derived from fundamental engineering knowledge, empirical data, or holistic guidelines; these models constrain the design variables \( z \) to feasible values. The function \( g(z) \) represents process inputs and outputs, the amounts of which are scaled by price data \( P \) to calculate the economic objective function \( Z_1 \). In a similar manner, the function \( h(z) \) represents inputs and outputs that are scaled by environmental intervention data \( B \) to calculate the environmental objective function \( Z_2 \). The exact forms of \( Z_1 \) and \( Z_2 \) vary from problem to problem. Process or production cost [101] and net present value [182] are commonly used economic objective functions. Early SPD studies frequently used multiple environmental objectives, including global warming potential (GWP), water pollution and acidification. [26, 31, 265] The majority of more recent SPD studies consider single environmental objectives, with the most common being Eco-Indicator 99 [123, 249, 250], greenhouse gas emissions [157, 199, 319] and GWP [44, 298]. Multi-objective optimization techniques are used to locate designs that offer compromises between the economic and environmental objectives [64, 124, 225] and are occasionally applied to identify trade-offs between multiple environmental objectives. [43, 76]
$P$ and $B$ are quantified at different scales: $P$ consists of price data for inputs and outputs of the system of interest, while $B$ consists of data on emissions and environmental impacts for the system of interest and its life cycle. In practice, $B$ consists of emissions factors, assumed to be fixed and linearly scalable, obtained from life cycle inventory data available from a commercial database or LCA modeling software.
Chapter 3: Life cycle assessment of an integrated anaerobic digestion plant

3.1 Introduction

Anaerobic digestion (AD) is a process that uses microorganisms in an oxygen-deprived environment to convert organic wastes into biogas, a mixture of gases consisting primarily of methane and carbon dioxide. [177] Biogas can be compressed to produce a bio-based product equivalent to compressed natural gas (CNG) transportation fuel, combusted in a gas turbine for heat and electricity production, or converted to liquid hydrocarbon transportation fuels via Fischer-Tropsch synthesis. [53, 54] The AD process also produces digestate, an organic slurry rich in carbon, nitrogen and other compounds that under some circumstances can be applied to agricultural fields as a soil amendment or as a partial replacement for chemical fertilizers. [151, 210]

The appeal of AD lies in its versatility and its simplicity. Liquid AD (L-AD) can utilize food and beverage waste as feedstock, while solid state AD (SS-AD) can utilize a wide variety of agricultural residues, yard waste and forest residues as well as municipal solid organic waste. SS-AD can also utilize cellulosic energy crops such as switchgrass, low input high diversity (LIHD) grasses and miscanthus as feedstocks.
AD is, unlike other processes that convert biomass into energy, a “one-pot” process that requires minimal feedstock processing and less product upgrading than do cellulosic ethanol production, pyrolysis, gasification and other conversion processes. Because AD is a simpler process, it is also more economically feasible to establish pilot-scale AD plants near sources of organic waste than it would be to do the same for other biomass conversion processes. As a result, AD is widely utilized in Europe and in developing countries as a source of renewable energy and as a way to treat and manage organic waste streams.

This chapter analyzes a novel AD system configuration, the integrated anaerobic digestion system (iADs). iADs combines a L-AD unit with a SS-AD unit by using the SS-AD unit to further treat the digestate of the L-AD unit. As a result, biogas production is increased and the iADs unit is capable of utilizing a wider variety of feedstocks compared to either L-AD or SS-AD alone. The LCA study focuses on an iADs plant located in Zanesville, which is owned and operated by quasar energy group.

Work presented in this chapter was completed in collaboration. Sections indicated with an asterisk contain work performed wholly or primarily by Varsha Gopalakrishnan.

3.2 Goal and scope definition

The primary objective of the iADs LCA is to quantify how the environmental performance of the iADs process is affected by the combination of feedstocks used and by the combination of final biogas products produced. To accomplish this objective, nine different configurations of the iADs system are assessed; these configurations
cover the possible combinations of three cellulosic biomass feedstocks fed to the SS-AD unit and three possible end products produced from biogas. The three SS-AD feedstocks considered are corn stover, miscanthus and yard waste collected from the local community. Corn stover collected from local farms is currently utilized in the quasar plant, and an experimental field plot of miscanthus was established in 2013, although to date miscanthus has not yet been used as an iADs feedstock. Similarly, there are plans to collect yard waste from local residential communities, but they have not yet been implemented. The only L-AD feedstock considered is a food and beverage waste stream collected from local Kroger stores. Although the quasar plant currently converts biogas only to heat and electricity via CHP and to compressed natural gas (CNG) for use in company vehicles, there are plans to implement a biogas-to-liquids (BTL) Fischer-Tropsch reaction system for converting biogas into syngas and then into liquid hydrocarbon fuel, comparable to biodiesel produced from syngas. Therefore, the three biogas end products examined here are electricity, CNG and liquid hydrocarbon fuels.

3.3 Process based inventory analysis

Inventory data for background and upstream life cycle processes was obtained primarily from the NREL LCI database. [219] Plant-specific data for the iADs process was obtained from the quasar energy group as a plant-wide heat and mass balance, shown in Figure 3.1. [291] The process of purifying biogas and converting it to liquid hydrocarbon fuels was modeled with data taken from the ecoinvent (v2.2) database, as the necessary data was not available in the NREL database. [275] Data for other
Figure 3.1: iADs plant data used to develop the life cycle models [291].

Note:
1. The alkali loading is 8% of dry corn stover.
2. Biogas yield for SSAD is 0.4 m³/kg VS.
3. Methane content of biogas is 60% and the compression ratio is 1:100.4. Generator electrical efficiency is 35%.
5. Liquid hydrocarbon fuel yield is 0.042 gallon/m³. The parasitic electric load/biogas equivalence for the AD is 15%. The biogas used for heating in the BTL process is 0.15 m³ for 1 m³ biogas processed.
life cycle processes was obtained as necessary from published literature and other sources; further details are given in the following sections.

Both a process based and a tiered hybrid inventory were assembled for this study. openLCA, an open-source life cycle assessment software, was used to build the process based inventory, to quantify the upstream cutoff flows for the tiered hybrid inventory, and to generate results for the process based study. [120]

3.3.1 Miscanthus farming and collection

Data on fertilizer application, fuel and equipment use, and approximate biomass yields were obtained from [300] and used to create a custom openLCA process for miscanthus farming. The temporal variability of miscanthus farming could not be captured in the life cycle model, thus all input and output values were averaged over the lifetime of the miscanthus stand, which was assumed to be 15 years. [71, 234] For instance, miscanthus rhizomes were assumed to be used on a 7,000 unit/acre basis. [149] The lifetime average input of rhizomes was then calculated as

\[
\text{average rhizome input} = \frac{7,000 \text{ units/acre}}{15 \text{ years}} = 467 \text{ units/acre-year} \quad (3.1)
\]

The lifetime average values for other inputs and outputs were calculated similarly. In calculating the average miscanthus yield, it was assumed that no harvest took place in years 1 or 2 and yield for those years was therefore zero. [21]

Table 3.1 represents a “farm-to-gate” process. The process captures all farming activities including biomass harvesting, baling and loading onto trucks. Production and distribution of all chemical and fuel inputs was modeled using system processes in the NREL database. Rhizome production, which was assumed to be via harvest
Table 3.1: Inputs and outputs of the miscanthus farming openLCA process. Values represent lifetime averages on an annual basis.

<table>
<thead>
<tr>
<th>Input</th>
<th>Amount</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rhizomes</td>
<td>467</td>
<td>units/acre-year</td>
</tr>
<tr>
<td>Diesel fuel</td>
<td>9.06</td>
<td>gallons/acre-year</td>
</tr>
<tr>
<td>Nitrogen fertilizer</td>
<td>31.42</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Phosphorus (P$_2$O$_5$) fertilizer</td>
<td>10.97</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Potassium (K$_2$O) fertilizer</td>
<td>44.74</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Herbicide (glyphosate)</td>
<td>1.08</td>
<td>kg/acre-year</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Output</th>
<th>Amount</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Miscanthus biomass</td>
<td>8.93</td>
<td>dry tons/acre-year</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Emissions</th>
<th>Amount</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$</td>
<td>5.99</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Volatile organic compounds (non-methane)</td>
<td>$6.23 \times 10^{-3}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>$3.44 \times 10^{-2}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Nitrogen oxides</td>
<td>$5.56 \times 10^{-2}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>PM10 (dust)</td>
<td>$5.62 \times 10^{-3}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>PM2.5</td>
<td>$5.45 \times 10^{-3}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Sulfur oxides</td>
<td>$6.23 \times 10^{-4}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Methane</td>
<td>$4.89 \times 10^{-5}$</td>
<td>kg/acre-year</td>
</tr>
<tr>
<td>Nitrous oxide</td>
<td>$7.14 \times 10^{-5}$</td>
<td>kg/acre-year</td>
</tr>
</tbody>
</table>
from established miscanthus stands [21], was not accounted for in the process LCA but was included in the tiered hybrid LCA.

Emissions to air were calculated based on the diesel fuel consumption. Emission factors obtained from GREET 2014 [30] for diesel fuel burned in a farming tractor were used to convert the average amount of diesel fuel used annually to quantities of emissions. Any emissions resulting from land use, such as nitrogen volatilization or carbon released from the soil, were not accounted for.

3.3.2 Corn stover farming and collection

Corn stover collection and the additional inputs to corn farming due to stover removal were both modeled using system processes in the NREL database. These additional inputs include nitrogen fertilizer, phosphorus fertilizer, potassium fertilizer (K$_2$O), transportation of these fertilizers, and hay grown for feed as a stover replacement. Inputs and emissions associated with corn farming other than those mentioned here are not accounted for. Corn grain and stover was assumed to be harvested with a single pass method, thus no extra diesel fuel was consumed for stover collection.

3.3.3 Yard waste collection

Collection of yard waste from local communities is currently modeled as a simple transportation process using a compressed natural gas (CNG) powered light duty truck (see Section 3.3.5 for details). A round-trip distance of 30 km, with each trip transporting the maximum payload of yard waste on a dry basis, was assumed.
3.3.4 Food waste collection*

Based on the provided iADs plant data, the total amount of food waste collected annually is 30,000 tons. [291] Food waste is assumed to come from three sources: the Central Food Facility in Athens, OH, and two local Kroger stores. The Central Food Facility is a 151.2 km round trip from the quasar plant and is assumed to provide 55 wt% of the total food waste steam. The first Kroger is a 30.21 km round trip from the quasar plant and is assumed to provide 22.5 wt% of the total food waste. The second Kroger is a 37.4 km round trip from the quasar plant and is assumed to provide 22.5 wt% of the total food waste. All distances were calculated using the two point method. The total amount of food waste collected per year is 27,215,542 kg (assuming “tons” in [291] refer to short tons, or 907.18 kg). Using the assumed percentages above, 6,123,497 kg waste comes from Kroger 1, 6,123,497 kg waste comes from Kroger 2 and 14,968,548 kg waste comes from the Central Food Facility. Based on the assumed maximum payload for the CNG-powered light duty trucks used for transportation, transporting waste from Kroger 1 requires 3,374 round trips for a total of 101,928 km per year. Transporting waste from Kroger 2 waste requires 3,374 round trips for a total of 126,188 km per year. Transporting waste from the Central Food Facility waste 8,248 round trips for a total of 1,247,098 km per year. The total distance traveled annually for food waste transportation is thus 1,475,214 km. Emissions associated with burning CNG as a transportation fuel were calculated based on this distance using emissions factors from GREET 2014. [30]
Table 3.2: Model of feedstock transportation via CNG-powered light duty truck.

<table>
<thead>
<tr>
<th>Input</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNG from biogas</td>
<td>0.154</td>
<td>kg/km</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Output</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Transportation</td>
<td>1,815</td>
<td>kg/km</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Emission</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO(_2)</td>
<td>1.81\times10^{-1}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Volatile organic compounds (non-methane)</td>
<td>1.07\times10^{-4}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>2.63\times10^{-3}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Nitrogen oxides</td>
<td>1.23\times10^{-4}</td>
<td>kg/km</td>
</tr>
<tr>
<td>PM10 (dust)</td>
<td>1.62\times10^{-5}</td>
<td>kg/km</td>
</tr>
<tr>
<td>PM2.5</td>
<td>7.46\times10^{-6}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Sulfur oxides</td>
<td>6.21\times10^{-7}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Methane</td>
<td>8.64\times10^{-5}</td>
<td>kg/km</td>
</tr>
<tr>
<td>Nitrous oxide</td>
<td>4.35\times10^{-6}</td>
<td>kg/km</td>
</tr>
</tbody>
</table>

3.3.5 Use of CNG-powered vehicles for feedstock transportation

All vehicles used for feedstock collection and transportation to the iADs plant are run on CNG produced from biogas. [20] Sufficient information was not available to calculate emissions factors per ton-kilometer, as is commonly done for goods transportation processes. Instead, emissions factors and fuel mileage for a 2010 light-duty truck running exclusively on CNG were obtained from GREET 2014 and used in a custom openLCA transportation process. [30] The truck was assumed to have a maximum payload of 1,815 kg; this value was used to calculate the number of trips required and total distance traveled for all feedstock transportation processes.

The life cycle of the vehicles themselves are not currently included in the process based inventory. The necessary life cycle processes were not available in the NREL inventory database nor in the GREET vehicle life cycle model. [29, 219] Instead,
the CNG vehicles were accounted for as part of the tiered hybrid study discussed in Section 3.4.

3.3.6 quasar iADs plant

The iAD units and all downstream biogas processing stages were modeled as separate processes in openLCA to facilitate comparisons between various configurations of the iADs plant. Parasitic heat and energy requirements, including heat added to the AD units and power required to operate the various biogas processing units, were assumed to be supplied by biogas CHP. [291] Therefore, no grid electricity or fuel other than biogas is consumed within the plant and no heat leaves the plant as a useful output.

Cellulosic feedstock size reduction

Cellulosic feedstocks go through a size reduction unit before being sent to the SS-AD unit. [291] No further information on the type of equipment or power consumption was available, thus the size reduction unit was modeled in openLCA as a process with no other inputs than feedstock and no other outputs than size-reduced feedstock.

Anaerobic digestion units

The L-AD unit takes only food waste as feedstock; the SS-AD unit uses either corn stover, miscanthus or yard waste as feedstock. Biogas yields for both units were given on an annual basis. [291] The SS-AD biogas yield is assumed to be constant for the three cellulosic feedstocks, as biogas yield data using a plant-scale SS-AD unit was not available.
It was assumed that both AD units are maintained at mesophilic conditions, which are 35°C and 1 atm. [301] Heat produced via biogas CHP is added to the AD units to maintain this temperature. This parasitic energy requirement was specified in [291] as 15% (assumed volume percent) of the total biogas produced per year, which is 3,428,000 m³ at 35°C, 1 atm. From this quantity and the energy content of biogas calculated below, the heat input for the iAD units was calculated as 1,632,073 MJ per year.

Alkali was added to the SS-AD unit at a rate of 3% (assumed by mass) of the cellulosic feedstock. [291] This rate was assumed to remain constant for all three cellulosic feedstocks, and sodium hydroxide (NaOH) was assumed to be the alkali used. [322] Because the NREL inventory database did not contain any processes related to the production of NaOH, it was excluded from the process analysis inventory but was included in the tiered hybrid inventory.

Fugitive methane and carbon dioxide emissions from the iAD units were estimated from literature as ranging from 0 - 8.4% of biogas produced in digesters, with the most likely value being around 3%. [77, 106, 210] The rate of fugitive emissions was modeled in openLCA as a parameter with a triangular distribution with min = 0.0, max = 0.084 and mode = 0.03.

**Raw biogas purification***

Before being converted to syngas and then undergoing the Fischer-Tropsch synthesis, the biogas is purified to increase the methane concentration and remove any components that would interfere with the conversion. The purification process involves removal of H₂S and gas conditioning as well as methane enrichment. This
process yields biogas at 5 bar (4.93 atm) that is 96 vol% methane, with the remaining 4 vol% consisting of carbon dioxide.

The NREL database did not contain a relevant process for the purification step, thus process data was obtained from the ecoinvent (v2.2) database. [275] Relevant process data is given in Table 3.3; for brevity, the full list of environmental inputs and outputs is not given.

### Biogas conversion to syngas*

The purified biogas undergoes conversion to syngas before being converted to liquid hydrocarbon fuels via Fischer-Tropsch synthesis. This conversion step involves COS hydrolysis and sulfur and CO₂ removal, and yields syngas at 24.67 atm with a conversion of 99.9%. The data used to model conversion to syngas was taken from the ecoinvent (v2.2) database; a partial process model is given in Table 3.4.
Table 3.4: Model of the biogas-to-syngas conversion process.

<table>
<thead>
<tr>
<th>Input</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biogas, 96 vol% CH₄, 0°C and 4.93 atm</td>
<td>1.0</td>
<td>m³ at NTP</td>
</tr>
<tr>
<td>Electricity</td>
<td>3.48×10⁻³</td>
<td>kWh/m³ syngas at NTP</td>
</tr>
<tr>
<td>Zinc</td>
<td>8.65×10⁻⁴</td>
<td>kg/m³ syngas at NTP</td>
</tr>
<tr>
<td>Chemical waste disposal</td>
<td>1.0</td>
<td>kg/m³ syngas at NTP</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Output</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Syngas, 0°C, 24.67 atm</td>
<td>1.0</td>
<td>m³ syngas at NTP</td>
</tr>
</tbody>
</table>

Table 3.5: Model of Pd-Co catalyst production.

<table>
<thead>
<tr>
<th>Input</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alumina</td>
<td>0.011</td>
<td>kg/kg catalyst</td>
</tr>
<tr>
<td>Copper</td>
<td>0.016</td>
<td></td>
</tr>
<tr>
<td>Potassium chloride</td>
<td>7.41×10⁻³</td>
<td></td>
</tr>
<tr>
<td>Magnesium oxide</td>
<td>5.11×10⁻³</td>
<td></td>
</tr>
<tr>
<td>Zeolite powder</td>
<td>0.352</td>
<td></td>
</tr>
<tr>
<td>Iron</td>
<td>0.234</td>
<td></td>
</tr>
<tr>
<td>Titanium oxide</td>
<td>0.176</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Output</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pd-Co catalyst</td>
<td>1.0</td>
<td>kg</td>
</tr>
</tbody>
</table>

Fisher-Tropsch synthesis of liquid hydrocarbon fuels*

Data on the density of the exact fuel blend produced was unavailable; based on bench scale experiments, a density value of 832.0 kg/m³ was assumed. [317] Inputs to the Fischer-Tropsch synthesis are syngas, produced by the process described above, a Pd-Co-Mo catalyst [317] and electricity. Life cycle data on the Pd-Co-Mo catalyst was not available, thus data for a Pd-Co catalyst was substituted. [172] The process model for catalyst production is given in Table 3.5.
Table 3.6: Model of Fischer-Tropsch conversion of biogas to liquid hydrocarbon fuels.

<table>
<thead>
<tr>
<th>Input</th>
<th>Amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Syngas</td>
<td>6.969</td>
<td>m$^3$/m$^3$ fuel</td>
</tr>
<tr>
<td>Catalyst</td>
<td>0.0832</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>Electricity</td>
<td>0.001247</td>
<td>kwh/m$^3$</td>
</tr>
</tbody>
</table>

Table 3.6 gives the process model for Fischer-Tropsch conversion of bio-syngas to liquid fuel. The quantity of catalyst used is 100 g per ton of liquid fuel product. [172]

Biogas compression to CNG fuel

The compression process is assumed to be downstream of purification, such that biogas entering the compressor consists of 96 vol% CH$_4$ at a pressure of 5 bar. To simplify the compression calculations, and due to the lack of other information, the temperature of the purified biogas entering compression is assumed to be 0°C. The compressor is assumed to have an isothermal efficiency of 60% which is in the center of the standard isothermal efficiency range for compressors. [229]

A “compression ratio” of 1:100 is specified for the biogas compression unit [291], but the interpretation of this value is unclear. CNG is commonly provided at a pressure of 3,000 - 3,600 PSI. [19] For the compressor power calculations detailed below, a delivery pressure of 3,300 PSI was assumed.

The compressor power was calculated assuming isothermal compression of an ideal gas. Under these conditions, the power required to compress 1 pound-mass (lb$_m$) of
biogas to from 5 bar to 3,300 PSI is (Equation 21 on page 524 of [229])

\[
\text{Power} = \frac{1}{0.6} p_1 \nu_1 \ln \left( \frac{p_2}{p_1} \right) \tag{3.2}
\]

where 0.6 is the isothermal efficiency of the compressor, \( p_1 \) is the intake pressure (10442.7 lb\( f \)/ft\(^2 \)), \( \nu_1 \) is the reciprocal of the biogas density at intake conditions (2.924 ft\(^3 \)/lb\( f \)) and \( p_2 \) is the delivery pressure (475200.0 lb\( f \)/ft\(^2 \)). Using these values, the compressor power required is calculated as 3.181 MJ per m\(^3\) purified biogas at 0°C, 5 bar, which produces 5.477 kg of CNG at 3,300 PSI. This value is used to quantify the compressor’s parasitic energy requirement which is supplied by the biogas CHP unit.

**Combined heat and power unit**

The biogas CHP unit is assumed to be upstream of all biogas purification and compression units [291], thus biogas entering CHP is raw, consisting of 60 vol% \( \text{CH}_4 \) and 40 vol% \( \text{CO}_2 \), and is at 35°C and 1 atm. Under these conditions, and assuming that the energy content of biogas is due entirely to methane, the energy content of raw biogas is calculated as 7.244 MJ/m\(^3\) (LHV). This value was obtained using the methane energy content (LHV) given in GREET 2014 (962 BTU/ft\(^3\)) [30] and converting the energy content at GREET conditions (0°C and 1 atm) to the conditions at which biogas leaves the AD units by assuming ideal gas behavior. The generator electrical efficiency is specified to be 35% (Figure 3.1), thus 35% of the biogas energy content is converted to power. Electricity yield is calculated as 2.535 MJ per m\(^3\) raw biogas at 35°C and 1 atm. This value represents gross electricity production; part of this electricity goes to supply parasitic energy requirements, and the remainder is available for sale as a final product. There was no distinction made between heat
and power production in the process models, as no data was available to make such a distinction.

### 3.4 Tiered hybrid inventory analysis

In a tiered hybrid LCA, any input flows that cannot be included in a process based inventory are quantified in monetary units as upstream cutoff flows and treated as the final demand in an EEIO model. More information on hybrid LCA is given in Section 2.1.5. For this study, Eco-LCA, an ecologically-extended input-output model, was used as the EEIO model. [18] Cutoff flows for the iADs life cycle models were quantified from information already in the NREL database, and from inputs for which accurate process based inventory data was not available. Cutoff flows already within the NREL database are marked as “dummy” flows. Price data for these flows was used to convert physical cutoff amounts into monetary final demand, based on the amount of each flow required to produce a particular functional unit. Some dummy flows were neglected due to their extremely small magnitude ($< 1 \times 10^{-10}$, various units). Other flows were neglected because due to an ambiguous product name, it was not possible to determine a market price. Relatively few of the dummy flows were neglected.

Life cycle processes that could not be modeled within the process based inventory were manufacturing of the CNG-powered light-duty truck, production of miscanthus rhizomes and production of sodium hydroxide. The next several sections discuss how these flows were quantified as final demand.
3.4.1 CNG light-duty truck

As part of the calculations involved in generating the process based inventory, the total distance traveled by a CNG vehicle in the production of each functional unit was calculated. This distance was divided by the total distance that a typical CNG truck could be expected to travel during its useful lifetime to yield a percentage. The CNG truck was assumed to last for 15 years and travel 90,000 miles annually [185], for a lifetime distance of 2,172,614 km. The final demand was calculated as the total purchase price of a CNG truck ($33,150, online retailer), multiplied by the percentage of the truck’s lifetime distance used to produce each functional unit.

3.4.2 Miscanthus rhizome production

The lifetime average input of rhizomes to the miscanthus farming process is 467 units/acre-year (Table 3.1), and the process LCA calculations yield the number of rhizomes needed to produce each functional unit. A price of $0.09 per rhizome was assumed and was used to quantify the final demand. [149]

3.4.3 Sodium hydroxide production

The amount of sodium hydroxide needed to produce each functional unit was calculated similarly to the rhizome input. A market price of $0.65/kg [165] was used to quantify the final demand.

3.5 Results and discussion

Three different functional units were analyzed: 1 MJ of biogas electricity, 1 MJ of CNG and 1 MJ liquid hydrocarbon fuels. For each functional unit, three different AD feedstock combinations were analyzed: corn stover and food waste, miscanthus...
and food waste, and yard waste and food waste, for a total of nine sets of results representing the possible configurations of the iADs life cycle network. Life cycle interventions for three conventional products were obtained from GREET 2014 for purposes of comparison to the iADs end products; these conventional products were U.S. average grid electricity, fossil natural gas produced in the U.S. and soybean biodiesel. [30]

A total of six different product systems were created in openLCA; three systems contained processes related to the BTL conversion and three did not. All six systems contained processes related to biogas purification, compression, and CHP, as both CNG and biogas electricity was required to power various processes in the iADs network. Electricity and CNG based functional units represent production in excess of these parasitic requirements.

After obtaining the process based and tiered hybrid inventories, it was found that the hybrid inventory was not significantly different from the process based inventory. For this reason, only the process based results are presented in this section. Both the process based and EEIO inventories are given in tabular form in Appendix A.

The results in the following two sections represent environmental interventions, physical amounts of pollutants, rather than impacts, effects on environmental and human systems. Impact assessment has not yet been performed for this study, due to the need for verifying the data used in the process based inventory. This is discussed further in Section 3.6.
3.5.1 End products compared across different feedstocks

Figures 3.2 - 3.4 show results from the process based LCA for each end product. Different bars within each graph represent different cellulosic feedstocks and the conventional product.

Results for liquid hydrocarbon fuel production from iADs biogas (blue, red and green bars) are given in Figure 3.2 and compared to soybean biodiesel (yellow bar). From this graph, it appears that the three cellulosic feedstocks have approximately the same environmental performance across the emissions shown. However, all three feedstocks out-perform soybean biodiesel in all categories save for CO₂ emissions, which for biodiesel were negative due to carbon sequestration in the farming stage. Carbon sequestration at the farming stage was not accounted for in this study; were it to be included, it is possible that both miscanthus and corn stover CO₂ emissions would be negative as well. Sequestration for the yard waste feedstock, because it comes from a variety of sources and land management practices, cannot be predicted.

Results for compressed natural gas from iADs biogas (blue, red and green bars) and from fossil sources (yellow bar) are shown in Figure 3.3. For the most part, the iADs products out-perform fossil CNG here as well; the only exception is carbon monoxide emissions for which fossil CNG has slightly lower emissions. Miscanthus and yard waste appear basically equivalent for CNG, and corn stover performs slightly better than either.

Interestingly, U.S. grid electricity (yellow bar) appears to be practically equivalent if not superior to electricity produced from iADs biogas, as shown in Figure 3.4. This may once again be due to the neglected carbon sequestration at the farming
Figure 3.2: Life cycle emissions for 1 MJ liquid hydrocarbon fuel produced from different feedstocks. The CO$_2$ emissions for soybean biodiesel were -55.77 kg and are not shown due to the log scaling on the y-axis.
Figure 3.3: Life cycle emissions for 1 MJ CNG transportation fuel produced from different feedstocks.
Figure 3.4: Life cycle emissions for 1 MJ electricity produced from different feedstocks.

stage. The three feedstocks, as for liquid hydrocarbon fuels, appear here to have approximately the same environmental performance across all emissions shown.

Overall, the results in this section indicate that none of the three cellulosic feedstocks are significantly environmentally superior to the others.

3.5.2 Feedstocks compared across different end products*

Figures 3.5 - 3.7 show results from the process based LCA for each feedstock; different bars within each graph represent different end products. Results for the three conventional end products are not shown in these figures.
Figure 3.5: Life cycle emissions for 1 MJ of each end product produced from miscanthus.

All three figures indicate that liquid hydrocarbon fuels (yellow bars) have the lowest life cycle emissions per MJ regardless of feedstock. This is not necessarily due to the environmental superiority of the end product, but rather due to the physical amount of liquid fuel that contains 1 MJ of energy. Because the liquid fuels are extremely energy dense, the 1 MJ functional unit is equal to a fraction of a kilogram of fuel; therefore the low life cycle emissions are due primarily to the scaling down of the life cycle. Correcting this issue can be done with a different functional unit, which is discussed further in Section 3.6.
Figure 3.6: Life cycle emissions for 1 MJ of each end product produced from corn stover.
Figure 3.7: Life cycle emissions for 1 MJ of each end product produced from yard waste.
3.6 Ongoing work

Before proceeding to impact assessment and final LCA results, the models and data discussed in Sections 3.3 and 3.4 must be verified and updated if necessary based on information from the quasar energy group. Once completed, results will be re-generated both for the 1 MJ functional unit used in this chapter and for a distance-driven functional unit, representing the amount of each end product consumed in driving 1 km in a light-duty passenger vehicle.
Chapter 4: Statistical modeling for streamlined life cycle assessment

4.1 Introduction

The methods for streamlining LCA discussed in Section 2.1.6 share an approach: these methods all focus on identifying the minimum amount of inventory data that must be collected in order to generate the desired life cycle results. The disadvantage of this approach is that the amount of error incurred in using streamlined inventory data rather than complete data is unknown. Without knowledge of the complete inventory, the accuracy and completeness of the streamlined inventory cannot be quantified, and collecting the complete inventory for the purpose of calculating the accuracy of the streamlined inventory defeats the purpose of streamlined LCA. The uncertainty in life cycle results due to streamlining is therefore unknown and unknowable under conventional streamlining methods.

This chapter presents an alternative approach to streamlined LCA. Rather than identifying the minimum amount of new inventory data that must be gathered to perform a streamlined LCA, the proposed approach attempts to extract useful information from available inventory data and uses that information to generate new streamlined inventories. This approach, regression streamlining, combines the use of
proxy indicators [142] and correlated impacts [159, 220, 224] with statistical model building techniques. Linear regression models that predict a variety of environmental interventions or impacts from a small number of key predictor quantities that are highly correlated with the interventions of interest. Cumulative energy demand (CED) and carbon footprint (CF) are the two predictor quantities used in this chapter.

An advantage of building models to predict new inventory data from available data is that cross-validation techniques can be applied to estimate the accuracy of the regression models. Leave-one-out cross-validation (LOOCV), a form of bootstrapping, tests the accuracy of regression models by building models on the entire data set less one data point and then testing the model using the left out data point. [186] The procedure is repeated for all points in the data set, resulting in a distribution of error values.

A practical advantage of regression streamlining is that predicting life cycle results using indicators is an easily understood and intuitive method that can be used by practitioners without extensive experience with LCA or statistical modeling.

Regression streamlining has some features in common with the streamlining methodology developed by Park and Seo [226], but there are a few significant differences. Park and Seo’s method begins with a large group of dissimilar products, and various clustering methods are applied to separate the products into similar groups. Neural networks are then used to predict impacts from environmental impact drivers and the results from those networks are verified by multiple regression analysis. In contrast, regression streamlining begins with a group of similar products; similarity is determined according to various product characteristics. Linear regression techniques are
used to build impact models instead of neural networks, which are nonparametric, nonlinear modeling tools. [22, 321] Using a linear model is sufficient to predict life cycle results due to the assumed linearity of the life cycle system [138] and the fact that the relationship between various impacts (if one exists) is rarely higher than first order.

Huijbregts and colleagues proposed using cumulative energy demand (CED) as an indicator for various life cycle impacts. [158, 159] Their analysis focused on using the $R^2$ statistic to evaluate correlation between CED and other impacts. An $R^2$ value close to 1 or -1 indicates strong correlation. [186]

The data sets used in [158, 159] were log transformed before $R^2$ was calculated and all results were presented in the log domain. Transforming the impact data is counterproductive for two reasons. First, any impacts predicted from transformed data will also be in the log domain. A reverse transformation is necessary before the results can be applied or interpreted; the transformation therefore adds unnecessary complexity to the calculation procedure. Huijbregts and colleagues state that the log transform was done to improve the highly skewed distribution of the dataset (ecoinvent v1.3, [275]) and bring the distribution closer to a Gaussian or normal distribution. However, no statistical analysis beyond calculating $R^2$ was done and no inference was done on the regression coefficients. The non-Gaussian distribution would only become problematic if such further analysis was performed. $R^2$ can be calculated and is valid for any data set regardless of the underlying distribution, thus the skewness of the data did not need to be corrected.

A second reason why the log transform is counterproductive is that the transformation may exaggerate the prediction capabilities of CED. The value of a regression
model used for streamlining lies in its ability to predict streamlined life cycle results in the original domain. The best regression model is the most accurate model, not necessarily the model with the highest $R^2$, and models must be evaluated in the original, untransformed domain to obtain practically relevant information on model accuracy.

This chapter consists of previously published material that appears in [131].

4.2 Methodology

For regression streamlining to be successful, that is for the streamlined results to have a reasonable degree of accuracy, it must be applied to homogeneous sets of products. Products that are similar to each other will most likely have impacts that are highly correlated. This will result in regression models of greater accuracy than if the models were built for sets of dissimilar products. Models will be built using data in the original domain as well as transformed data. By comparing the accuracy of the two models, the effect of the log transform, if any, will be determined.

Regression streamlining begins with a set of results from a full-scale LCA performed on a product set of interest. Product sets consist of similar products, with similarity determined by product characteristics, use or type. Because this methodology is intended for use in the manufacturing industries, a convenient way to group products is by manufacturer or manufacturing site. A set of laundry detergents sold under a particular brand is one example of a set of similar products; the set of computer mice produced by a particular electronics manufacturer is another. A larger set of products will give more accurate results than a small set so long as the products are fairly homogeneous. Including several different kinds of products in the data set will,
at least theoretically, make the resulting regression models more widely applicable, but the accuracy of the models may suffer.

A preliminary examination of correlation amongst the various impacts and emissions of interest is done to determine if CED is an acceptable predictor variable or if some other impact is more highly correlated with the results of interest. Stepwise model building techniques, which choose one or more predictor variables based on statistical significance, can be used if more than one indicator has a high degree of correlation. More than one predictor variable may also be chosen using methods such as LASSO or principle component regression. [311] However, when regression streamlining is used in applications, more predictor variables will mean more data that must be collected to apply the models. One predictor variable was found to be adequate in both case studies performed for this work.

In this work, the statistical computing program R was used to perform ordinary least-squares (OLS) linear regression and least absolute deviations (LAD) linear regression. [235] OLS calculates a regression line based on the $l_2$ norm or squared distance between the regression line and the data points, while LAD uses an $l_1$ norm or absolute value distance. [49] Regression models were evaluated using the percent error ($\epsilon\%$):

$$\epsilon\% = \frac{100}{n} \sum_{i=1}^{n} \frac{|Y_i - \hat{Y}_i|}{Y_i}$$  

(4.1)

which is an $l_1$ norm. The $Y_i$s in Equation (4.1) are the original impact data (response variable) and $\hat{Y}_i$ are the predicted impacts.

The primary advantage of using $\epsilon\%$ over other statistical metrics such as mean squared error (MSE) or $R^2$ is that it is more easily interpreted, particularly by a layperson. LAD models, which minimize the $l_1$ norm rather than the $l_2$ norm, will
always have a lower $\epsilon\%$ than OLS models, but the reduction in error was found to be very small in all cases. For this reason only OLS results are presented for the two case studies.

Once the models are built, leave-one-out cross-validation (LOOCV) is performed to obtain estimates of the error in each model. LOOCV involves building as many regression models as there are data points, each time leaving out a different data point. \[239\] The result is a collection of slightly different models. $\epsilon\%$ is calculated for each of these models and then averaged over the number of models. LOOCV provides a way to test the robustness of the models to different data sets. LOOCV also corresponds with the way regression streamlining will be used: applied regression streamlining models will be built using an entire data set and then used to predict results for new products. For these reasons, LOOCV was chosen over other cross-validation techniques.

The error estimates referred to here apply to new products, not to products in the original data set. The error is the difference between the streamlined LCA results calculated from the regression models and the full-scale LCA results, which is unknown for new products.

To demonstrate the efficacy and advantages of the proposed regression streamlining method, two case studies were performed. The first case study looked at packaging options for soft goods and demonstrates the value of using a homogeneous product set for building regression models. This study also demonstrates how the streamlined results are affected when the data is log transformed. The second case study included several different types of materials, and serves as an example of streamlining accuracy when the product set under study is heterogeneous.
4.3 Case study: Packaging

Franklin Associates assembled a life cycle inventory on 26 packaging options for soft goods such as clothing, books, and other items that can be safely sent through the mail without excessive packaging. Each option consisted of a cardboard box, a plastic bag or a paper bag plus some type of filler or padding material.

The two predictor variables considered for this case study were CED and total CO$_2$ emissions. A stepwise model-building technique (Type III sum of squares) was used to identify the most significant predictor or predictors for each impact under study. CED was the only significant predictor for most impacts and was used as the predictor variable throughout. Using LOOCV, distributions of $\epsilon_\%$ were obtained for each impact.

Due to the extreme skewness of the $\epsilon_\%$ distributions, the medians are presented rather than the means. The error bars indicate the 25$^{th}$ and 75$^{th}$ quantiles of the distributions. In all of the following figures, bars or error bars that reach the top of the plot indicate bars that continue above the viewing window.

Fig. 4.1 shows median $\epsilon_\%$ for the testing data sets. These are the quantities that would be used as error estimates for new products in the same product set, thus they are of primary interest from an application-oriented view. For this particular data set, the log transform has no consistent effect on model accuracy. The difference in model accuracy is also quite small ($< 10\%$) in all cases.

The packaging data set did not display a high degree of skewness; although results for boxes and bags were in two distinct clusters, both clusters had fairly symmetric distributions. This lack of skewness is likely the reason for the minimal effect of the log transform.
Figure 4.1: Median percent error for regression streamlining applied to the packaging data set (testing data).

4.4 Case study: Materials

The second product set used for a case study was a set of materials that included several types of metal, wood, glass, and ceramic. [246] Results are presented in Fig. 4.2 as medians with 25th and 75th quantiles for the error bars.

The median $\epsilon$%s for the testing set are, in general, high enough that these models would not be acceptable for streamlining use. The data for this product set was highly skewed, and the log transform tends to decrease $\epsilon$%, resulting in more accurate models. However, the error bars in this study were in general very large. Were these models applied to new products in the same product set, the actual accuracy of the streamlining results could vary widely from the predicted accuracy.
4.5 Discussion

Regression streamlining is simple, intuitive and provides a way to estimate streamlining error for products without the need for further life cycle data. Regression streamlining is not entirely objective, as predictor variables and regression techniques must be chosen by the practitioner. The success (accuracy) of the streamlining models depends heavily on the product set used to build models: although streamlining models for the heterogeneous materials data set used the same predictor variable and many of the same emissions as the homogeneous packaging data set, the models were much less accurate. Exactly how similar products must be, and what metric should be used to judge similarity, will need to be determined on a case-by-case basis. Given a
homogeneous product set that is not highly skewed, the log transformed and untransformed models have nearly equivalent accuracy. In contrast, the log transformed models for a skewed data set tended to be more accurate than the untransformed models. This indicates that the log transform is only useful when the original data set is highly skewed, and is unnecessary otherwise.
Chapter 5: Addressing the ill-posed nature of allocation in life cycle inventories

5.1 Introduction

There are two key debates regarding multi-functionality in life cycle assessment. The first is whether system expansion or allocation should be applied. As discussed in Section 2.2, each of these methods is useful in some situations, and neither method can be applied in all situations. The second debate deals with partitioning allocation, and which partitioning criterion to use. [80, 297] For many inventories, allocation has such a drastic effect that it is possible to “game” life cycle impacts by assigning allocation weights that correspond with the objectives of a particular study. For instance, lignocellulosic ethanol produced from corn stover can appear either superior or inferior to corn ethanol, depending on whether or not stover is treated as a waste.

There is no consensus on which partitioning criterion is best: different organizations and practitioners prefer or recommend different partitioning criteria. [79, 216] Moreover, it is difficult to defend any single criterion: for many multi-functional processes, there are multiple criteria that provide logical partitioning, but no one criterion provides logical partitioning for all products. Mass allocation works well in manufacturing processes but cannot be applied to energetic outputs such as electricity;
energetic allocation is not intuitive for products not commonly quantified according
to energy content; economic allocation is problematic for products that are typically
treated as waste, such as corn stover, and products with volatile prices, such as fuels.

Applying multiple partitioning criteria and obtaining results for multiple allocated
inventories has recently become popular as a way to avoid choosing and justifying a
single criterion. [107, 274] However, differences in the allocated inventories can lead to
contradictory conclusions [63, 200, 211, 299] This is particularly true for comparative
life cycle studies that examine several functionally equivalent products with the goal
of determining the preferred product, which is the product with the lowest life cycle
impacts. Many case studies have shown that the preferred product is not necessarily
consistent across different partitioning criteria. [161, 175, 320] In such cases, the
comparisons are not robust to allocation, thus no definite conclusions can be drawn
from the case study.

Recent work has used linear model theory to gain mathematical insight into the
issues surrounding partitioning allocation. Using the matrix notation for life cycle
inventory data, [136] the calculation of impacts for a multi-functional inventory is
seen as an ill-posed problem with infinite solutions that are highly sensitive to the ap-
plied allocation method. [74, 75] The implication for LCA is that any given allocated
inventory is only one of infinitely many possible inventories, and that inventories ob-
tained from different partitioning criteria will vary widely from one another. Because
allocation assumptions made in the inventory phase are propagated through to the
impact assessment and interpretation phases, any decisions made based on allocated
inventories are controlled by the allocation method rather than by differences in the
inventory data.
If only partitioning allocation is applied in a comparative study, there is no way to determine conclusively whether or not the results of the study are robust to allocation. When multiple partitioning criteria are applied, the end result is a finite subset of the possibly infinitely many inventories. Conclusions based on partitioning therefore ignore a large amount of information on how the inventory is affected by allocation, and can lead to poor decision making due to neglecting this information. Specifically, the conclusions of comparative studies may be incorrect – the preferred product identified as such may not have the lowest environmental impacts in reality – due to non-robustness not detectable by conventional sensitivity analyses.

The calculation procedure developed in this chapter, the Comprehensive Allocation Investigation Strategy (CAIS), uses the matrix notation for inventory data to parameterize the allocation decisions within an arbitrary multi-functional inventory, essentially writing the inventory as a function of allocation decisions. CAIS thus enables inventory analysis without previously restricting allocation decisions to individual partitioning criteria and provides previously unobtainable insight into how inventories and product preferences change as a result of allocation. By applying CAIS in the inventory analysis phase of a LCA, subsequent phases of the study will be based upon complete information rather than the partial set of information obtainable via partitioning allocation.

A key advantage of CAIS is the ability to represent all allocation decisions simultaneously, which allows for the effects of allocation to be examined quantitatively, by applying optimization and other mathematical procedures, as well as qualitatively through graphics. CAIS is also capable of representing all possible allocation methods, including non-traditional methods in which inputs and interventions are
allocated according to several different partitioning criteria and methods in which mass and energy balances over the life cycle are not preserved. The effects of system expansion, which have been shown to be equivalent to independently allocated inputs and impacts [69], are also captured by CAIS.

All non-robustness to allocation is detectable when CAIS is applied, even non-robustness that is not detectable using standard sensitivity analyses. When comparisons are not robust, CAIS provides information about how allocation affects the inventories being compared. For some comparisons, the product preference may change only for extreme allocation schemes, or one product may never be preferred. In such situations it may be possible to use CAIS results to decide on a preferred product. For other comparisons, the inventories may be too similar or too dependent on allocation choices to determine a preferred product. In these cases, the only way to determine a preferred product is by incorporating new data external to the original inventories. CAIS does not solve the ill-posed allocation problem, but rather provides a general, systematic method for parameterizing the allocated inventory and extracting useful information that can then be used in impact assessment, interpretation and eventually in decision support.

5.2 Motivating example

Ethanol is a transportation fuel that can be produced from a variety of feedstocks and conversion pathways. Allocation is required in virtually all ethanol production pathways, and previous studies have shown that ethanol life cycle inventories are sensitive to allocation choices. [55, 179] Consider three ethanol production pathways: corn grain fermentation, corn stover hydrolysis and corn stover gasification. It is
Table 5.1: Life cycle CO₂ emissions for three ethanol production pathways under mass and economic allocation. A bold entry indicates the preferred pathway.

<table>
<thead>
<tr>
<th>Pathway</th>
<th>kg CO₂ emissions per L ethanol</th>
<th>Mass allocation</th>
<th>Economic allocation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn grain fermentation</td>
<td>5.46</td>
<td>7.88</td>
<td></td>
</tr>
<tr>
<td>Corn stover hydrolysis</td>
<td>1.77</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>Corn stover gasification</td>
<td>3.14</td>
<td>0.14</td>
<td></td>
</tr>
</tbody>
</table>

of interest to determine which of these pathways should be implemented, based on which pathway has the lowest life cycle CO₂ emissions. Inventory data for ethanol production is available in the literature. The data used in this study was obtained from [41, 214, 263] and the inventories are given in Appendix C, Tables C.2 - C.10. Allocation is required in all three pathways at the farming process and in the grain fermentation and stover hydrolysis pathways at the ethanol production process. Both mass and economic allocation are applied.

Results given in Table 5.1 indicate that different pathways are preferred under the two allocation methods. Therefore the comparison is not robust and, using only partitioning allocation, the only conclusion that can be reached is that grain fermentation should probably not be implemented. Moreover, based on results from only mass or only economic allocation, it is not apparent that the comparison is not robust.

CAIS provides complete information on how the inventories are affected by allocation decisions. Figure 5.1 compares results from CAIS (vertical lines) and partitioning allocation (points). Each line represents the range of values that can be assigned to CO₂ emissions by changing the allocation methods. Note the large overlap between the lines for the three life cycles. Within this region of overlap, different partitioning
Figure 5.1: Life cycle CO$_2$ emissions for three ethanol production pathways under mass and economic partitioning allocation and as calculated by CAIS. CAIS results are shown as bars that indicate the variation in CO$_2$ emissions due to allocation decisions in each pathway. Partitioning allocation results are shown as points. Allocation methods will prefer different pathways. For example, the CO$_2$ emissions of the two corn stover pathways fall in this region: stover hydrolysis is preferred under mass allocation (squares) while stover gasification is preferred under economic allocation (triangles). From the overlapping CAIS results, the non-robustness of the ethanol pathways comparison is easily determined. Based solely on Figure 5.1, the preferred pathway cannot be determined, but a decision may be possible when the results of the CAIS procedure are examined in more quantitative detail.

5.3 Allocation as an ill-posed problem

Throughout the following discussion, inventories that contain multi-functional processes are assumed to contain more products than processes. For simplicity, each
multi-functional process is assumed to provide one primary product and one by-
product, and it is also assumed no product is being produced by more than one pro-
cess. While the CAIS procedure and related concepts apply to inventories for which
these assumptions do not hold, modifications to the calculation procedure are neces-
sary to accommodate differences in the way allocation decisions are modeled. Only the
situation corresponding to these simplifying assumptions is discussed here in detail.

As discussed in Sections 2.1.3 and 2.2.2, a life cycle inventory can be represented
as a technology matrix $X$. An inventory that does not require allocation results in a
square technology matrix. When the inventory contains multi-functional processes,
$X^{-1}$ does not exist in this situation and Equation (2.2) cannot
be applied immediately. Partitioning allocation enables the calculation of $X^{-1}$ by
expanding $X$ to a square $p \times p$ matrix $X_*$, as follows:

$$\begin{bmatrix}
 X_{11} & -X_{12} & -X_{13} \\
 -X_{21} & X_{22} & -X_{23} \\
 0 & X_{32} & 0 \\
 -X_{41} & -X_{42} & X_{43}
\end{bmatrix}
\xrightarrow{\text{Partitioning}}
\begin{bmatrix}
 X_{11} & -w_1 X_{12} & -(1 - w_1) X_{12} & -X_{13} \\
 -X_{21} & X_{22} & 0 & -X_{23} \\
 0 & 0 & X_{32} & 0 \\
 -X_{41} & -w_2 X_{42} & -(1 - w_2) X_{42} & X_{43}
\end{bmatrix}
$$

(5.1)

The expansion separates multi-functional processes into artificial mono-functional
sub-processes. [271, 304] Inputs and intervention data for the original process are
divided amongst the sub-processes with allocation weights $w$, and each of the sub-
processes is scaled independently. In Equation (5.1), $w_1$ and $w_2$ may be calculated
from a common partitioning criterion ($w_1 = w_2$, the industry-technology assumption)
or they may be calculated from different criteria ($w_1 \neq w_2$, the commodity-technology
assumption). $B$ is likewise expanded to an $r \times p$ matrix $B_*$, and $s$ is expanded to a
$p \times 1$ vector $s_*$ with the addition of scaling factors for each allocated sub-process. $g$
for the allocated system, denoted $g_*$, is then calculated by applying Equation (2.2)
5.3.1 Emergy method for multi-functional inventory analysis

Emergy is defined as the total solar energy consumed directly or indirectly to provide a product or service. [221] Unlike energy and mass, emergy is not necessarily conserved within a system, [59] implying that when emergetic content is used as a partitioning criterion, energy and mass are likewise not necessarily conserved within a life cycle. Emergetic allocation is thus fundamentally different from conventional partitioning allocation which preserves mass and energy balances. However, emergetic and partitioning allocation are implemented similarly within the matrix notation:

\[
g_* = B \cdot X^{-1} f
\]

Moreover, emergetic and partitioning allocation yield identical results for specific allocation weight values. A demonstration is given in Appendix C. Emergetic allocation can thus be viewed as a special case of partitioning allocation, despite the methodological differences between the two methods.

5.3.2 Insight from linear model theory

Equation (2.1), reproduced below for reference, is a system of linear equations:

\[
Xs = f
\]
When $X$ is square, the system has one unique solution which is used to calculate $g$.

When $p > n$, Equation (2.1) becomes an *overdetermined* system of equations,

$$
\begin{bmatrix}
  x_{11} & -x_{12} & -x_{13} \\
  -x_{21} & x_{22} & -x_{23} \\
  0 & x_{32} & 0 \\
  -x_{41} & -x_{42} & x_{43}
\end{bmatrix}
\begin{bmatrix}
  s_1 \\
  s_2 \\
  s_3
\end{bmatrix}
=
\begin{bmatrix}
  f_1 \\
  f_2 \\
  f_3 \\
  f_4
\end{bmatrix}
$$

(5.4)

and in general has no exact solution.

Using partitioning allocation to expand $X$ to $X_*$ allows $g_*$ to be calculated; however, the system of equations now involves the allocation weights $w$, which are themselves *independent variables*. The system is now underdetermined with four equations and either five or six unknowns, as follows,

$$
\begin{bmatrix}
  x_{11} & w_1 x_{12} & -(1 - w_1) x_{12} & -x_{13} \\
  -x_{21} & x_{22} & 0 & -x_{23} \\
  0 & x_{32} & 0 & 0 \\
  -x_{41} & -w_2 x_{42} & -(1 - w_2) x_{42} & x_{43}
\end{bmatrix}
\begin{bmatrix}
  s_1 \\
  s_{2a} \\
  s_{2b} \\
  s_3
\end{bmatrix}
=
\begin{bmatrix}
  f_1 \\
  f_2 \\
  f_3 \\
  f_4
\end{bmatrix}
$$

(5.5)

The underdetermined nature of the system leads to the insight that partitioning allocation is a fundamentally ill-posed problem with the following characteristics: there are infinitely many values of $s_*$ and $w$ that satisfy Equation (5.5), and $s_*$ and $g_*$ are highly sensitive to allocation choices quantified in the value of $w$. [73–75]

An ill-posed problem can be turned into a well-posed problem by incorporating data external to the original problem. A well-posed problem, if it has a solution, will have one unique solution. In the context of life cycle inventory, Equation (5.5) can be turned into a well-posed problem by incorporating additional equations that impose restrictions on $s_*$ and $w$. Partitioning allocation appears to solve the ill-posed allocation problem by using product mass, energetic content or other information to fix the value of $w$. This does not provide an adequate solution, because the information used to fix $w$ is not external to the life cycle inventory: all commonly
used partitioning criteria are based on process output data, which is already in the inventory, plus a conversion factor to change the units.

One non-partitioning attempt at solving the ill-posed allocation problem used ordinary, total and data least squares to find optimal solutions to Equation (2.1), concluding that total least squares was the best method of solution. [202, 203] The least squares methods find minimal corrections to $X$ and $f$ such that Equation (2.1) has a solution; this allows $g$ to be calculated for inventories that require allocation without performing partitioning allocation. However, corrections made to the inventory data $X$ may not be consistent with the physical system being represented: small flows can reverse direction, zero flows can become non-zero and vice-versa. There is no way to guarantee that the corrections made to $X$ and to $f$ are consistent with system-wide mass and energy balances, and thus no guarantee that $g$ and further results based on $g$ calculated from these techniques are valid. [73–75] If least squares methods are to yield consistent, meaningful results, further constraints must be imposed on the methods, including but not limited to mass and energy balances and constraints that prevent process data from becoming unrealistic.

5.4 The comprehensive allocation investigation strategy

CAIS is applicable to any life cycle inventory that requires allocation in an arbitrary number of multi-functional processes. Flows in the inventory that must be allocated are written as functions of allocation weights $w$. Thus the inventory itself, specifically the matrices $X$ and $B$, become functions of $w$. This allows the impact vector $g$ to be calculated, also as a function of $w$. This section provides a brief overview
of the calculations involved in CAIS. Further details on the calculation procedure and an illustrative example of its application are provided in Appendix C.

The first step in CAIS is locating multi-functional processes. For small inventories this can be done by inspection and for large inventories the process is easily automated. The technology matrix $X$ is decomposed into a make matrix $V'$ and a use matrix $U$ using the following relationships: 

$$ v_{ji} = \begin{cases} x_{ij} & \text{if } x_{ij} > 0 \\ 0 & \text{otherwise} \end{cases} \quad (5.6) $$

$$ u_{ij} = \begin{cases} |x_{ij}| & \text{if } x_{ij} < 0 \\ 0 & \text{otherwise} \end{cases} \quad (5.7) $$

After this decomposition, $V'$ contains only process outputs and $U$ contains only process inputs such that Equation (5.8) holds.

$$ X = V' - U \quad (5.8) $$

Multi-functional processes correspond to columns in $V'$ with more than one non-zero element.

Next, the multi-functional processes must be divided into mono-functional processes and inputs to the mono-functional processes written as functions of $w$. $V'$ is expanded by moving off-diagonal elements to the diagonal and adding columns where necessary, resulting in the diagonal (square) matrix $V'_{\star}$. $U$ is expanded by adding columns where multi-functional processes are being divided; elements in these new columns and in the original columns corresponding to multi-functional processes are written as functions of $w$, resulting in the square matrix $U_{\star}(w)$. $B$ is expanded using the procedure for $U$. Finally, $V'_{\star}$ and $U_{\star}(w)$ are recombined using Equation (5.8) to obtain $X_{\star}(w)$. Equation (2.2) is now applied to obtain $g_{\star}(w)$, a vector of $R$ inventory
functions:

\[ \mathbf{g}_s(w) = \begin{bmatrix} g_{s1}(w) \\ \vdots \\ g_{sR}(w) \end{bmatrix} \]  \hspace{1cm} (5.9) 

A diagram of CAIS calculation procedure is shown in Figure 5.2.

5.5 Representing, interpreting and applying results

After obtaining the inventory function vector \( \mathbf{g}_s(w) \) for each product, the information in \( \mathbf{g}_s(w) \) must be interpreted correctly and compared between products. The focus of this section is on determining if a given product comparison is robust to allocation and if not, determining the extent of non-robustness. The most direct way to determine robustness is to compare the \( r^{th} \) inventory function for each product
and determine if *equality sets*, sets of points in the allocation space $0 \leq w \leq 1$ for which two or more inventory functions are equal, exist for any of the interventions of interest. An equality set for products $A$ and $B$ and intervention $r$ is defined as the set $\{w_e\}$ for which

$$g^A_{sr}(w_e) = g^B_{sr}(w_e), \quad \forall \ w_e \in \{w_e\}$$

(5.10)

The existence of an equality set for two or more products implies that the intervention functions for those products overlap, as seen in Figure 5.1 for the three ethanol pathways. If no equality sets exist, then the product comparison is robust.

If equality sets exist among the products and interventions of interest, then the comparison is *potentially* non-robust. Before conclusively determining non-robustness, the equality set(s) must be tested to determine if it is also a *preference boundary*. A preference boundary is an equality set that divides the allocation space into preference regions, within each of which a single product is preferred. In other words, product preference only changes across a preference boundary. Figure 5.3 shows two preference boundaries that exist between the three ethanol production pathways for $\text{N}_2\text{O}$ emissions. Equation (5.10) was applied to locate the equality sets. As can be seen in Figure 5.3, the product preference on either side of the two equality sets is different, thus both equality sets are also preference boundaries.

The problem of locating preference boundaries can be separated into two tasks: (1) Locating equality sets $\{w_e\}$ at which the inventory functions of two products are equal, and (2) Testing the product preferences in the regions separated by $\{w_e\}$ to determine if $\{w_e\}$ is a preference boundary. Given two products $A$ and $B$, the
The equality set found using Equation (5.11) is then evaluated further to determine if the product preference changes from product A on one side of the boundary to product B on the other side, or vice versa. This step is necessary because it is possible for the inventory functions of two products to be equal without either product being preferred, for instance if a third product in the set being compared has lower interventions at points in the equality set. Another possibility is that only a portion of an equality set qualifies as a preference boundary. This situation is expected to arise only when more than two products are being compared.
Each point \( w_p \in \{w_p\} \) for which a solution \( \Delta w_p \) exists to the following optimization problem,

\[
\begin{align*}
\text{minimize} & \quad \Delta w_p \\
\text{subject to} & \quad \min \left\{ g^A_{sr}(w_p - \Delta w_p), g^B_{sr}(w_p - \Delta w_p), \ldots \right\} = g^A_{sr}(w_p - \Delta w_p) \quad (5.13) \\
& \quad \min \left\{ g^A_{sr}(w_p + \Delta w_p), g^B_{sr}(w_p + \Delta w_p), \ldots \right\} = g^B_{sr}(w_p + \Delta w_p) \quad (5.14) \\
& \quad 0 \leq \Delta w_p \leq \epsilon \quad (5.15)
\end{align*}
\]

is defined as a point on the preference boundary between products \( A \) and \( B \) for intervention \( r \). Constraints (5.13) and (5.14) impose the requirement that the product preference - the product with minimum intervention \( r \), among all products being compared - changes across the preference boundary. In Equation (5.15), \( \epsilon \) is some small number that constrains \( \Delta w_p \) such that \( w_p - \Delta w_p \) and \( w_p + \Delta w_p \) represent points in the preference regions separated by \( \{w_p\} \).

For product comparisons involving two or fewer allocation weights, such as the comparison between ethanol pathways discussed in the motivating example, preference regions and boundaries can be represented graphically. Figure 5.4 shows two such preference plots for CO\(_2\) emissions (Figure 5.4a, top) and for CO emissions (Figure 5.4b, bottom). Different preference regions are indicated by color, and preference boundaries divide one region from another. In Figure 5.4, \( w_F \) and \( w_P \) indicate the allocation weight for the farming process and for the ethanol production process, respectively. \( w_F \) is the fraction of farming inputs and interventions allocated to the primary product, which is corn grain for the grain fermentation pathway and corn stover for the other two pathways. \( w_P \) is the fraction of ethanol production inputs...
and interventions allocated to ethanol, thus \(1 - w_P\) is the fraction assigned to the co-product, which is dried distiller’s grains and solubles for grain fermentation and lignin electricity for stover hydrolysis. As stover gasification does not involve allocation at the ethanol production process, \(w_P\) is undefined for that pathway. The inventory functions for stover gasification therefore do not depend on \(w_P\).

Figure 5.4 also shows the intervention magnitude of the preferred product at each point, demonstrating that both the preferred product and the interventions of the preferred product are sensitive to allocation. For \(\text{CO}_2\) emissions shown in Figure 5.4a, stover hydrolysis is the preferred product over the majority of the allocation space. Stover gasification is preferred only when \(w_F < 0.1\) and \(w_P > 0.8\), and grain fermentation is preferred only when \(w_P < 0.1\). In contrast, grain fermentation and stover hydrolysis are preferred almost equally for \(\text{CO}\) emissions shown in Figure 5.4b, with stover gasification being preferred only when \(w_F < 0.4\) and \(w_P > 0.8\).

5.5.1 Using CAIS results for decision support

In practice, impact assessment (weighting and normalization) would be performed on the inventory functions prior to using them for decision support. In this section the inventory functions are used as-is for simplicity and for illustrative purposes.

In Figure 5.4a, stover hydrolysis is preferred over the majority of the allocation space. It is therefore not unreasonable to conclude that, when considering \(\text{CO}_2\) emissions, stover hydrolysis is the preferred pathway. When there is no one product preferred over the majority of the allocation space, as for the \(\text{CO}\) emissions shown in Fig. 5.4b, the product preference is less obvious. More quantitative information is
Figure 5.4: Preference plots show the different preference regions in the allocation space. For comparisons involving up to two allocation weights, preference plots can be used to locate preference boundaries instead of or in addition to Equations (5.12) - (5.15).
required to determine a preferred product, and even then it may not be possible to reach a definite conclusion.

The sizes (length, area, volume, etc.) of the preference regions expressed as a fraction of the allocation space, the preference percentages, can be used to determine if one product is preferred over the majority of the space or if products are preferred more equally. Comparing an arbitrary number of products yields $M$ preference boundaries $\{w_p\}_1, \ldots, \{w_p\}_M$ and some number of preference regions for an intervention $r$. To calculate the $r^{th}$ preference percentage for each product, first determine the preferred product in each preference region by choosing an arbitrary point in the region and finding the product with the minimum inventory function value at that point. This is the preferred product in that preference region. Then, for each preference region, quantify the size by integrating between preference boundaries. The dimensionality of the integration will be determined by the number of allocation weights. The $r^{th}$ preference percentage for product $j$ is equal to the size of product $j$’s preference region for intervention $r$ expressed as a percentage of the total allocation space.

Preference percentages can also be calculated by defining a grid of values of $w$ in the allocation space and finding the preferred product at each point and for each intervention $r$. Then the number of points for which product $j$ is preferred, $PP_j$, divided by the total number of points $N$, is approximately the preference percentage for that product and intervention:

$$PP_j \approx \frac{1}{N} \sum_{j=1}^{N} H_j, \quad H_j = \begin{cases} 1 & \text{Product } j \text{ is preferred} \\ 0 & \text{otherwise} \end{cases} \quad \text{(5.16)}$$

Preference percentages estimated from Equation (5.16) are given for the ethanol pathways comparison in Table 5.2. Stover gasification is preferred only in small
Table 5.2: Preference percentages by emission for the ethanol production pathways.

<table>
<thead>
<tr>
<th>Pathway</th>
<th>kg CO₂</th>
<th>kg CO</th>
<th>kg CH₄</th>
<th>kg NOₓ</th>
<th>kg N₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain fermentation</td>
<td>9.1</td>
<td>50.4</td>
<td>9.1</td>
<td>50.4</td>
<td>9.1</td>
</tr>
<tr>
<td>Stover hydrolysis</td>
<td>89.2</td>
<td>44.6</td>
<td>15.7</td>
<td>48.8</td>
<td>47.9</td>
</tr>
<tr>
<td>Stover gasification</td>
<td>1.7</td>
<td>5.0</td>
<td>75.2</td>
<td>0.8</td>
<td>43.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pathway</th>
<th>kg SO₂</th>
<th>kg coal</th>
<th>kg crude oil</th>
<th>kg natural gas</th>
<th>kg water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain fermentation</td>
<td>17.3</td>
<td>83.5</td>
<td>9.1</td>
<td>91.7</td>
<td>91.7</td>
</tr>
<tr>
<td>Stover hydrolysis</td>
<td>81.8</td>
<td>13.2</td>
<td>66.1</td>
<td>5.0</td>
<td>2.5</td>
</tr>
<tr>
<td>Stover gasification</td>
<td>0.8</td>
<td>3.3</td>
<td>24.8</td>
<td>3.3</td>
<td>5.8</td>
</tr>
</tbody>
</table>

fractions of the space, except for CH₄ and N₂O emissions; grain fermentation performs slightly better, and stover hydrolysis appears to have the overall best performance.

5.6 Case study: Production of 1,3-propanediol

Urban and Bakshi performed a cradle-to-gate comparative LCA of 1,3-propanediol (PDO) produced from fossil-based and biomass-based feedstocks. [285] The fossil-based process begins with syngas, a mixture of H₂ and CO, and ethylene oxide, which react together over a silver catalyst to produce PDO. None of the processes in the fossil-based PDO life cycle are multi-functional. The biomass-based process uses corn as a feedstock, which is milled to produce starch and starch by-products. The starch, which contains glucose, is fermented to produce PDO. The corn wet milling process produces is multi-functional, providing both starch, the primary product, and valuable starch by-products. After applying the total allocation procedure, it was found that regardless of allocation, biomass-based PDO was preferred over fossil-based for nine out of eleven interventions considered. The comparison was not robust
Table 5.3: Preference percentages by emission for fossil and biomass-based 1,3-propanediol.

<table>
<thead>
<tr>
<th>Pathway</th>
<th>g CO</th>
<th>g CO₂</th>
<th>MJ non-renewable energy</th>
<th>g NOₓ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fossil-based</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>5.5</td>
</tr>
<tr>
<td>Biomass-based</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>94.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pathway</th>
<th>g N₂O</th>
<th>CH₄ (g CO₂-eq)</th>
<th>g PM₁₀</th>
<th>g SOₓ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fossil-based</td>
<td>20.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Biomass-based</td>
<td>80.0</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pathway</th>
<th>CFC (g CO₂-eq)</th>
<th>g Lead</th>
<th>g VOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fossil-based</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Biomass-based</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

For N₂O and NOₓ emissions, most likely due to the farming process in the biomass-based PDO life cycle. For these two interventions, fossil-based PDO was preferred only for relatively high values of \( w > 0.8 \) and \( w > 0.945 \) respectively. Table 5.3 contains the preference percentages for the eleven emissions considered.

Because biomass-based PDO is preferred exclusively for the majority of interventions considered, and because it is preferred in a small fraction of the allocation space even for N₂O and NOₓ, the conclusion is that it is the preferred product.
Chapter 6: The process to planet modeling framework for sustainable engineering applications

6.1 Introduction

Sustainable engineering methods tend to follow a “bottom up” approach, modeling the system of interest in detail at the smallest relevant scale [50] and capturing that system’s life cycle using empirical data that represents average production technology. [137, 138] Such approaches are a simple and appealing way of incorporating life cycle considerations into engineering design, as the addition of life cycle data does not require significant changes to the traditional engineering design problem. However, the simplicity of this approach leads to some serious shortcomings. The prevalent method for quantifying life cycle considerations in engineering design is process based LCA, in which a system boundary is defined by choosing which parts of the life cycle are considered to be most important. As discussed in Section 2.1.2, process based LCA accounts for a relatively small proportion of the complete life cycle, estimated at 20 - 50%. [189] Because a significant portion of the life cycle is neglected, any design or other decisions based on a process based life cycle are based on incomplete life cycle information; these decisions may therefore be sub-optimal. In particular, a narrow life cycle boundary allows environmental impacts to be shifted outside the life
A complete life cycle is infinite due to the interconnections between industries and cannot be modeled feasibly using process LCA. Cycle, resulting in an apparent decrease in impacts when in reality net impacts may not change at all or may even increase. [121]

Current approaches to sustainable engineering design rely on the life cycle boundary shown in Figure 6.1 as dark red circles. In order to ensure correct, optimal design decisions and to avoid causing unintended externalities, the full life cycle (both dark and light circles in Figure 6.1) must be accounted for in the sustainable engineering design problem. [32, 47] Process LCA requires that each life cycle process and each connection between processes be modeled individually; therefore, expanding the life cycle boundary using the current approach is impractical and computationally intractable for moderately large life cycle networks, as the number of connections in any life cycle network is essentially infinite. [66]
The challenges of using bottom up models in a sustainable design context also apply to LCA and footprint studies that apply similar models in a sustainability assessment context. To address some of the system boundary issues of bottom up methods, “top down” methods have been developed for modeling and analyzing 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 [193, 194, 222], and has been applied to sustainability assessment studies up to the global scale. [65] Economic [68], general equilibrium [40] and partial equilibrium models [95] are other top down methods applied to national scale sustainability analyses. Although top down models are comprehensive, particularly compared to process LCA, they lack detail at sub-national and -regional scales and do not benefit from the fundamental engineering models available at the equipment (plant) scale.

This chapter develops a multi-scale “process to planet” (P2P) modeling framework that integrates engineering models, life cycle process models, and EEIO models to capture systems with components at multiple spatial scales in multiple levels of detail. The P2P modeling framework connects detailed fundamental models of individual processes and unit operations at the equipment scale with linear, empirical models of life cycle processes at the value chain scale and input-output models of the regional, national or global economic system at the economy scale. The framework is based upon hybrid LCA methods that connect models at the value chain and economy scales; by extending these existing models to the equipment scale, the P2P framework 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, and can be implemented within an optimization formulation to solve a wide variety of sustainable engineering problems. [134]

Material in this chapter has been previously published in references [132] and [134].

6.2 Process to planet modeling framework

The P2P modeling framework represents system components at three distinct scales: equipment, value chain and economy. Conventional models and modeling techniques have been developed for systems at all three scales; the P2P approach integrates these separate models into a single cohesive multi-scale model representing a national life cycle.

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 macro-economic system. Mining, grain farming and power generation are examples of economic sectors. National economy scale models are available from tools such as EIO-LCA [119] and Eco-LCA [18]
as well as from governmental sources for some countries. [286] Planetary scale economy models have also been developed that use multi-regional input-output (MRIO) models to represent the global economy. [191, 283] The P2P framework developed in this chapter extends only to the national scale; extension of the framework to the planetary scale is discussed in Section 9.2.3.

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 and 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 U.S., 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 [275] and the US NREL database. [219] The combination of the value chain and equipment scales represents the usual scope for conventional sustainable process design problems.

For the remainder of the dissertation, the overbar notation will continue to indicate models and quantities at the economy scale. Because value chain activity models are essentially the same models used in process LCA, the underbar notation will indicate value chain models. No bars on a quantity indicates the equipment scale. A combined over- and underbar, \( \overline{\underline{X}} \), is used to indicate the complete P2P system. A superscript
star * denotes a component model that has been disaggregated as discussed in Section 6.2.3. Other subscripts and superscripts used in the notation will be defined as they occur. Table D.1 contains a list of terms along with their definitions and first appearance in the dissertation.

An illustrative P2P system is shown in Figure 6.2. System components are sectors ($S_1$, $S_2$ and $S_3$) modeled at the economy scale, activities ($S_4$ and $S_5$) at the value chain scale and processes ($S_6$) at the equipment scale. $S_6$ may represent a single production facility or a supply chain. 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 equipment scale 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 6.2 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.

6.2.1 System component models

In Figure 6.2, 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 determined empirically. Each sector and activity model is a vector of inputs and outputs, $\mathbf{x}_j^2$.

$^2$Not to be confused with $\mathbf{x}$, the vector of total sector outputs used to derive the direct requirements matrix, which does not have a subscript.
and $\mathbf{x}_j$ respectively. $\mathbf{x}_j$ and $\mathbf{x}_l$ are the columns of matrices $\mathbf{X}$ and $\mathbf{X}$:

$$
\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_J \end{bmatrix}
$$ (6.1)

$$
\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_L \end{bmatrix}
$$ (6.2)

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 $\mathbf{A}$ and Leontief inverse are derived from $\mathbf{X}$, the transactions matrix, as discussed in Section 2.3. $\mathbf{X}$, 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 Section 2.1.2.

Environmental interventions for both scales are specified as vectors of inputs from and outputs to the environment. $\mathbf{b}_j$ contains interventions per dollar of output from sector $j$, while $\mathbf{b}_l$ contains interventions corresponding to the level of production of activity $l$ specified in $\mathbf{x}_l$. $\mathbf{b}_j$ and $\mathbf{b}_l$ are collected into interventions matrices $\mathbf{B}$ and $\mathbf{B}$:

$$
\mathbf{B} = \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_J \end{bmatrix}
$$ (6.3)

$$
\mathbf{B} = \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \cdots & \mathbf{b}_L \end{bmatrix}
$$ (6.4)

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

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 non-linear. 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
Figure 6.3: Process model \( n \) consists of a set of fundamental unit operation models \( h_n \) involving design variables \( z_n \). Inputs and outputs of process \( n \) are written as functions of \( z_n \), \( x_n(z_n) \), which are derived from \( h_n(z_n) \).
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 $x_n(z_n)$ which is exactly analogous to those used to model value chain activities. Figure 6.3 demonstrates this for a process with five design variables, in which $z_n = \{z_{n1}, z_{n2}, z_{n3}, z_{n4}, z_{n5}\}$. For process $n$ in Figure 6.3, the input-output vector $x_n(z_n)$ is

$$x_n(z_n) = \begin{bmatrix} -x_{n1}(z_n) \\ -x_{n2}(z_n) \\ +x_{n3}(z_n) \\ +x_{n4}(z_n) \end{bmatrix}$$

(6.5)

$\{z\}$ denotes the entire set of unit operation variables: $\{z\} = \{z_1, \ldots, z_N\}$.

$x_n(z_n)$ differs from $x_l$ in that the elements of $x_n(z_n)$ are variable and dependent on the values of process $n$’s design variables $z_n$. No information is lost in using this vector notation, as the fundamental models $h_n(z_n)$ 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 $X(\{z\})$, in which any or all of the elements
may be functions, and a set of fundamental models for each process, as follows:

\[
X(\{z\}) = \begin{bmatrix} x_1(z_1) & \cdots & x_N(z_N) \end{bmatrix}
\]

\[
H(\{z\}) \geq 0
\]  

(6.6)

\[
H(\{z\}) \text{ denotes the entire set of fundamental models: } H(\{z\}) = \{h_1(z_1), \ldots, h_N(z_N)\}.
\]

The environmental intervention matrix for the equipment scale is likewise dependent on unit operation variables, and is also derived from \(H(\{z\})\):

\[
B(\{z\}) = \begin{bmatrix} b_1(z_1) & \cdots & b_N(z_N) \end{bmatrix}
\]

(6.7)

6.2.2 Interactions between scales

Thus far the component models have described only exchanges between system components at the same scale. Interactions between components at different scales are captured in matrices containing upstream and downstream cutoff flows. Cutoff flows are inputs or outputs of components at one scale that are modeled as being produced (inputs) or consumed (outputs) at a different scale. Throughout this discussion and the rest of the dissertation, the descriptors “upstream” and “downstream” are always used in reference to the smaller scale. For instance, flows produced at the economy scale and consumed at the value chain scale are referred to as value chain upstream cutoff flows. Similarly, flows 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 upstream cutoff flows are inputs to value chain activities that are produced at the economy scale. Data on value chain upstream cutoffs is obtained from the same sources as exchanges within the value chain, and is 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 build the P2P model. The value chain upstream cutoff matrix $X_u$ has $L$ columns, one for each value chain activity, and $I$ rows, one for each economic commodity. Figure 6.4 shows $X_u$ in the context of the entire P2P system.
Downstream cutoff flows for the value chain scale are activity outputs that are consumed at the economy scale. 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 before being used in the P2P modeling framework. This normalized value chain downstream cutoff matrix is denoted \( \mathbf{A}_d \). However, when the downstream cutoff matrix is used in the disaggregation calculations of Section 6.2.3, it is not normalized and is denoted \( \mathbf{X}_d \). The relevant flow in Figure 6.4 is thus labeled as both \( \mathbf{X}_d \) and \( \mathbf{A}_d \). Both \( \mathbf{A}_d \) and \( \mathbf{X}_d \) have \( J \) columns, one for each sector, and \( K \) rows, one for each value chain product.

Equipment scale cutoff matrices are analogous to value chain cutoff matrices, although a superscript \( E \) or \( V \) is added to indicate whether the cutoff flows connect to the economy scale or to 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 \( \mathbf{X}_{\text{eu}}^{\text{E}}(\{z\}) \) 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 \( \mathbf{X}_{\text{vu}}^{\text{V}}(\{z\}) \) 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 \( \mathbf{A}_{\text{du}}^{\text{E}}(\{z\}) \) are...
normalized by the total output of each destination sector; the equipment-economy
downstream cutoff matrix used in disaggregation, $X_d^E(\{z\})$, is not normalized, just
as $A_d$ was normalized and $X_d$ was not. However, the elements of the equipment-value
chain downstream cutoff matrix, $X_d^V(\{z\})$, do not need to be normalized by the total
output of the destination activity in the P2P model. The relevant flows are labeled
in Figure 6.4.

6.2.3 Model disaggregation

The multi-scale nature of the system in Figure 6.2 leads to inevitable overlap be-
tween models. It is common for value chain activity models and process models to
be contained within sector models, and for process models to likewise be contained
within value chain activity models. In this situation, the smaller scale models are repre-
sented twice in the P2P modeling framework – once explicitly and once implicitly
– leading to double-counting of the smaller scale’s technological and environmental
flows. The inputs and outputs of sector $S_3$ in Figure 6.5a, for instance, also contain
inputs and outputs of activity $S_4$. Generally, more detailed data or models are avail-
able for the smaller scale system components, the constituents, than for the larger
scale components, the parents. Constituent value chain activities, being less aggre-
gated, are modeled in more detail than their parent sectors, and constituent processes
are modeled in still more detail than their parent value chain activities. To accommo-
date this extra information and to avoid double-counting, the parent component is
split into two or more sub-components: the constituent component(s) for which more
detailed data or models are available, and the remainder of the parent component.
The constituent components are modeled separately at the smaller scale(s), while the remainder of the parent component remains as part of the parent scale model.

In Figure 6.5a, \( S_4 \) represents constituent value chain activity(ies) and \( S_3 \) represents the parent industrial sector such that \( S_4 \in S_3 \). Figure 6.5b illustrates the system after disaggregation; \( S_3^* \), called the adjusted sector, represents the remainder of \( S_3 \). The relationship between \( S_3 \), \( S_3^* \) and \( S_4 \) is

\[
S_3 = S_3^* \cup S_4
\]  

(6.8)

As an example, suppose \( S_3 \) represents the power generation sector and \( S_4 \) represents a coal-burning electricity generation activity, for which more detailed empirical data is available. To model \( S_3 \) and \( S_4 \) without overlap, the power generation sector is divided into the coal-based activity \( S_4 \) and all other electricity generating activities, \( S_3^* \). \( S_4 \) is then modeled separately from the EEIO model at the value chain scale using the more detailed data.

Suppose that \( S_4 \) also has a constituent process, \( S_7 \) (not shown in Figure 6.5). Two disaggregations would be needed in this case, one for \( S_3^* \) and one for \( S_4^* \); the relationship between \( S_3 \) and its constituents is expressed as

\[
S_3 = S_3^* \cup S_4^* \cup S_7
\]  

(6.9)

where \( S_4 \) in (6.8) has been disaggregated as follows:

\[
S_4 = S_4^* \cup S_7
\]  

(6.10)

Standalone components that do not overlap with any larger scale system components are less common than constituent components. Standalone processes may represent newly developed technology that cannot be classified into existing sectors
Figure 6.5: When smaller scale system components overlap with larger scale components as shown on the left, the parent components ($S_3$ and $S_2$) must be disaggregated into constituent activities and/or processes ($S_4$ and $S_6$), which are modeled in detail at smaller scales, and adjusted components ($S_3^*$ and $S_2^*$), which remain in the original parent model as shown on the right.
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 6.5, $S_5$ is a standalone activity. $S_5$, like the constituent activity $S_4$, interacts with other system components, but as it does not have a parent component no disaggregation need be performed.

Component model 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 associated with the parent component in the larger scale model. To accomplish this subtraction, the constituent and parent component models must be on an equivalent time basis; in other words, all models involved in disaggregation must represent the same amount of time. This time basis will in general be one year, as most EEIO models are assembled on the basis of one year and the smaller scale models can be scaled up more easily than the EEIO model can be scaled down.

The disaggregation of $S_3$ and $S_2$ shown in Figure 6.5 is accomplished by subtracting off flows originating in the constituent components:

\[
x_{35} = x_{35} - p_{45}y_{45}
\]

\[
x_{25} = x_{25} - p_{65}y_{65}
\]

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

\[
x_{kl} = p_{kl}y_{kl}
\]
Price data for equipment scale flows, \( p_{mn} \), is used analogously.

\[ x_{mn} = p_{mn}y_{mn} \] (6.14)

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 generating electricity, the value chain scale price of coal electricity is averaged over all coal power plants in a particular region, while the equipment scale price is specific to a single power plant. Equations (6.11) and (6.12) implicitly assume that product flows \( x_{13} \) and \( x_{32} \) belong, respectively, to the commodities represented by flows \( \bar{x}_{13} \) and \( \bar{x}_{32} \), which in general is a valid assumption to make for products of constituent components at both the value chain and process scale. Environmental interventions are similarly disaggregated:

\[ \bar{b}_3 = b_3 - b_3 \] (6.15)

In general, P2P systems contain multiple parent components at different scales, each with multiple constituents. Manual disaggregation, as shown in Equations (6.11) - (6.15), becomes complex and time-consuming in this situation. A more efficient way to disaggregate the economy and value chain models is through the make and use matrices discussed in Section 2.3.2. 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: \( \bar{U} \) is \( I \times J \), \( \bar{U} \) is \( K \times L \) and \( U \) 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 \( \mathbf{\nabla} \), \( L \times K \) for \( \mathbf{\mathbf{V}} \) and \( N \times M \) for \( \mathbf{V} \). [209] 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 how equipment scale products, value chain products and commodities relate to each other and information on relationships between all constituent and parent components. [267] This information is quantified in product and process permutation matrices, which then are used in the disaggregation calculations.

Definitions for previously undefined matrices appearing in the following equations are given in Table D.1. As discussed previously, the equipment scale models are dependent on design variables \( \{z\} \). \( \{z\} \) is propagated throughout the models via the disaggregation process, resulting in both the economy and value chain models being dependent on unit operation design variables.

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

\[
\mathbf{\nabla}^*(\{z\}) = \mathbf{\nabla} - \hat{p}(\mathbf{P}_P)^T \mathbf{\mathbf{V}}(\mathbf{P}_P)^T - \hat{p}(\mathbf{P}_E)^T \mathbf{\mathbf{V}}(\{z\})(\mathbf{P}_E)^T
\]

\[
\mathbf{\mathbf{U}}^*(\{z\}) = \mathbf{\mathbf{U}}
\]

\[
- (\hat{p}\mathbf{P}_P \mathbf{U}\mathbf{P}_P + \hat{p}\mathbf{P}_P \mathbf{X}_d + \mathbf{X}_u \mathbf{P}_P)
\]

\[
- (\hat{p}\mathbf{P}_E \mathbf{U}(\{z\})\mathbf{P}_P + \hat{p}\mathbf{P}_E \mathbf{X}_d(\{z\}) + \mathbf{X}_u(\{z\})\mathbf{P}_E)
\]

in which

\[
\mathbf{P}_F = \{p_F\}
\]

\[
p_{Fik} = \begin{cases} 
  1 & \text{if value chain product } k \text{ belongs to commodity } i \\
  0 & \text{otherwise}
\end{cases}
\]

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The permutation matrices defined in Equation (6.18) - (6.21) contain information on the relationships between parent sectors and constituent activities and processes. These matrices along with price data vectors $\hat{p}$ and $p$ are used to “translate” the various make and use matrices from one scale to another. Superscripts on the equipment scale permutation matrices in Equations (6.20) and (6.21) are used to specify the scale to which flows are being translated. $\mathbf{P}_E$ for instance relates equipment scale products to economic (E) commodities, while $\mathbf{P}_V$ in Equation (6.24) 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 Equations (6.18) and (6.19).

Note that in Equations (6.16) and (6.17), the original value chain make and use matrices are used rather than the disaggregated matrices. This is because, in the situation that a constituent activity also contains an activity-constituent process, removing the undisaggregated activity also removes the activity-constituent process. Disaggregation of the value chain scale make and use matrices to $\mathbf{V}^*\{\{z\}\}$ and $\mathbf{U}^*\{\{z\}\}$
is analogous to the economy scale:

$$V^*(\{z\}) = V - \hat{p}(P^V_P)^T V (\{z\}) (P^V_P)^T$$

(6.22)

$$U^*(\{z\}) = U - \hat{p}P^V_U (\{z\}) P^V_P - \hat{p}P^V_U X^V_U (\{z\}) - X^V_u (\{z\}) P^V_P$$

(6.23)

in which

$$P^V_F = \{p^V_F\}$$

(6.24)

$$p^V_{Fkm} = \begin{cases} 
1 & \text{if product } m \text{ belongs to the product set represented by value chain product } k \\
0 & \text{otherwise}
\end{cases}$$

(6.25)

$$P^V_P = \{p^V_P\}$$

$$p^V_{Pnl} = \begin{cases} 
1 & \text{if process } n \text{ is constituent to value chain activity } l \\
0 & \text{otherwise}
\end{cases}$$

Readers familiar with integrated hybrid LCA will notice similarities between Equations (6.16), (6.17), (6.22) and (6.23) and Equations (A6) and (A7) in [267]. The first two terms in Equations (6.16) and (6.17) are identical to the disaggregation equations, (A7) and (A6) respectively, used in integrated hybrid LCA. The final terms in (6.16) and (6.17) deal with fundamental models at the engineering scale and introduce unit operation variables and non-linearities to the economy scale make and use matrices. These terms are among the contributions of this work. Equations (6.22) and (6.23) are directly analogous to (A7) and (A6), although they are applied to the value chain technology matrices and once again introduce variables and non-linearities from the equipment scale models.

To summarize, the disaggregated make and use matrices represent only production and consumption by components at 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, either value chain activities or processes. As a result of the disaggregation, parent sectors and activities become smaller: the portion of the parent’s output produced by constituent process(es) is subtracted, reducing the total output and therefore the “size” of the parent components. Tables 6.1 and 6.2 give the physical interpretation of each factor in Equations (6.16), (6.17), (6.22) and (6.23).

The disaggregated economy scale make and use matrices are used to calculate the disaggregated direct requirements matrix as in Equation (2.30):

\[
\overline{A}^*({\{z\}}) = \overline{U}^*({\{z\}}) \left( \overline{V}^{*T}({\{z\}}) \right)^{-1}
\]  

(6.26)

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

\[
\overline{A}^*({\{z\}}) \overline{V}^{*T}({\{z\}}) \left( \overline{V}^{*}({\{z\}}) \right)^{-1} = \overline{U}^*({\{z\}}) \left( \overline{V}^{*}({\{z\}}) \right)^{-1}
\]

(6.27)

a system of linear equations in which \(\overline{V}^{*T}({\{z\}}) \ 1\) is the vector of total sector outputs after disaggregation, \(\overline{x}^*({\{z\}})\), and all matrices are known except for \(\overline{A}^*({\{z\}})\).

1 denotes a vector of all 1’s; multiplication by 1 produces a vector of row sums.

The quantity \(\overline{V}^{*T}({\{z\}}) \ 1\) is then a vector of column sums of \(\overline{V}^*\). The solutions to Equations (6.26) and (6.27) are equivalent when the make and use matrices are square and for the same values of ({\{z\}}).

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

\[
\overline{X}^*({\{z\}}) = \overline{V}^{*T}({\{z\}}) - \overline{U}^*({\{z\}})
\]

(6.28)

Environmental interventions for the parent components must be disaggregated as well to avoid counting the interventions of both the parents and constituents. The
Table 6.1: Explanation of factors involved in economy and value chain model disaggregations given in Equations (6.16) and (6.17).

<table>
<thead>
<tr>
<th>Factor</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{V}$</td>
<td>Economy scale make matrix: commodities produced by sectors</td>
</tr>
<tr>
<td>$\hat{p}(\mathbf{P}_P)^T \mathbf{V}(\mathbf{P}_F)^T$</td>
<td>Products produced by sector-constituent value chain activities, calculated from value chain scale make matrix $\mathbf{V}$</td>
</tr>
<tr>
<td>$\hat{p}(\mathbf{P}_P)^T \mathbf{V}({z})(\mathbf{P}_F)^T$</td>
<td>Products produced by sector-constituent processes, calculated from equipment scale make matrix $\mathbf{V}({z})$</td>
</tr>
<tr>
<td>$\mathbf{U}$</td>
<td>Economy scale use matrix: commodities consumed by sectors</td>
</tr>
<tr>
<td>$\hat{p}\mathbf{P}_P \mathbf{U}\mathbf{P}_P$</td>
<td>Products consumed and produced by sector-constituent activities, calculated from value chain scale use matrix $\mathbf{U}$</td>
</tr>
<tr>
<td>$\hat{p}\mathbf{P}_P \mathbf{X}_d$</td>
<td>Products consumed by sectors and produced by sector-constituent activities, calculated from value chain scale downstream cutoff matrix $\mathbf{X}_d$</td>
</tr>
<tr>
<td>$\mathbf{X}_u \mathbf{P}_P$</td>
<td>Products consumed by sector-constituent activities and produced by sectors, calculated from value chain scale upstream cutoff matrix $\mathbf{X}_u$</td>
</tr>
<tr>
<td>$\hat{p}\mathbf{P}_E^E \mathbf{U}({z}) \mathbf{P}_P^E$</td>
<td>Products consumed and produced by sector-constituent processes, calculated from equipment scale use matrix $\mathbf{U}({z})$</td>
</tr>
<tr>
<td>$\hat{p}\mathbf{P}_E^E \mathbf{X}_d^E({z})$</td>
<td>Products consumed by sectors and produced by sector-constituent processes, calculated from equipment-economy downstream cutoff matrix $\mathbf{X}_d^E({z})$</td>
</tr>
<tr>
<td>$\mathbf{X}_u^E({z}) \mathbf{P}_P^E$</td>
<td>Products consumed by sector-constituent processes and produced by sectors, calculated from equipment-economy upstream cutoff matrix $\mathbf{X}_u^E({z})$</td>
</tr>
</tbody>
</table>
Table 6.2: Explanation of actors involved in value chain disaggregations given in Equations (6.22) and (6.23).

<table>
<thead>
<tr>
<th>Factor</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V )</td>
<td>Value chain scale make matrix (not disaggregated): commodities produced by activities</td>
</tr>
<tr>
<td>( \hat{p}(P_d^V)^TV({z})(P_F^V)^T )</td>
<td>Products produced by activity-constituent processes, calculated from equipment scale make matrix ( V({z}) )</td>
</tr>
<tr>
<td>( U )</td>
<td>Value chain scale use matrix (not disaggregated): commodities consumed by activities</td>
</tr>
<tr>
<td>( \hat{p}P_k^V U({z})P_p^V )</td>
<td>Products consumed and produced by activity-constituent processes, calculated from equipment scale use matrix ( U({z}) )</td>
</tr>
<tr>
<td>( \hat{p}P_F^V X_d^V({z}) )</td>
<td>Products consumed by activities and produced by activity-constituent processes, calculated from equipment-value chain downstream cutoff matrix ( X_d^V({z}) )</td>
</tr>
<tr>
<td>( X_u^V({z})P_p^V )</td>
<td>Products consumed by activity-constituent processes and produced by activities, calculated from equipment-value chain upstream cutoff matrix ( X_u^V({z}) )</td>
</tr>
</tbody>
</table>
interventions matrix used in EEIO models, $\mathbf{B}$, is normalized to the total output of each sector, as discussed in Section 2.3.3; $\mathbf{B}$ 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 and do not represent an average value. $\mathbf{R}$ denotes the total interventions matrix for the economy scale. The value chain interventions $\mathbf{B}$ are not normalized by activity output but represent total environmental interventions for the level of production specified in the activity model. The disaggregated economy scale environmental interventions matrix $\mathbf{B}^*(\{z\})$ is calculated from data in the original and disaggregated make matrices:

$$ \mathbf{R}^*(\{z\}) = \mathbf{R} - \mathbf{B}\mathbf{P}_P - \mathbf{B}(\{z\})\mathbf{P}_E^E $$

(6.29)

$$ \mathbf{B}^*_j(\{z\}) = \frac{1}{(\mathbf{V}^*T(\{z\})\mathbf{1})}_j \mathbf{r}^*(\{z\})_j $$

(6.30)

Taking the transpose of the matrix before multiplying by 1, as in Equation (6.30), produces a vector of row sums. The vector $\mathbf{V}^*T(\{z\})\mathbf{1}$ therefore contains total outputs by industrial sector after disaggregation. $(\mathbf{V}^*T(\{z\})\mathbf{1})_j$ refers to the $j^{th}$ element in $\mathbf{V}^*T(\{z\})\mathbf{1}$, which is the total output of disaggregated sector $j$. $\mathbf{r}^*(\{z\})_j$ and $\mathbf{r}_j$ similarly refer to the $j^{th}$ column of the disaggregated and total interventions matrices $\mathbf{R}^*(\{z\})$ and $\mathbf{R}$, respectively. The disaggregated value chain scale interventions matrix $\mathbf{B}^*(\{z\})$ is calculated similarly:

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

(6.31)

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

Following disaggregation, the component models, listed and defined in Table 6.3, are integrated into a single P2P transactions matrix $\mathbf{X}(\{z\})$ and a P2P environmental interventions matrix $\mathbf{B}(\{z\})$, both shown in Table 6.4. $\mathbf{X}(\{z\})$ captures flows within and between the sectors, activities and processes. Each row corresponds to flows of a particular commodity or product that is produced and consumed within the system, and each column corresponds to one system component and includes upstream cutoffw, downstream cutoffw and intra-scale flows. $\mathbf{B}(\{z\})$ captures flows between system components and the environment; each row corresponds to one environmental intervention and each column corresponds to one system component.

The P2P transactions matrix functions analogously to the direct requirements matrix $\mathbf{A}$ used in economic input-output analysis (see Section 2.3) or the technology matrix $\mathbf{X}$ used in process based LCA (see Section 2.1.2). Both $\mathbf{A}$ and $\mathbf{X}$ represented systems that were assumed to scale linearly, and both system models were multiplied by a vector of scaling factors ($\mathbf{x}$ and $\mathbf{s}$, respectively) determined from the final demand or functional unit vector, in order to calculate system-wide environmental interventions. $\mathbf{X}(\{z\})$ 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

$$\mathbf{s} = \begin{bmatrix} \mathbf{s} \\ \mathbf{S} \\ \mathbf{s} \end{bmatrix}$$ \hspace{1cm} (6.32)

and consists of three sub-vectors, each of which correspond to the models at one scale of the system. $\mathbf{s}$ has the same interpretation as the throughput vector $\mathbf{x}$ of Section
Table 6.3: System component models to be included in the P2P modeling framework.

<table>
<thead>
<tr>
<th>Scale</th>
<th>Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Economy</strong></td>
<td>$\tilde{A}^*({z})$</td>
<td>Disaggregated direct requirements matrix</td>
</tr>
<tr>
<td></td>
<td>$\tilde{B}^*({z})$</td>
<td>Disaggregated economy scale environmental interventions</td>
</tr>
<tr>
<td></td>
<td>$\tilde{f}$</td>
<td>Final demand from economy (generally zero)</td>
</tr>
<tr>
<td></td>
<td>$\tilde{s}$</td>
<td>Sector scaling vector (variable, analogous to throughput vector $\bar{x}$)</td>
</tr>
<tr>
<td><strong>Value chain</strong></td>
<td>$X^*({z})$</td>
<td>Disaggregated value chain model</td>
</tr>
<tr>
<td></td>
<td>$X_u({z})$</td>
<td>Value chain upstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$\Delta_d({z})$</td>
<td>Normalized value chain downstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$B^*({z})$</td>
<td>Disaggregated value chain environmental interventions</td>
</tr>
<tr>
<td></td>
<td>$f$</td>
<td>Final demand from value chain (generally zero)</td>
</tr>
<tr>
<td></td>
<td>$s$</td>
<td>Value chain activity scaling vector (variable)</td>
</tr>
<tr>
<td><strong>Process</strong></td>
<td>$X({z})$</td>
<td>Equipment model matrix</td>
</tr>
<tr>
<td></td>
<td>$X^E_u({z})$</td>
<td>Equipment-economy upstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$X^V_u({z})$</td>
<td>Equipment-value chain upstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$A^E_d({z})$</td>
<td>Normalized equipment-economy downstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$X^V_d({z})$</td>
<td>Equipment-value chain downstream cutoff matrix</td>
</tr>
<tr>
<td></td>
<td>$B({z})$</td>
<td>Equipment environmental interventions</td>
</tr>
<tr>
<td></td>
<td>$f$</td>
<td>Final demand from equipment scale process(es)</td>
</tr>
<tr>
<td></td>
<td>$s$</td>
<td>Equipment scaling vector (variable or fixed)</td>
</tr>
<tr>
<td><strong>Unit operation</strong></td>
<td>$H({z})$</td>
<td>Unit operation models external to $X({z})$</td>
</tr>
</tbody>
</table>
Table 6.4: P2P transactions matrix and environmental interventions matrix. Sub-matrices are colored according to scale.

<table>
<thead>
<tr>
<th>( \mathbf{X}({z}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbb{I} - \mathbf{A}^*({z}) )</td>
</tr>
<tr>
<td>( - \mathbf{A}_d({z}) )</td>
</tr>
<tr>
<td>( - \mathbf{A}_E^E({z}) )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \mathbf{B}({z}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{B}^*({z}) )</td>
</tr>
</tbody>
</table>

2.3 and scales the economic sector models as well as the value chain and equipment-economy downstream cutoff flows. \( \mathbf{s} \) scales the value chain activities, the value chain upstream cutoffs and the equipment-value chain downstream cutoffs. Both \( \tilde{\mathbf{s}} \) and \( \mathbf{s} \) are standard, linear scaling vectors because the economic sector and activity models are assumed to scale linearly. The last sub-vector of \( \tilde{\mathbf{s}} \) 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 non-linear such as \( s^0.7 \). To avoid finding the exact form of each element of \( \mathbf{s} \), \( \tilde{\mathbf{s}} \) can also be fixed in order to fix the scale of the process models at whatever scale is represented in the process models \( \mathbf{H}(\{z\}) \).

The complete P2P modeling framework consists of a set of balance equations on the system’s commodities and products,

\[
\mathbf{X}(\{z\})\tilde{\mathbf{s}} = \mathbf{f} \quad (6.33)
\]

and a set of fundamental models for each process,

\[
\mathbf{H}(\{z\}) \geq 0 \quad (6.34)
\]
that are specified externally to $\mathbf{X}(\{z\})$ as discussed in Section 6.2.1. Equation (6.33) constrains the variable elements of $\mathbf{g}$ such that net production of each commodity, value chain product and equipment scale product is at least equal to the final demand placed on the entire system. Equation (6.33) also forms one set of constraints on the design variables $\{z\}$. The variables are further constrained by the fundamental models in Equation (6.34).

6.3 Illustrative example and comparison to conventional methods

In this section, the data and calculations involved in representing a system using the P2P modeling framework are demonstrated with a toy example. As each component model used to represent the toy system is discussed, 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 two economic sectors, two value chain activities and two processes. Each process involves two unit operation design 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 the disaggregation procedure need be applied only to the economic system. The structure of the system, including all
Figure 6.6: The toy system modeled in Section 6.3 consists of two parent sectors, two non-parent value chain activities and two processes.

exchanges between components and all parent-constituent relationships, is shown in Figure 6.6.

### 6.3.1 Economy model

Sectors 1 and 2, $S_1$ and $S_2$ in Figure 6.6, are modeled with an economic input-output model. Commodity exchanges between $S_1$ and $S_2$ are captured in monetary units by the following make and use matrices,

\[
\mathbf{V} = \begin{bmatrix}
700 \\
0
\end{bmatrix}
\]

(6.35)

\[
\mathbf{U} = \begin{bmatrix}
150 \\
300
\end{bmatrix}
\begin{bmatrix}
200 \\
100
\end{bmatrix}
\]

(6.36)
For this example, $\mathbf{U}$ and $\mathbf{V}$ are given in dollars; note that input-output tables are commonly specified in millions of dollars. The elements of $\mathbf{V}$ are interpreted as commodity flows from producing sectors; the elements of $\mathbf{U}$ are interpreted as commodity flows to consuming sectors. For instance, the $(1, 1)th$ element of $\mathbf{V}$ is $500$, indicating that sector 1 produces $500$ worth of commodity 1. The $(1, 1)th$ element of $\mathbf{U}$ is $150$, indicating that of the $500$ worth of commodity 1 that sector 1 produced, $150$ worth was consumed by sector 1. This flow is indicated by the arrow in Figure 6.6 that originates and terminates at $S_1$.

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

$$
\mathbf{B} = \begin{bmatrix} 0.40 & 0.20 \\
\end{bmatrix} \quad (6.37)
$$

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 $\mathbf{B}$ 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 $\mathbf{R}$, is required. Unlike the data in $\mathbf{B}$, which is normalized by each sector’s total output, $\mathbf{R}$ gives unnormalized flows of environmental interventions for each sector. For this toy economic system, $\mathbf{R}$ is as follows:

$$
\mathbf{R} = \begin{bmatrix} 200 & 140 \\
\end{bmatrix} \quad (6.38)
$$

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

$$\mathbf{R} \mathbf{x}^{-1} = \begin{bmatrix} 200 & 140 \\ 500 & 700 \end{bmatrix}^{-1} = \begin{bmatrix} 0.40 & 0.20 \end{bmatrix}$$  \hfill (6.39)

If only one of $\mathbf{R}$ and $\mathbf{B}$ is known, Equation (6.39) can be used to obtain the other.

### 6.3.2 EEIO model

Given the data in Equations (6.35) - (6.37), an environmentally extended input-output model can be derived. The direct requirements matrix is obtained from the make and use matrices according to Equation (2.30):

$$\mathbf{A} = \mathbf{U} (\mathbf{V}^T)^{-1} = \begin{bmatrix} 0.30 & 0.29 \\ 0.60 & 0.14 \end{bmatrix}$$  \hfill (6.40)

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

$$\mathbf{x} = (\mathbf{I} - \mathbf{A})^{-1} \bar{f} = \begin{bmatrix} 0.70 & -0.29 \\ -0.60 & 0.86 \end{bmatrix}^{-1} \bar{f}$$  \hfill (6.41)

$\mathbf{B}$ and the Leontief inverse of Equation (6.41) are used to calculate the total environmental interventions $\bar{g}$ generated as a consequence of producing $\bar{f}$:

$$\bar{g} = \mathbf{B} (\mathbf{I} - \mathbf{A})^{-1} \bar{f} = \begin{bmatrix} 0.40 & 0.20 \end{bmatrix} \begin{bmatrix} 0.70 & -0.29 \\ -0.60 & 0.86 \end{bmatrix}^{-1} \bar{f}$$  \hfill (6.42)

This EEIO model is utilized in macro-scale or top-down analyses such as policy analysis and EIO-LCA, as discussed in Section 2.3.3. It is also used in combination with process LCA in hybrid LCA models.

### 6.3.3 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, $S_1$ and $S_2$ in Figure 6.6, is represented by the make and use matrices $V$ and $U$:

$$V = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} \quad (6.43)$$

$$U = \begin{bmatrix} 15 & 8 \\ 5 & 10 \end{bmatrix} \quad (6.44)$$

Columns of $X$, derived from $V$ and $U$ as follows,

$$X = V^T - U = \begin{bmatrix} 35 & 0 \\ 0 & 50 \end{bmatrix} - \begin{bmatrix} 15 & 8 \\ 5 & 10 \end{bmatrix} = \begin{bmatrix} 20 & -8 \\ -5 & 40 \end{bmatrix} \quad (6.45)$$

are models of the individual activities: activity 1 (column 1 of $X$) consumes 5 units of product 2 and 15 units of product 1 for every 35 units of product 1 it produces.

The value chain environmental interventions matrix $B$ for this system is defined as

$$B = \begin{bmatrix} 8 & 5 \end{bmatrix} \quad (6.46)$$

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

### 6.3.4 Process LCA

In process LCA, Equations (6.43) and (6.44) are used to derive the technology matrix $X$ as in Equation (6.45). The inventory vector $g$ for the production of the functional unit $f$ is then calculated by applying Equation (2.2):

$$g = BX^{-1}f = \begin{bmatrix} 8 & 5 \end{bmatrix} \begin{bmatrix} 20 & -8 \\ -5 & 40 \end{bmatrix}^{-1}f \quad (6.47)$$
6.3.5 Connecting the economy and value chain models

As seen in Figure 6.6, both value chain activities draw inputs from the economy scale in addition to the inputs drawn from the other activity. These inputs are value chain upstream cutoff flows, defined for the toy system as

\[
\mathbf{X}_u = \begin{bmatrix} 0 & \$20 \\ 12 & 0 \end{bmatrix}
\]  

(6.48)

Because the flows originate at the economy scale, they are given in monetary units.

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 6.6 as

\[
\mathbf{X}_d = \begin{bmatrix} 8 & 0 \\ 0 & 0 \end{bmatrix}
\]  

(6.49)

After normalization by the total output of the destination sector, Equation (6.49) becomes

\[
\mathbf{A}_d = \begin{bmatrix} 8 & 0 \\ \frac{8}{500} & 0 \end{bmatrix}
\]  

(6.50)

In Figure 6.6, the arrow originating at \( S_1 \) and terminating at \( \overline{S}_1 \) represents this downstream cutoff flow.

6.3.6 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 (\( f \)), 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: [61, 171, 269]

\[
\bar{g}_t = g + \bar{g} = B X^{-1} \bar{f} + \bar{B} (\bar{I} - \bar{A})^{-1} \bar{f} 
\]

\[
= \begin{bmatrix} 8 & 5 \end{bmatrix} \begin{bmatrix} 20 & -8 \end{bmatrix}^{-1} \bar{f} + \begin{bmatrix} 0.40 & 0.20 \end{bmatrix} \begin{bmatrix} 0.70 & -0.29 \end{bmatrix}^{-1} \bar{f}
\]

where

\[
\bar{f} = \begin{bmatrix} $20 \\ $12 \end{bmatrix}
\]

Note that the data in Equation (6.48) and in Equation (6.52) is the same. The interpretation is largely the same as well. Equation (6.48) 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 (6.52) 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.

### 6.3.7 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. [267] This is accomplished by using the economy and value chain models to construct a hybrid transaction matrix \( \overline{X}_i \) and a hybrid interventions matrix \( \overline{B}_i \), analogous to those in Table 6.4:

\[
\overline{X}_i = \begin{bmatrix} I - \overline{A}^* \\ -A_d \\ \overline{X} \end{bmatrix} \begin{bmatrix} -X_s \\ \overline{X} \end{bmatrix}
\]

\[
\overline{B}_i = \begin{bmatrix} \overline{B}^* \\ B \end{bmatrix}
\]

in which \( \overline{A}^* \) has been disaggregated according to Equation (6.16) and (6.17), with the equipment scale terms neglected. As the equipment scale is neglected, both matrices
contains only constant terms and, assuming $\overline{X}_i$ to be square, Equation (2.2) is used to calculate the integrated hybrid interventions vector:

$$\overline{g}_i = \overline{B}_i \overline{X}_i^{-1} \overline{f}_i$$  \hspace{1cm} (6.55)

6.3.8 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 $h_i(z_{11}, z_{12}, z_{21})$ for process 1 impose constraints on $z_{11}$, $z_{12}$ and $z_{21}$ and are defined as

$$h_{11}(z_{12}, z_{21}): z_{12} - 0.129 z_{21} = 0$$  \hspace{1cm} (6.56)

$$h_{12}(z_{11}, z_{12}): \frac{z_{11} z_{12}}{7} \left(1 - \frac{z_{12}}{7}\right) - 0.12 \leq 0$$  \hspace{1cm} (6.57)

$$h_{13}(z_{11}, z_{12}): - \frac{z_{11} z_{12}}{7} \left(1 - \frac{z_{12}}{7}\right) \leq 0$$  \hspace{1cm} (6.58)

$$h_{14}(z_{11}): z_{11} - 0.8 \leq 0$$  \hspace{1cm} (6.59)

$$h_{15}(z_{11}): 0.3 - z_{11} \leq 0$$  \hspace{1cm} (6.60)
For process 2, models $h_2(z_{21}, z_{22})$ impose constraints on $z_{21}$ and $z_{22}$ and are defined as

$$h_{21}(z_{21}, z_{22}): 4.2z_{21}(z_{22} - 104) - 3000.0 \leq 0 \quad (6.61)$$

$$h_{22}(z_{21}): 14 - z_{21} \leq 0 \quad (6.62)$$

$$h_{23}(z_{21}): z_{21} - 50 \leq 0 \quad (6.63)$$

$$h_{24}(z_{22}): 120 - z_{22} \leq 0 \quad (6.64)$$

$$h_{25}(z_{22}): z_{22} - 140 \leq 0 \quad (6.65)$$

To include the process models in the P2P framework, the information in process models $h_1(z_{11}, z_{12}, z_{21})$ and $h_2(z_{21}, z_{22})$ must be represented in make, use and interventions matrices. While these matrices are derived from the process model equations, the process models are not duplicated verbatim. The process models contain information on how unit operations within each process function, and the matrices contain information on how each process interacts with the other process(es) and with the environment, as follows:

$$U(\{z\}) = \begin{bmatrix} z_{12} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad (6.66)$$

$$V(\{z\}) = \begin{bmatrix} 0 & z_{12} \left(z_{11} - \frac{z_{11}z_{12}}{7} \left(1 - \frac{z_{12}}{7}\right)\right) & z_{12} \left(\frac{z_{11}z_{12}}{7} \left(1 - \frac{z_{12}}{7}\right)\right) \\ 0 & 0 & 0 \end{bmatrix} \quad (6.67)$$

The elements of $U(\{z\})$ and $V(\{z\})$ 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 $U(\{z\})$ because, as described above, $z_{12}$ is the volumetric flow rate of the stream entering $S_1$ from $S_2$, shown in Figure 6.6. Its placement in the $1^{st}$ row indicates that this stream consists of product 1. In a similar manner, the $(1,2)th$ and $(1,3)th$ elements of $V(\{z\})$ are the flow rates of the streams out of $S_2$ (not shown in Figure 6.6, 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 Equations (6.56) - (6.65) to produce the equipment scale environmental interventions matrix,

\[
B\{z\} = \begin{bmatrix}
1.78 z_{12} \left( \frac{z_{11} z_{12}}{7} (1 - \frac{z_{12}}{7}) \right) & 1.4 z_{12} + 2 z_{22}
\end{bmatrix}
\]  

(6.68)

The first element of \(B\{z\}\) 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 \(B\{z\}\) 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 (\(z_{22}\)).

6.3.9 Process, product and supply chain design

Equations (6.56) - (6.65), 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:

maximize

$$0.65 z_{12} \left( \frac{z_{11} z_{12}}{7} \left( 1 - \frac{z_{12}}{7} \right) \right) - 0.45 z_{12} + 0.074 z_{21} (z_{22} - 104)$$

subject to

$$z_{12} - 0.129 z_{21} = 0$$
$$\frac{z_{11} z_{12}}{7} \left( 1 - \frac{z_{12}}{7} \right) - 0.12 \leq 0$$
$$- \frac{z_{11} z_{12}}{7} \left( 1 - \frac{z_{12}}{7} \right) \leq 0$$
$$z_{11} - 0.8 \leq 0$$
$$0.3 - z_{11} \leq 0$$
$$4.2 z_{21} (z_{22} - 104) - 3000.0 \leq 0$$
$$14 - z_{21} \leq 0$$
$$z_{21} - 50 \leq 0$$
$$120 - z_{22} \leq 0$$
$$z_{22} - 140 \leq 0$$

(6.69)

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

### 6.3.10 Equipment scale cutoff flows

Not all inputs to processes 1 and 2 are represented at the equipment scale; several inputs are upstream cutoff flows that originate in the value chain or economy scales. The equipment-value chain upstream cutoff matrix is defined as

$$X_u^V(z) = \begin{bmatrix} 0.79 z_{12} & 0 \\ 0 & 0.129 z_{21} \end{bmatrix}$$

(6.70)
and the equipment-economy upstream cutoff matrix is defined as

\[
X_u^E(\{z\}) = \begin{bmatrix}
0.45z_{12} & 0.074z_{21}(z_{22} - 104) \\
0 & 0 \\
0 & 0 \\
\end{bmatrix}
\]  \hspace{1cm} (6.71)

The flows in Equation (6.70) are in mixed physical units and the flows in Equation (6.71) are in monetary units. Although both processes receive inputs from the two larger scales as indicated by Equations (6.70) and (6.71), no equipment scale products are sold back to the system, thus both downstream process cutoff matrices consist of all zeros:

\[
X_d^V = \begin{bmatrix}
0 & 0 \\
0 & 0 \\
\end{bmatrix}
\]  \hspace{1cm} (6.72)

\[
X_d^E = \begin{bmatrix}
0 & 0 \\
0 & 0 \\
\end{bmatrix}
\]  \hspace{1cm} (6.73)

### 6.3.11 P2P model

All flows shown in Figure 6.6 between the system components have now been defined. The value chain and economy scales must now be disaggregated as discussed in Section 6.2.3. 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. \( \mathcal{S}_1 \) has one constituent activity, and \( \mathcal{S}_2 \) 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 (6.74) - (6.75) define the permutation matrices that relate the constituent
activity \( S_2 \) to its parent sector \( S_1 \):

\[
P_F = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{6.74}
\]

\[
P_P = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{6.75}
\]

The location of the 1 in Equation (6.74) indicates that value chain product 2 (1 is in the second column) belongs to commodity 1 (1 is in the first row). Equation (6.75) indicates that \( S_2 \) (1 is in the second row) is constituent to \( S_1 \) (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,

\[
P^V_F = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{6.76}
\]

Equipment scale product 1 belongs to commodity 2, as indicated by

\[
P^E_F = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{6.77}
\]

Finally, \( S_1 \) is constituent to \( S_2 \):

\[
P^E_P = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{6.78}
\]

but is not constituent to either \( S_1 \) or \( S_2 \),

\[
P^V_P = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{6.79}
\]

Equations (6.35) - (6.78) 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 is required in order to translate flows from one scale to another. This price data is given for the value chain products in Equations (6.80) and for the equipment scale products in Equation (6.81).

\[
p = \begin{bmatrix} \$4 & \$6 \end{bmatrix} \tag{6.80}
\]

\[
p = \begin{bmatrix} \$9 & \$5 \end{bmatrix} \tag{6.81}
\]

The adjusted use matrix \( U^* \) is calculated from Equation (6.17):

\[
U^* \{ z \} = \begin{bmatrix} \$150 & \$200 \\ \$300 & \$300 \end{bmatrix} - \begin{bmatrix} \$4 & 0 \\ 0 & \$6 \end{bmatrix} \begin{bmatrix} 0 & 1 & 15 & 8 & 0 & 0 \\ 0 & 0 & 5 & 10 & 1 & 0 \end{bmatrix} - \begin{bmatrix} \$4 & 0 \\ 0 & \$6 \end{bmatrix} \begin{bmatrix} 0 & 1 & 8 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} \$9 & 0 \\ 0 & \$5 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} - \begin{bmatrix} \$0 & 0 \\ \$0.45z_{12} & \$0.074z_{21}(z_{22} - 104) \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}
\]

\[
U^* = \begin{bmatrix} \$90 & \$200 - 0.45z_{12} \\ \$300 & \$300 - 5z_{12} \end{bmatrix} \tag{6.83}
\]

\( U^* \) contains only economy-level flows that are both produced and consumed at the economy scale.

The adjusted make matrix \( V^* \) is calculated from Equation (6.16):

\[
V^* \{ z \} = \begin{bmatrix} \$500 & 0 \\ 0 & \$700 \end{bmatrix} - \begin{bmatrix} \$4 & 0 \\ 0 & \$6 \end{bmatrix} \begin{bmatrix} 0 & 1 & 35 & 0 & 0 & 0 \\ 0 & 0 & 50 & 1 & 0 \end{bmatrix} - \begin{bmatrix} \$9 & 0 \\ 0 & \$5 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & z_{12}(z_{11} - \frac{z_{11}z_{12}}{7} (1 - \frac{z_{12}}{7})) \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}
\]

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The matrix subtracted from $\mathbf{V}$ in Equation (6.84) represents in monetary units flows produced by value chain activities, thus $\mathbf{V}^*$ in Equation (6.85) represents the total output of the sectors less the output of their constituent activity and process.

As seen by comparing Equation (6.35) with Equation (6.85), the disaggregated sectors have a lower total output. This reduction in total output is also applied to the total interventions matrix $\mathbf{R}$, as follows.

$$
\mathbf{R}^* = \begin{bmatrix} 200 & 140 \\ 8 & 5 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 192 & 135 \end{bmatrix}
$$

(6.86)

$\mathbf{R}^*$ is then normalized to the level of sector output given in $\mathbf{V}^*$ to calculate the adjusted economy scale interventions matrix $\mathbf{B}^*$, as shown in Equation (6.87).

$$
\mathbf{B}^* = \begin{bmatrix} 192 \\ 300 \end{bmatrix} \begin{bmatrix} 135 \\ 700 \end{bmatrix}
$$

(6.87)

The final calculation before combining the three models is calculating the adjusted total requirements matrix. $\mathbf{A}^*$, the adjusted direct requirements matrix, is calculated from $\mathbf{U}^*$ and $\mathbf{V}^*$ according to Equation (6.26) (re-stated as Equation (6.88)), as follows.

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

(6.88)

$$
\mathbf{A}^* = \begin{bmatrix} 0.30 & 0.29 - 6.43 \times 10^{-4} z_{12} \\ 1.00 & 0.14 - 7.1 \times 10^{-3} z_{12} \end{bmatrix}
$$

(6.89)
Table 6.5: Sub-matrices required to assemble the P2P transactions and interventions matrices.

<table>
<thead>
<tr>
<th>P2P transactions sub-matrices</th>
<th>P2P interventions sub-matrices</th>
</tr>
</thead>
<tbody>
<tr>
<td>(6.89)</td>
<td>(6.87)</td>
</tr>
<tr>
<td>(6.48)</td>
<td>(6.46)</td>
</tr>
<tr>
<td>(6.71)</td>
<td>(6.68)</td>
</tr>
<tr>
<td>(6.50)</td>
<td></td>
</tr>
<tr>
<td>(6.43), (6.44)</td>
<td></td>
</tr>
<tr>
<td>(6.70)</td>
<td></td>
</tr>
<tr>
<td>(6.73)</td>
<td></td>
</tr>
<tr>
<td>(6.72)</td>
<td></td>
</tr>
<tr>
<td>(6.67), (6.66)</td>
<td></td>
</tr>
</tbody>
</table>

The effects of disaggregation can be seen by comparing Equation (6.40) with Equation (6.89).

The P2P transactions and interventions matrices shown in Table 6.4 can now be assembled from the equations given in Table 6.5:

\[
\mathbf{X}(\{z\}) =
\begin{bmatrix}
0.70 & 6.43 \times 10^{-4}z_{12} - 0.29 & 0 & -820 & -0.45z_{12} & -0.074z_{21}(z_{22} - 104) \\
-1.00 & 7.1 \times 10^{-3}z_{12} - 0.14 & -812 & 0 & 0 & 0 \\
-8 & 0 & 20 & -8 & -0.79z_{12} & 0 \\
0 & 0 & -5 & 40 & 0 & -0.129z_{21} \\
0 & 0 & 0 & 0 & z_{12}(z_{11} - \frac{z_{12}}{7} (1 - \frac{z_{12}}{7})) & 0.129z_{21} \\
0 & 0 & 0 & 0 & z_{12}(\frac{z_{11}z_{12}}{7} (1 - \frac{z_{12}}{7})) & 0 \\
0 & 0 & 0 & 0 & 1.78z_{12}(\frac{z_{11}z_{12}}{7} (1 - \frac{z_{12}}{7})) & 1.4z_{12} + 2.0z_{22}
\end{bmatrix}
\]

(6.90)

\[
\mathbf{B}(\{z\}) = \begin{bmatrix}
0.64 & 0.19 & 8 & 5 & 1.78z_{12}(\frac{z_{11}z_{12}}{7} (1 - \frac{z_{12}}{7})) & 1.4z_{12} + 2.0z_{22}
\end{bmatrix}
\]

(6.91)

The final component of the P2P model is the set of constraints on the unit operation variables, given in Equations (6.56) - (6.65).

### 6.4 P2P sustainable process design problem

Using the P2P modeling framework, a general SPD problem can be stated as a (MI)NLP with both economic and environmental objective functions. The economic
objective function, \( Z_1 \), remains unchanged from the conventional SPD problem given in Equation (2.39): although the P2P framework captures a different system than the conventional approach, only the economics of the equipment scale are of interest in the design problem. \( Z_1 \) is defined as

\[
Z_1 = \sum_{n=1}^{N} Z_{1n}(\{z_n\})
\]  

(6.92)

with the economic objective for each process \( n \) given by

\[
Z_{1n} = p(\{z\}) \cdot s, \quad \forall n \in N
\]  

(6.93)

The environmental objective function for intervention \( r \),

\[
\overline{Z}_{2r} = \overline{B}_r(\{z\}) \cdot \overline{s}
\]  

(6.94)

contains interventions generated at the economy scale as well as at the process and value chain scales captured by conventional SPD methods. To see this more clearly, Equation (6.94) is rewritten as

\[
\overline{Z}_{2r} = \overline{B}_r(\{z\}) \cdot \overline{s} + \overline{B}_r^*(\{z\}) \cdot \overline{s} + B_r(\{z\}) \cdot s
\]  

(6.95)

Emissions factors \( B \) and \( \overline{B} \), which are fixed in conventional SPD, are now functions of unit operation design variables.

The decision variables \( \overline{s} \) and \( \{z\} \) are constrained with a set of system-wide balance equations on production and consumption, defined as

\[
\begin{bmatrix}
\mathbf{I} - \mathbf{A}^* (\{z\}) & -\mathbf{X}_u (\{z\}) & -\mathbf{X}_V (\{z\}) \\
-\mathbf{A}_d (\{z\}) & \mathbf{X}^* (\{z\}) & -\mathbf{X}_V (\{z\}) \\
-\mathbf{A}_d^E (\{z\}) & -\mathbf{X}_V^E (\{z\}) & \mathbf{X} (\{z\})
\end{bmatrix}
\begin{bmatrix}
\overline{s} \\
\mathbf{s} \\
\mathbf{s}
\end{bmatrix}
= 
\begin{bmatrix}
\overline{f} \\
\mathbf{f} \\
\mathbf{f}
\end{bmatrix}
\]  

(6.96)

Fundamental engineering process models further constrain the unit operation design variables \( \{z\} \) to feasible values:

\[
\mathbf{H}(\{z\}) \geq 0
\]  

(6.97)
in which $H(\{z\})$ represents the entire set of fundamental models, $\{h_1(z_1), \ldots, h_N(z_N)\}$.

Due to the integrated nature of the P2P framework, the decision variables are optimized *simultaneously* and *in the context of the entire system*. There are no sequential decisions, and each decision variable within the system affects all other decision variables regardless of scale.

6.4.1 Conventional SPD as a special case of the P2P problem

A conventional SPD problem was stated in Equation (2.39) and is re-stated here using the notation introduced in Chapter 6:

$$\begin{align*}
\text{maximize} & \quad Z_1(p, \{z\}) \\
\text{minimize} & \quad Z_2(\{z\}, B, B(\{z\})) \\
\text{subject to} & \quad H(\{z\}) \geq 0
\end{align*}$$

The economic objective function $Z_1$ is a function of price data $p$ and the equipment scale design variables $\{z\}$. $Z_2$ is a function of the value chain and equipment scale environmental interventions matrices $B$ and $B(\{z\})$. Note that in this problem, $B$ is not a function of $\{z\}$.

Conventional SPD problems such as the one stated in Equation (6.98) consider only the equipment and value chain scales. Figure 6.7 compares the system boundary of a conventional SPD problem, in dark colors, to the boundary of the P2P modeling framework which encompasses the entire figure. Interactions with system components outside these scales, including inputs produced by the economy and environmental interventions generated from economic activity, are neglected. The design problem consists of choosing the optimal values of the unit operation design variables $\{z\}$. As in the P2P framework, value chain activity models are empirical and fixed while
Figure 6.7: Conventional SPD accounts only for the process(es) of interest ($S_6$) and select processes in the value chain ($S_4$ and $S_5$). Feedback to the value chain ($y_{65}$) is rarely accounted for, and all interventions with the economy ($S_1$, $S_2$ and $S_3$) are neglected. The P2P approach for SPD accounts for all the components and exchanges shown in this figure.

process models are theoretical and are functions of unit operation variables. No disaggregation of the value chain models is performed, thus all environmental interventions at the value chain scale are constant and independent of the design solution.

6.5 Life cycle assessment with the P2P framework

The P2P framework is applicable to attributional life cycle assessment, with some minor modifications. In performing attributional LCA, the system model is fixed; that is, there are no design alternatives at any scale. This distinction separates the SPD design problem from the life cycle assessment problem. The calculation of life cycle impacts is formulated as an optimization problem, similar to the SPD design
problem, as follows:

\[
\begin{align*}
\text{minimize} \quad & \mathbf{g}_r = \mathbf{B}_r(\{z_0\}) \cdot \mathbf{s} \\
\text{subject to} \quad & \mathbf{X}(\{z_0\}) = \mathbf{f} \\
& \mathbf{s} \geq 0
\end{align*}
\]  

(6.99)

in which the notation \(\{z_0\}\) indicates that the equipment scale decision variables are fixed at some predetermined values. Equation (6.99) is thus a linear program. The objective function minimizes the amount of some intervention \(r\) produced by the P2P life cycle, which due to the linearity of the problem is equivalent to minimizing the sum of the P2P scaling factors. For a square P2P transactions matrix, Equation (6.99) reduces to a matrix inversion calculation:

\[
\mathbf{g} = \mathbf{B}(\{z_0\}) \left[ \mathbf{X}(\{z_0\}) \right]^{-1} \mathbf{f}
\]  

(6.100)

\(\mathbf{g}\) is the inventory vector of life cycle environmental interventions which is used in impact assessment and subsequent stages of the LCA study.

Note that, while Equation (6.99) minimizes only intervention \(r\), Equation (6.100) calculates the amounts of all interventions simultaneously. This is not a failing of the optimization formulation. Recall that the system model used for LCA has no design alternatives or decision variables. Therefore, the optimal scaling vector \(\mathbf{s}\) that minimizes intervention \(r\) will also minimize all other interventions, because there is at most one value of \(\mathbf{s}\) that satisfies the P2P product balance constraint. This value of \(\mathbf{s}\) is also calculated in Equation (6.100) as \(\left[ \mathbf{X}(\{z_0\}) \right]^{-1} \mathbf{f}\). Once \(\mathbf{s}\) is found for one intervention, the objective function of Equation (6.99) is re-calculated for each intervention \(r\), yielding the complete inventory vector \(\mathbf{g}\).
Inventory vectors representing process based and conventional hybrid LCAs can also be obtained, by changing the objective function in Equation (6.99). The P2P product balance constraints and the requirement that all scaling factors are greater than or equal to zero remain as they are in Equation (6.99). For process based LCA, the objective function involves only the value chain scale:

\[ g = b_r(z_0) \cdot s \]  

(6.101)

Including the equipment and value chain scales in the objective function yields a process based LCA with greater detail but essentially the same system boundary as a typical process LCA. For conventional hybrid LCA, the objective function includes the economy and value chain scales:

\[ g_{conv} = b_r(z_0) \cdot s + b_r(z_0) \cdot s \]  

(6.102)

Once again, including the equipment scale as in Equation (6.99) yields a more detailed inventory.

In addition to the relatively small scale SPD problem described in Section 6.4, the P2P framework can be applied to macro-scale or “top down” design and assessment problems, including economic policy design. This requires extending the P2P framework to include more flexible economy scale models, and is discussed further in Chapter 8.
Chapter 7: Sustainable engineering design by the P2P modeling framework

7.1 Introduction

This chapter applies the P2P modeling framework to several chemical and process systems engineering design problems. The purpose of doing so is to (a) demonstrate the practical aspects of the P2P framework and its implementation within an optimization problem and (b) compare optimal designs obtained using the P2P framework and using conventional SPD methods.

Intuitively, the P2P framework offers an improved approach to SPD over methods currently in use. Although conventional SPD methods rely on the latest developments in mathematical programming, optimization algorithms and PSE modeling, the techniques used to perform a LCA and utilize the results within the SPD problem have not substantially changed since the mid-1990s. As discussed in Chapter 6, the analysis boundary of conventional SPD problems is always restricted to the process based life cycle. The process based LCI commonly excludes contributing processes past second or third order as well as a portion of the inputs to the life cycle. Inputs such as chemical process equipment, maintenance services and plant construction are rarely included in the inventory. (The exceptions are [112] and [113] which include chemical
process equipment manufacturing in the life cycle inventory.) A probable reason for the exclusion of these potentially significant inputs is the lack of life cycle inventory data. The P2P framework offers a convenient way to include currently neglected flows even without inventory data: the flows are modeled as upstream cutoffs, or inputs that originate in the economy scale. The only data required is the market prices of the input flows and knowledge of the sector in which the inputs are produced.

Conventional SPD also models environmental interventions generated within the life cycle with fixed “emissions factors” [111, 168, 230], the values of which are assumed to be independent of the life cycle structure and of the system being designed. Using fixed emissions factors is valid for applications that deal with static systems, including straightforward life cycle assessment. However, when a system model involves variables, such as in a design context, the emissions factors are in reality dependent on the design solution. The dependence is caused by avoided production of co-products utilized in the life cycle and the aggregated nature of the life cycle inventory and economy scale models. Avoided production is the situation where a by-product of a process displaces another, functionally equivalent product, thereby avoiding production of the equivalent product. For example, the production and sale of lignin electricity as a by-product of cellulosic ethanol production avoids production of grid electricity. Avoided production results in changes in the emissions factors for the affected life cycle process(es), and is particularly significant for large-scale engineering design problems. [100, 315] Failing to account for variable emissions factors results in inaccurate life cycle models, which in turn lead to sub-optimal or infeasible designs.
The level of aggregation in the life cycle and economy models can also lead to inaccurate emissions factors. “Processes” modeled in life cycle inventories do not represent individual plants but rather aggregates of several production technologies for one type of process in a given region. Economic sectors are even more highly aggregated, generally by the type of commodity each sector produces. In the case that only some of the production technologies in a life cycle process or sector are utilized by the system of interest, these production technologies can be modeled in greater detail at a smaller scale, necessitating disaggregation of the larger scale models. Disaggregation separates system components into two portions, one which is modeled at a smaller scale and the remainder of the original component, which is modeled at the original scale. [132, 267] Both technological interventions and environmental interventions, represented by emissions factors, are disaggregated, resulting in emissions factors for large scale models that are dependent on smaller scale models and in particular on equipment scale design variables.

This chapter discusses two sustainable process design case studies, one which focuses on a toy supply chain (Section 7.2) and another which focuses on a corn ethanol plant (Section 7.3). A third case study presented in Section 7.4 deals with the design of a renewable energy production system at both the equipment and value chain scales.

Material in this chapter has been previously published as [133] (Section 7.2) and [134] (Section 7.3).
7.2 Demonstration: Polymer supply chain design

The P2P modeling framework is demonstrated with a toy process and supply chain design problem. The supply chain involves the production of two polymer products, only one of which is of interest, from electricity, monomer and catalyst. Figure 7.1 shows the superstructure of potential supply chain processes, with similar processes grouped by process type. Of the supply chain processes, only the model for expanded and thermoformed polymer production (ETPP), the process of interest, involves design variables; the supply chain processes have fixed, linear process models. The ETPP model depends on two variables, $X$ and $C$, which are roughly analogous to reaction conversion and catalyst consumption rate. The desired product of ETPP is expanded polymer; ETPP also produces thermoformed polymer as a by-product which is sold back to the economy. Due to the simplicity of this system, the value chain scale is neglected, leaving only the supply chain (equipment) and economy scales.

The polymer production system shown in Figure 7.1 exists within an eight-sector economy with four parent sectors and four non-parent sectors. Three of the parent sectors have two constituent processes each and the fourth has one constituent process; all of the supply chain processes have parent sectors. The eight industrial sectors of the economic system are water and sewage (WS), coal mining (CM), crude oil extraction (OE), natural gas extraction (NGE), power generation and supply (PGS), organic chemical manufacturing (OCM), specialty chemical manufacturing (SCM) and plastics manufacturing (PM), with the latter four sectors being the parent sectors. Plastics manufacturing is the parent sector of polymer production, and the other three sectors are the parent sectors for the supply chain processes.
Because the ETPP process model involves two unit operation variables $X$ and $C$, all inputs and outputs to this process as well as its environmental interventions are dependent on $X$ and $C$. Figure 7.2 shows the relationships between parent sectors, constituent processes and unit operation variables in this production system. PM, the parent sector for ETPP, is disaggregated into two components: ETPP, modelled theoretically at the process scale, and all other plastic production processes which remain in the economy-scale model. Through the disaggregation, the entire multi-scale model of the disaggregated PM sector is dependent on $X$ and $C$, even though the variables exist at a much smaller scale. The PM sector is connected through its inputs and outputs to all other sectors in the economy, both parent and non-parent. Thus the entire economic model and all economy-scale environmental interventions are dependent, albeit indirectly, on unit operation variables. This interaction between
model scales is captured *without* needing to specify the exact relationship between the unit operation variables and each sector, which could prove prohibitively difficult for more realistic systems.

Equations (6.16) and (6.17) are applied to disaggregate the economy scale model. The polymer supply chain consists of models at only two scales, equipment and economy, thus the last term in Equation (6.16) and the terms in Equation (6.17) that refer to sector-constituent processes are neglected. Both the make and use matrices are square at the economy scale; \( \mathbf{V} \) is therefore invertible and the adjusted direct requirements matrix \( \mathbf{A}^* \) is calculated from Equation (6.26) rather than by solving the system of linear equations given in Equation (6.27).

The upstream and downstream cutoff matrices \( \mathbf{X}_u(X, C) \) and \( \mathbf{X}_d(X, C) \) contain, respectively, inputs to the supply chain processes produced by economic sectors and by-products of the supply chain processes which are consumed by the economy. Elements in these two matrices corresponding to ETPP are dependent on the unit operation variables, causing the level of production required from the economy and the level of *avoided* production caused by the sale of thermoformed polymer to vary according to \( X \) and \( C \). In the model, the thermoformed polymer is arbitrarily sold back to the PM sector. However, the framework can also be used to identify the optimal market or combination of markets for by-products with respect to economic and/or environmental criteria of interest.

Data and models used in this section are given in Appendix E.
Figure 7.2: The toy polymer production system consists of an eight-sector economic system with four parent sectors, six supply chain processes and one process of interest. All processes are constituent processes, and all save ETPP have empirical, linear process models. ETPP is dependent on two variables at the equipment scale, $X$ and $C$. 
7.2.1 Results and discussion

Optimizing the polymer supply chain involved selecting the optimal mix of electricity, monomer and catalyst production processes from the superstructure and choosing the optimal values of \( X \) and \( C \). In this particular model, it is possible for the best combination of processes to include duplicates, for instance a 50/50 mix of coal and natural gas electricity. As an alternative, integer variables could be used to choose the technology mix such that only one of each type of process is allowed to be active in the value chain. This would be the better modeling choice when designing a new supply chain rather than choosing which of several existing processes to utilize, as was assumed to be the case for this problem.

The system was first optimized separately under an economic objective, total production cost, and two environmental objectives, total \( \text{CO}_2 \) emissions for the supply chain alone and for the life cycle which includes both the supply chain and the economy. Both the P2P framework and the conventional SPD approach described in Section 6.4 were used to obtain supply chain designs in order to compare results of the two approaches. Designs obtained under the conventional SPD approach were evaluated using the P2P framework in order to compare the two sets of designs using the same system boundary. Two-dimensional Pareto curves were obtained using the \( \epsilon \)-constraint method. Points on the Pareto curves are supply chain designs that represent compromises between two of the three competing objectives: cost and supply chain \( \text{CO}_2 \), cost and life cycle \( \text{CO}_2 \), and supply chain and life cycle \( \text{CO}_2 \).

Major conclusions of this case study are as follows.

- A process design that is optimal in a restricted analysis boundary is not necessarily optimal when the boundary is expanded. See Figure 7.3.
• Emissions produced by the process of interest and the supply chain are an order of magnitude less than the emissions produced by the economic activity necessary to support the supply chain. See Figure 7.4.

• For the same environmental objective, the P2P framework produces a better (lower emissions) supply chain design than does the conventional SPD approach. See Figure 7.5.

• For the same combination of objectives, the P2P design problem resulted in a greater number of unique designs on the Pareto curve compare to the conventional SPD problem, although the shape of the Pareto curves were nearly identical between the two approaches. See Figures 7.6 - 7.9.

• Supply chain processes that provide inputs to multiple other processes (in this case, the electricity processes) have a large influence on both economic and environmental aspects of the supply chain. See Figure 7.12.

Designs for ETPP (values of $X$ and $C$) were obtained as part of both the conventional SPD problem and P2P design problem. For comparison purposes, ETPP was also optimized as a standalone process. Figure 7.3 shows the three ETPP designs in Figure 7.3a as well as the CO$_2$ emissions and production costs of those designs in Figure 7.3b. It is immediately apparent that the designs obtained by considering ETPP as a standalone process are drastically different from the designs obtained from either the conventional or P2P approach. As a standalone process, $X$ and $C$ are at the extremes of their ranges, compared to the more moderate values of the conventional and P2P approaches. While not surprising, these results demonstrate the necessity
Figure 7.3: ETPP designs, CO₂ emissions and production costs for minimum CO₂ and minimum cost designs. Both conventional SPD (left) and the P2P approach (center) were applied, and ETPP was optimized as a standalone process as well (right).
of designing processes in the context of a supply chain or other system; if this is not done, the resulting system is far from optimal.

The ETPP supply chain was optimized for production cost, supply chain CO\textsubscript{2} emissions and life cycle CO\textsubscript{2} emissions. Using the conventional SPD approach, the life cycle of ETPP consists of the supply chain and four processes in the value chain; using the P2P framework, the life cycle consists of the supply chain and the macro-economic system in which the supply chain operates. The two design approaches yielded identical minimum cost supply chain designs. It was expected that the two approaches would be equivalent under minimum cost; the two approaches differ only

---

Figure 7.4: Comparison of total CO\textsubscript{2} emissions and production cost for minimum CO\textsubscript{2} supply chain designs obtained using the P2P framework and the conventional SPD approach.
at the value chain and larger scales. At the supply chain scale, which is the only scale relevant to the economic objective function, the two approaches are identical. Minimum supply chain and life cycle CO\textsubscript{2} results, shown in Figure 7.4, differed widely between the two approaches. Although Figure 7.4 seems to indicate that the conventional SPD approach yielded far superior designs, much of the difference between the two sets of results is due to the different analysis boundaries. The conventional SPD approach neglects the economy and includes only select processes at the value chain scale, while the P2P framework includes interactions with the economy but does not explicitly model processes in the value chain. Figure 7.5 shows CO\textsubscript{2} emissions of the four supply chain designs represented in Figure 7.4, with the emissions for the conventional SPD approach designs calculated using the P2P framework. The minimum CO\textsubscript{2} designs obtained with the P2P framework have lower emissions than the conventional SPD approach designs in both cases. For supply chain emissions, the reduction is approximately 5\% and for life cycle emissions the reduction is approximately 4\%.

Combining the Pareto curves of Figures 7.6 - 7.8 into three-dimensional plots gives Figures 7.9 and 7.10. Although the exact values of supply chain and life cycle CO\textsubscript{2} emissions are different between the two approaches, the shape of the combined curve is quite similar. The Pareto solutions that consider cost-supply chain CO\textsubscript{2} and supply chain-life cycle CO\textsubscript{2} all fall on roughly the same curve, while the cost-life cycle CO\textsubscript{2} solutions fall in a group apart from the curve. The cost-life cycle CO\textsubscript{2} Pareto solutions include the lowest production costs as well as the lowest life cycle CO\textsubscript{2} and thus represent “win-win” designs, in which both an economic and an environmental benefit is realized.
Figure 7.5: Minimum CO₂ supply chain designs obtained under the conventional SPD approach are evaluated using the P2P framework (left-hand set of bars) and compared to minimum CO₂ designs obtained under the P2P framework (right-hand set).

The set of Pareto designs for the ETPP process and supply chain are shown in Figures 7.11 - 7.14. The far right column of each plot contains the designs obtained under a single objective, for comparison to the Pareto designs. The two approaches found very similar sets of designs; the most significant difference was that P2P design resulted in monomer B production rather than monomer A production for some solutions both Pareto and single objective, while the conventional SPD approach resulted in monomer A for all solutions. The choice of electricity process was by far the most variable, with both approaches selecting a wide range of electricity combinations. This is because the electricity process(es), unlike other processes in the supply chain, provides inputs to the rest of the supply chain. The electricity process has the highest activity level and therefore the highest individual CO₂ emissions in the supply chain, making the choice of electricity process(es) more dependent on the
Figure 7.6: The trade-off between supply chain CO₂ emissions and production cost is nearly identical for the P2P approach and the conventional SPD approach, although the P2P approach produced a greater number of unique designs.
Figure 7.7: The Pareto curve between the minimum life cycle CO₂ and minimum cost solutions.
Figure 7.8: The Pareto curve between the minimum life cycle CO\textsubscript{2} and supply chain CO\textsubscript{2} solutions.
Figure 7.9: The Pareto points for the P2P approach, shown separately in Figures 7.6, 7.7 and 7.8, are combined into a single three-dimensional curve.
Figure 7.10: The Pareto points for the conventional SPD approach, shown separately in Figures 7.6, 7.7 and 7.8, are combined into a single three-dimensional curve.
Figure 7.11: ETPP designs that fall on the Pareto curve.
Figure 7.12: Electricity mixes in supply chains on the Pareto curve.
Figure 7.13: Monomer mixes in supply chains on the Pareto curve.
Figure 7.14: Catalyst mixes in supply chains on the Pareto curve.
different objective functions. In particular, the electricity choice was more variable than the choice of $X$ and $C$, implying that for some systems the structure of the supply chain is more influential than the design of the process of interest.

7.3 Case study: Corn ethanol plant design

The P2P framework was applied to the design and optimization of an ethanol production system consisting of a dry-grind corn ethanol process and its life cycle, shown in Figure 7.15. Detailed engineering models for the ethanol plant were obtained from [17, 174] and were implemented in the Python language. The original model was simplified from a MINLP superstructure optimization to a NLP parametric optimization with fifteen independent design variables, defined in Table 7.2. The plant capacity was set by fixing the input rate of corn grain at 18 kg/s; only the operating conditions of the plant were variable.

Empirical models for value chain activities were obtained from the GREET 2014 fuel cycle model. [30] Environmental interventions for corn farming, corn transportation and ethanol transportation included vehicle production and distribution, and all activities included interventions related to upstream fuel production and distribution activities, back to fossil resource extraction. Data on the use of corn seeds in the corn farming activity was not included in the GREET model and was obtained from [13]. Water consumption data was available for all value chain activity models of interest except for the production and distribution of $\alpha$-amylase, gluco-amylase and yeast; the water use by these activities was thus not modeled explicitly. Default values were used for all GREET input parameters.
Figure 7.15: P2P model of the dry-grind corn ethanol process and its value chain, showing upstream connections to the economy. Downstream connections to the economy that were not captured in the P2P model are shown in lighter colors.
Table 7.1: Inputs to the ethanol process and its life cycle were modeled at either the value chain scale (V) or at the economy scale (E) as an upstream cutoff flow. Both model A and model B account for all of the inputs shown here.

<table>
<thead>
<tr>
<th>Input</th>
<th>Model A</th>
<th>Model B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen fertilizer</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>P₂O₅ fertilizer</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>K₃O fertilizer</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>CaCO₃ fertilizer</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>Herbicide</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>Insecticide</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>Corn seeds</td>
<td>E</td>
<td>E</td>
</tr>
<tr>
<td>Corn</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>Corn transportation</td>
<td>V</td>
<td>V</td>
</tr>
<tr>
<td>Natural gas</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>Coal</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>US grid electricity</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>α-amylase</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>Yeast</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>Urea</td>
<td>V</td>
<td>E</td>
</tr>
<tr>
<td>Corn grits</td>
<td>E</td>
<td>E</td>
</tr>
<tr>
<td>Water</td>
<td>E</td>
<td>E</td>
</tr>
<tr>
<td>Ethanol transportation</td>
<td>V</td>
<td>V</td>
</tr>
</tbody>
</table>
Table 7.2: List and description of unit operation design variables present in the ethanol plant model.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_1$</td>
<td>Mass flow of water stream entering mixer after corn is ground</td>
</tr>
<tr>
<td>$z_2$</td>
<td>Mass flow of water (steam) stream entering jet</td>
</tr>
<tr>
<td>$z_3$</td>
<td>Temperature (C) of jet stream</td>
</tr>
<tr>
<td>$z_4$</td>
<td>Mass flow of water entering mixer upstream of fermentation vessel</td>
</tr>
<tr>
<td>$z_5$</td>
<td>Mass flow of urea entering mixer upstream of fermentation vessel</td>
</tr>
<tr>
<td>$z_6$</td>
<td>Temperature of stream entering mixer upstream of fermentation vessel</td>
</tr>
<tr>
<td>$z_7$</td>
<td>Fraction of water from the incoming stream that goes into the liquid stream outlet of the mechanical press</td>
</tr>
<tr>
<td>$z_8$</td>
<td>Fraction of water in the feed solids that goes to the vapor stream</td>
</tr>
<tr>
<td>$z_9$</td>
<td>Fraction of stream leaving solids separation that is discarded</td>
</tr>
<tr>
<td>$z_{10}$</td>
<td>Temperature of stream entering the beer column</td>
</tr>
<tr>
<td>$z_{11}$</td>
<td>Recovery of water in beer column</td>
</tr>
<tr>
<td>$z_{12}$</td>
<td>Recovery of water in rectification column</td>
</tr>
<tr>
<td>$z_{13}$</td>
<td>Split fraction of impure ethanol stream sent to rectification column</td>
</tr>
<tr>
<td>$z_{14}$</td>
<td>Split fraction of impure ethanol stream sent to adsorption operation</td>
</tr>
<tr>
<td>$z_{15}$</td>
<td>Fraction of water removed from the mixture entering the adsorption operation</td>
</tr>
</tbody>
</table>
Both the ethanol plant and the corn farming activity provide by-products: the ethanol plant produces both ethanol and dried distiller’s grains and solubles (DDGS) while the corn farming activity produces both corn grain and stover. For simplicity, these by-products are neglected. Were they to be included in the model, by-products would be modeled as downstream cutoff flows. The corn stover would be a value chain downstream cutoff and the DDGS an equipment-economy downstream cutoff. Figure 7.15 accordingly shows the flow of by-products back to the economy in lighter colors, indicating that these flows were not captured in the model.

The equipment and value chain scales were expanded to a P2P model by using the EEIO model to capture the production and distribution of those inputs for which value chain scale data was not included in GREET 2014. For this case study, only the production and distribution of corn seeds, water and corn grits could not be modeled at the value chain scale. The P2P model includes these inputs as value chain upstream cutoffs.

Make and use tables (producer’s prices, after redefinitions) from the 2002 benchmark model developed by the U.S. Bureau of Economic Analysis were used to derive the economy scale model. [286] The tables were obtained at the detailed level of aggregation and originally consisted of 426 sectors and 430 commodities. The tables were transformed into square matrices by removing rest-of-world inputs and redistributing scrap production proportional to commodity production. [150] Sectors that were to be disaggregated and sectors that provided inputs to the value chain and the ethanol process were kept at the detailed level of aggregation. Remaining sectors were aggregated to the summary level, with the exception of the four retail sectors (441000, Motor vehicle and parts dealers; 445000, Food and beverage stores; 452000,
Table 7.3: Sources for price data used in the P2P ethanol production system model.

<table>
<thead>
<tr>
<th>Product</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuels (all)</td>
<td>[5, 7–10]</td>
</tr>
<tr>
<td>Electricity</td>
<td>[2]</td>
</tr>
<tr>
<td>Fertilizer</td>
<td>[4]</td>
</tr>
<tr>
<td>Herbicide and insecticide (approx.)</td>
<td>[6]</td>
</tr>
<tr>
<td>Corn seed</td>
<td>[13]</td>
</tr>
<tr>
<td>Corn grits</td>
<td>[3]</td>
</tr>
<tr>
<td>$\alpha$-amylase</td>
<td>[206]</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>[206]</td>
</tr>
<tr>
<td>Yeast</td>
<td>[206]</td>
</tr>
<tr>
<td>Urea</td>
<td>[206]</td>
</tr>
<tr>
<td>Water (approx.)</td>
<td>[46]</td>
</tr>
</tbody>
</table>

General merchandise stores and 4A0000, Other retail) which were aggregated into a single retail sector. The resulting make and use tables were square and consisted of 74 sectors and 74 commodities. Environmental intervention data was obtained from Eco-LCA [18, 259] and consisted of total fossil CO$_2$ emissions per sector for the year 2002. Sources for price data used to model products purchased from the economy are listed in Table 7.3; prices for inputs not listed in Table 7.3 were obtained from online retailers. When prices for 2002 were not available for a product, the most current price was found and converted to 2002 levels using commodity-specific producer’s price indexes (PPIs) obtained from the U.S. Bureau of Labor Statistics. [287]

No disaggregation was necessary at the value chain scale because the ethanol plant was modeled at the equipment scale rather than using GREET’s default ethanol production model. The ethanol plant model thus did not overlap with any of the value chain activity models. As a result, the value chain technology and environmental
interventions matrices were fixed instead of being functions of unit operation design variables. The EEIO was disaggregated to remove the value chain activities and the ethanol plant, resulting in several parent sectors having emissions factors that were dependent on the equipment scale design variables.

7.3.1 Optimization formulation

The objective of the case study was to optimize the ethanol plant design for minimum life cycle CO$_2$ emissions. In order to compare the results of a conventional SPD optimization with the results of the proposed P2P approach, the ethanol production system was optimized under two CO$_2$ objective functions. The objective function that corresponds to the conventional SPD approach includes CO$_2$ emissions from the value chain and equipment scales:

$$Z_{\text{conventional}}(\{z\}) = b \cdot s + b(\{z\}) \cdot s$$

(7.1)

The objective function that corresponds to the proposed P2P approach includes CO$_2$ emissions from the economy scale as well as the value chain and equipment scales:

$$Z_{\text{P2P}}(\{z\}) = \overline{b}^*(\{z\}) \cdot \overline{s} + b \cdot s + b(\{z\}) \cdot s$$

(7.2)

Plant economics are not considered as an objective function in this case study; as discussed in Section 6.4, the economically optimal plant designs will be identical under the conventional and P2P approaches.

The optimization formulation involves two sets of constraints. The first set consists of the P2P product balance, expressed as

$$\overline{X}(\{z\})\overline{s} = \overline{r}$$

(7.3)
In Equation (7.3), the equipment scale element of \( \overline{f} \) was set equal to the mass flow rate of ethanol produced by the ethanol plant. This ensured that the scaling factor for the ethanol plant was always equal to 1, and non-linear effects of scaling the ethanol plant did not need to be accounted for in the model.

The P2P scaling vector \( \bar{s} \) was calculated by inverting the P2P transactions matrix as follows:

\[
\bar{s} = \overline{X}(\{z\})^{-1} \overline{f} \tag{7.4}
\]

This has the effect of reducing solving time by reducing the number of decision variables in the optimization, as the elements of \( \bar{s} \) are calculated from (and therefore dependent on) the values of \( \{z\} \). Inverting \( \overline{X}(\{z\}) \) was possible due to the corn stover and DDGS by-products being neglected. Had these by-products been included, the P2P transactions matrix would be rectangular rather than square. In the case that inverting the P2P transactions matrix is not possible, Equation (7.3) would remain as constraints in the optimization problems and the elements of \( \bar{s} \) would remain decision variables.

The second set of constraints in the optimization formulation are those imposed on the unit operation design variables by the ethanol plant model, expressed as

\[
\{h_{1,...,173}(z_1, \ldots, z_{15}) \geq 0\} \tag{7.5}
\]

7.3.2 Results and discussion

The optimization formulation contained 15 continuous decision variables, 5 equality constraints and 63 inequality constraints. The ALGENCAN optimizer in the pyOpt package [227] was used to optimize the plant design under both the conventional SPD objective function of Equation (7.1) and the P2P objective function of
Figure 7.16: Results of the ethanol production system case study (original P2P model)

Equation (7.2), resulting in two unique optimal designs for the ethanol plant. Figure 7.16 shows CO₂ emissions from the equipment, value chain and economy scales of the P2P model for both designs.

The plant design obtained using the conventional approach to SPD has lower equipment and value chain emissions. However, this comes at the expense of much higher emissions at the economy scale, which are neglected under the conventional approach. Neglecting emissions attributable to the system of interest defeats the purpose of taking a life cycle approach to design. The design obtained using the P2P approach has lower total system-wide emissions. This result was expected based on the nature of the different objective functions used in each approach, as discussed in Section 7.3.1. The P2P design has total system-wide emissions that are 17% lower than the total system-wide emissions for the conventional design. Optimal values of
Table 7.4: Values of unit operation design variables for the two designs. Variables without specified units are unitless. Differences between the two designs are indicated by bold values.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
<th>Conventional approach</th>
<th>P2P approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>z₁</td>
<td>kg/s</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>z₂</td>
<td>kg/s</td>
<td>1.04</td>
<td>1.04</td>
</tr>
<tr>
<td>z₃</td>
<td>°C</td>
<td>120.0</td>
<td>120.0</td>
</tr>
<tr>
<td>z₄</td>
<td>kg/s</td>
<td>8.17</td>
<td>8.17</td>
</tr>
<tr>
<td>z₅</td>
<td>kg/s</td>
<td>0.086</td>
<td>0.086</td>
</tr>
<tr>
<td>z₆</td>
<td>°C</td>
<td>25.0</td>
<td>25.0</td>
</tr>
<tr>
<td>z₇</td>
<td>-</td>
<td>0.92</td>
<td>0.92</td>
</tr>
<tr>
<td>z₈</td>
<td>-</td>
<td>0.97</td>
<td>0.97</td>
</tr>
<tr>
<td>z₉</td>
<td>-</td>
<td>0.011</td>
<td>0.011</td>
</tr>
<tr>
<td>z₁₀</td>
<td>°C</td>
<td>94.6</td>
<td>94.6</td>
</tr>
<tr>
<td>z₁₁</td>
<td>-</td>
<td>0.20</td>
<td>0.20</td>
</tr>
<tr>
<td>z₁₂</td>
<td>-</td>
<td>0.14</td>
<td>0.14</td>
</tr>
<tr>
<td>z₁₃</td>
<td>-</td>
<td><strong>0.078</strong></td>
<td><strong>0.37</strong></td>
</tr>
<tr>
<td>z₁₄</td>
<td>-</td>
<td><strong>0.27</strong></td>
<td><strong>0.001</strong></td>
</tr>
<tr>
<td>z₁₅</td>
<td>-</td>
<td><strong>0.92</strong></td>
<td><strong>0.08</strong></td>
</tr>
</tbody>
</table>

The unit operation design variables for the conventional and P2P designs are given in Table 7.4, with variables that changed under the different approaches indicated in bold. The amounts of variable process inputs for the two designs are given in Table 7.5.

Variables $z_{13}$ and $z_{14}$ control the fraction of the ethanol-water stream going through each of the three drying unit operations. In the conventional design, 7.8% by mass of the ethanol/water stream is sent to the rectification column ($z_{13}$), 27% to corn grits adsorption ($z_{14}$) and 65.2% ($1 - z_{13} - z_{14}$) to the molecular sieve operation. In
Table 7.5: Summary of variable process input amounts for the two optimal process designs. Corn grain and yeast were modeled as fixed flow rates and are not shown here.

<table>
<thead>
<tr>
<th>Input</th>
<th>Conventional approach</th>
<th>P2P approach</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1.13</td>
<td>1.13</td>
<td>kg/s</td>
</tr>
<tr>
<td>Process energy</td>
<td>6.568×10⁴</td>
<td>7.168×10⁴</td>
<td>kJ/s</td>
</tr>
<tr>
<td>α-amylase</td>
<td>9.567×10⁻³</td>
<td>9.567×10⁻³</td>
<td>kg/s</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>2.297×10⁻²</td>
<td>2.297×10⁻²</td>
<td>kg/s</td>
</tr>
<tr>
<td>Urea</td>
<td>8.634×10⁻²</td>
<td>8.634×10⁻²</td>
<td>kg/s</td>
</tr>
<tr>
<td>Corn grits</td>
<td>7.372</td>
<td>0.124</td>
<td>kg/s</td>
</tr>
</tbody>
</table>

the P2P design, 37% of the ethanol/water stream is sent to rectification, 0.1% to adsorption (the minimum allowed by the model) and 62.9% to the molecular sieve. This change seems counter-intuitive at the equipment scale due to the high energy intensity of rectification; as seen in Table 7.5, the P2P design consumes more energy and therefore produces more equipment scale CO₂ emissions than the conventional design. However, when emissions from the entire P2P system are considered in the objective function, the environmental effect of purchasing corn grits outweighs the effect of an increase in process energy consumption, and the adsorption unit becomes virtually unused in favor of the rectification column and molecular sieve.

7.3.3 Alternative P2P model of the ethanol production system

GREET is a process based life cycle modeling tool that is more detailed and comprehensive than many life cycle models, particularly in accounting for greenhouse gases. As discussed in the previous sections, when GREET is used to model the value chain scale there are relatively few remaining inputs that must be captured at
the economy scale. However, modeling a life cycle entirely at the value chain scale is not practical for all systems. The time and effort required to construct a comprehensive process based inventory is quite large, and for new production technologies it is unlikely that the necessary data will be readily available. In this section an alternative P2P model of the ethanol production system is developed, based on the assumption that reliable value chain scale data was not available for the production and distribution of several inputs to the ethanol plant. For this particular case study, this assumption is completely artificial, but for the majority of SPD problems it is unlikely that a value chain scale model with the level of detail and comprehensiveness of GREET will be available. In fact, even GREET has a limited scope for material (non-fuel) inputs and for environmental interventions other than greenhouse gases.

In the alternative P2P model, shown in Figure 7.17, several plant inputs that were previously modeled as equipment-value chain upstream cutoffs (process energy, water, α-amylase, gluco-amylase, yeast, urea and corn grits) are now modeled as equipment-economy upstream cutoffs. The production of equipment-economy upstream cutoffs is then captured by the EEIO model, rather than the value chain model. This takes advantage of the EEIO model to reduce the amount of data needed to build the P2P model, by reducing the number of value chain activity models that must be included. However, although the alternative P2P model requires less data to build, it is likely to be less accurate than the original P2P model. The EEIO model is much coarser than the equivalent value chain model and the alternative P2P model therefore likely to have greater uncertainty than the original P2P model of the previous sections.

The alternative P2P model, like the original model, was optimized under both the conventional SPD approach and the P2P approach. The optimization formulation of
Figure 7.17: Alternative P2P model of the dry-grind corn ethanol process and its value chain, showing upstream connections to the economy. Downstream connections to the economy that were not captured in the model are shown in lighter colors.
Figure 7.18: Results of the ethanol production system case study (alternative P2P model)

Section 7.3.1 remains unchanged except for the dimensions of the P2P transactions matrix, final demand vector and scaling vector, all of which are smaller compared to the original model due to the reduced value chain model size. The original P2P transactions matrix was $91 \times 91$, and the alternative P2P transactions matrix is $84 \times 84$. Figure 7.18 shows equipment, value chain and economy scale CO$_2$ emissions for conventional and P2P plant designs obtained using the alternative P2P model.

Overall, conclusions of the original case study do not change when the alternative P2P model is optimized: the P2P approach still results in a significant 15% reduction in total CO$_2$ emissions compared to the conventional approach. Economy scale emissions for both the conventional and P2P designs are significantly higher under the alternative model, due to this model containing more equipment-economy upstream
cutoff flows. This increases the economic activity necessary to supply inputs and therefore increases emissions produced by the economy.

Table 7.6 gives the optimal design variable values for the conventional and P2P designs under the alternative model. The conventional approach designs obtained using the original and alternative models are identical. However, the P2P designs are different under the two models, although the difference (variables $z_2$ through $z_4$) represents a relatively small effect on the overall plant configuration. Variables $z_2$ through $z_4$ controlled the corn cooking step prior to fermentation. The decrease in $z_2$ and increase in $z_3$ implies that a smaller quantity of higher temperature steam was used to cook the corn prior to fermentation in the P2P design compared to the conventional design. The total amount of water added to the corn prior to fermentation is unchanged: the increase in $z_4$ (water added to mixer just upstream of the fermentation vessel) is the same magnitude as the decrease in $z_3$ (steam used to cook the corn). However, as seen in Table 7.7, the amount of water added elsewhere in the process has decreased as a result of the changing design variables, as the total water input to the process is reduced in the P2P process design.

Table 7.7 compares amounts of ethanol plant inputs for the conventional and P2P designs obtained using the alternative model. The P2P design under the alternative model has drastically decreased consumption of corn grits, just as the P2P design under the original model did. Consumption of water and enzymes has also decreased, and consumption of process energy has increased. These changes have the effect of reducing the economic activity compared to the conventional process design and both of the process designs obtained using the original P2P model.
Table 7.6: Values of unit operation design variables for the optimal process designs obtained from the alternative P2P model. Variables without specified units are unitless. Bold values indicate differences between the two designs.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
<th>Optimal values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Conventional approach</td>
</tr>
<tr>
<td>( z_1 )</td>
<td>kg/s</td>
<td>0.00</td>
</tr>
<tr>
<td>( z_2 )</td>
<td>kg/s</td>
<td>1.04</td>
</tr>
<tr>
<td>( z_3 )</td>
<td>°C</td>
<td>120.0</td>
</tr>
<tr>
<td>( z_4 )</td>
<td>kg/s</td>
<td>8.17</td>
</tr>
<tr>
<td>( z_5 )</td>
<td>kg/s</td>
<td>0.086</td>
</tr>
<tr>
<td>( z_6 )</td>
<td>°C</td>
<td>25.0</td>
</tr>
<tr>
<td>( z_7 )</td>
<td>-</td>
<td>0.92</td>
</tr>
<tr>
<td>( z_8 )</td>
<td>-</td>
<td>0.97</td>
</tr>
<tr>
<td>( z_9 )</td>
<td>-</td>
<td>0.011</td>
</tr>
<tr>
<td>( z_{10} )</td>
<td>°C</td>
<td>94.6</td>
</tr>
<tr>
<td>( z_{11} )</td>
<td>-</td>
<td>0.20</td>
</tr>
<tr>
<td>( z_{12} )</td>
<td>-</td>
<td>0.14</td>
</tr>
<tr>
<td>( z_{13} )</td>
<td>-</td>
<td>0.078</td>
</tr>
<tr>
<td>( z_{14} )</td>
<td>-</td>
<td>0.27</td>
</tr>
<tr>
<td>( z_{15} )</td>
<td>-</td>
<td>0.92</td>
</tr>
</tbody>
</table>

Table 7.7: Summary of variable plant inputs for the optimal designs obtained using the alternative P2P model. Corn grain and yeast are not shown.

<table>
<thead>
<tr>
<th>Input</th>
<th>Conventional approach</th>
<th>P2P approach</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1.13</td>
<td>0.99</td>
<td>kg/s</td>
</tr>
<tr>
<td>Process energy</td>
<td>6.568×10^4</td>
<td>7.171×10^4</td>
<td>kJ/s</td>
</tr>
<tr>
<td>( \alpha )-amylase</td>
<td>9.567×10^{-3}</td>
<td>9.497×10^{-3}</td>
<td>kg/s</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>2.297×10^{-2}</td>
<td>2.280×10^{-2}</td>
<td>kg/s</td>
</tr>
<tr>
<td>Urea</td>
<td>8.634×10^{-2}</td>
<td>8.634×10^{-2}</td>
<td>kg/s</td>
</tr>
<tr>
<td>Corn grits</td>
<td>7.372</td>
<td>0.124</td>
<td>kg/s</td>
</tr>
</tbody>
</table>
As discussed in Section 6.2.3, the disaggregation procedure caused the economy-scale emissions factors to become dependent on the plant design. Table 7.8 shows that the disaggregation procedure can either increase or decrease a sector’s emissions factors; the direction of change is determined by the constituent activity or process and whether that constituent has higher or lower emissions relative to the rest of the parent sector.

### 7.3.4 Findings

Based on the results of this case study, it can be concluded that the larger P2P analysis boundary reduces the chance of unintended harm caused by shifting of emissions and other environmental impacts outside the smaller system boundary used in conventional SPD. That this result is apparent even for a relatively small-scale design problem holds promise for future, larger-scale applications of the P2P modeling framework. For larger design problems such as regional supply chains, the effect of including emissions from the economy scale and the resulting net savings in emissions are both expected to be more significant than for this case study.

This case study also demonstrated that even very complete process based life cycle inventories, such as GREET, have gaps that can be filled relatively easily using the P2P approach. In particular, GREET does not include corn seed as an input to corn farming, nor does it account for emissions associated with water distribution. Both of these are captured with the P2P model using only the physical input amount and the current market price.

Finally, the different plant designs obtained under the conventional and P2P approaches indicate that accounting for a more complete life cycle in sustainable process
Table 7.8: Disaggregating the EIO model resulted in changes in emissions factors (elements of the environmental interventions matrix) for parent sectors.

<table>
<thead>
<tr>
<th>Sector</th>
<th>Original P2P model</th>
<th>Change in emissions factors, ( \bar{b}_j - \bar{b}_j^*({z}) ) (kg CO(_2)/MM$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sector</td>
<td>Conventional</td>
</tr>
<tr>
<td>Grain farming</td>
<td></td>
<td>6.60×10(^{-4})</td>
</tr>
<tr>
<td>Coal mining</td>
<td></td>
<td>7.68×10(^{-6})</td>
</tr>
<tr>
<td>Electric power generation, transmission and distribution</td>
<td></td>
<td>1.50×10(^{-5})</td>
</tr>
<tr>
<td>Natural gas distribution</td>
<td></td>
<td>1.01×10(^{-4})</td>
</tr>
<tr>
<td>Other basic organic chemical manufacturing</td>
<td></td>
<td>8.56×10(^{-4})</td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td></td>
<td>4.59×10(^{-3})</td>
</tr>
<tr>
<td>Pesticide and other agricultural chemical manufacturing</td>
<td></td>
<td>7.42×10(^{-5})</td>
</tr>
<tr>
<td>Rail transportation</td>
<td></td>
<td>5.39×10(^{-4})</td>
</tr>
<tr>
<td>Truck transportation</td>
<td></td>
<td>-8.93×10(^{-4})</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sector</th>
<th>Alternative P2P model</th>
<th>Change in emissions factors, ( \bar{b}_j - \bar{b}_j^*({z}) ) (kg CO(_2)/MM$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sector</td>
<td>Conventional</td>
</tr>
<tr>
<td>Grain farming</td>
<td></td>
<td>-4.44×10(^{-4})</td>
</tr>
<tr>
<td>Other basic organic chemical manufacturing</td>
<td></td>
<td>8.13×10(^{-4})</td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td></td>
<td>4.59×10(^{-3})</td>
</tr>
<tr>
<td>Pesticide and other agricultural chemical manufacturing</td>
<td></td>
<td>7.42×10(^{-5})</td>
</tr>
<tr>
<td>Rail transportation</td>
<td></td>
<td>5.39×10(^{-4})</td>
</tr>
<tr>
<td>Truck transportation</td>
<td></td>
<td>-9.77×10(^{-4})</td>
</tr>
</tbody>
</table>
design leads to unique plant designs with potentially non-intuitive characteristics. Using the value chain scale analysis boundary, the ethanol plant consumed less energy and a greater amount of corn grits in the adsorption unit; using the P2P boundary, the consumption of corn grits is seen as environmentally sub-optimal compared to energy consumption. This shows that in addition to using sophisticated optimization methods, as is quite common in current SPD work, it is also critical to define the proper system boundary and objective function to obtain the true optimum result.

7.4 Case study: Renewable energy production system design

Designing systems to produce renewable energy from biomass has been a focus of much recent work in PSE and SED; notable examples include [314], [101], and [318]. Decision variables in such design problems typically include the locations and capacities of biomass storage facilities and conversion processes. The type or types of biomass feedstock to utilize is occasionally treated as a variable [319], but is more generally modeled as an exogenous parameter with the supply chain facilities being located relative to the supply(ies) of biomass and the energy demand centers. [178]

This section presents a case study which expands the conventional design space for renewable energy production systems. Rather than considering a single energy production pathway, this case study begins with a superstructure of potential pathways; the objective is to select pathways from the superstructure based on several economic, energetic and ecological criteria. The design space thus includes decision variables in the land use stage of energy production as well as variables dealing with the conversion of biomass to fuel or electricity.
Decision variables in the land use stage include the type of cropping system to implement and the farming management practices to employ. The choice of cropping system determines the type and quantity of biomass that is produced, and if the biomass type remains constant every year or if different types are produced in alternating years (crop rotation). Farming management practices involve many interrelated variables, such as the amount of fertilizer and pesticides to apply, seeding density, irrigation, and tillage type. Some management practices offer situations in which the cost of producing biomass is decreased and the biomass yield is increased. For instance, using a no-till practice in continuous corn cropping systems has been shown in some areas to increase the annual per-acre corn grain and stover yield by approximately 5%. \[167\] The same no-till practice reduces fuel expenditures by reducing tractor and other equipment usage, which also reduces emissions from fuel combustion. However, no-till practices often involve increased inputs of herbicides and other agricultural chemicals \[309\] which increases emissions from upstream and life cycle activities and contributes to nutrient runoff. No-till practices may also require that agricultural residue such as corn stover is left on the field, rather than being removed and used as an energy feedstock. There are rarely any clear “win-win” decisions. Just as an apparently optimal plant design is seen as sub-optimal when the analysis boundary is expanded, so too farming management decisions should be made in the context of a larger system to ensure that practices are economically and environmentally optimal. \[82, 240\]

The superstructure of pathways considered in this case study, shown in Figure 7.19, contains two types of energy production pathways: agricultural pathways, which involve biomass farming followed by conversion of biomass to liquid fuel or electricity,
and technological pathways, which produce electricity directly through wind turbines or solar panels. Typically, energy systems are designed based on profitability and on emissions generation; the objective is to find the most profitable system with the life cycle that produces the least amount of carbon dioxide or other emissions. However, including agricultural activities in the design problem creates an opportunity to use additional, ecological design criteria. Agricultural activities are capable of providing *ecosystem services* such as carbon sequestration and air purification that can partially mitigate the environmental impacts of the entire system. In this case study, the energy system is designed for *net* environmental impacts – that is, for the difference between emissions generation and mitigation. The objective is to avoid exceeding the available mitigation capacity, or at least to reduce the extent to which the mitigation capacity
is exceeded; the latter is a much more likely scenario. This net impact approach to design decisions is expected to lead to novel, non-intuitive design decisions that may offer both economic and environmental benefits over designs obtained by minimizing gross environmental impacts. [37]

Ecosystem services considered in this case study are climate regulation, nitrogen cycle regulation and water purification. Climate regulation is quantified with carbon dioxide emissions and carbon sequestration (mitigation), respectively. Nitrogen cycle regulation is quantified with nitrous oxide and nitrogen oxide emissions, from fuel use and from soil emissions, and nitrogen fixation in the soil, provided by soybean farming and to a small extent by crop litter and seeds. For water purification, a local watershed has some nitrate runoff mitigation capacity quantified with the Total Maximum Daily Load (TMDL) for nitrification potential, and this balances nitrates in surface and sub-surface runoff that come from nitrogen fertilizer application.

The ecosystem services provided by the farmland are not insignificant, but they can be enhanced by considering services provided by local ecosystems. In this case study, two additional ecosystems are considered in addition to the land used for energy production: a forest ecosystem, established by reforesting local land that is assumed to be barren and unused, and the watershed ecosystem discussed above. Reforestation provides carbon sequestration in addition to what is provided by the farmland, and helps to further offset carbon dioxide emissions generated by the energy system. The watershed ecosystem provides water purification, which cannot be supplied by the land itself.
This work was completed in collaboration. Input and simulated data for all agricultural activities, for the use of reforestation as carbon sequestration, and for the soybean biodiesel process is attributed to Varsha Gopalakrishnan.

Details of the system component models used in this case study are given in Section 7.4.1. The formulation of this case study as an optimization problem, including decision variable descriptions and objective functions, is given in Section 7.4.2. Section 7.4.3 presents and discusses the optimal production system designs. Ongoing and future work for this case study is discussed in Section 9.2.4.

7.4.1 Model building

The economy scale was modeled with the same 2002 benchmark input-output model (after redefinitions, producers’ prices) [286] that was used in Section 7.3. The make and use tables were again converted to square matrices by removing the rest-of-world inputs and distributing scrap production for each sector among the various commodities produced by that sector. [150] Some aggregation from the detailed level of 426 sectors and commodities was necessary to perform the economy scale disaggregation. In the detailed model, several flows between sectors that were modeled at the value chain or equipment scale were zero at the economy scale. In order for the disaggregation procedure to result in positive flows at the economy scale, the following sectors were aggregated: Food manufacturing, Nonmetallic mineral product manufacturing, Engine, turbine, and power transmission equipment manufacturing and Semiconductor and other electronic component manufacturing. A composite sector for All federal, state and local government services and enterprises was also aggregated; this sector consisted of S00101, Federal electric utilities, through S00700,
General state and local government services. The resulting model consisted of 360 sectors and 360 commodities. Environmental intervention data for CO₂ emissions was obtained at the detailed level of aggregation from [18, 259] and was aggregated following the same procedure to 360 sectors.

All land use options were modeled at the value chain scale. As shown in Figure 7.19, three cropping systems with two management practice options each were included in the superstructure. Each combination of cropping system and management practice was modeled as a separate agricultural activity, such that there were multiple value chain activities producing each type of biomass. The agricultural activities were simulated for central Ohio using WinEPIC, a Microsoft Windows implementation of the Environmental/Policy Integrated Climate model developed by the US Department of Agriculture. [48] Input data for WinEPIC consisted of information on the local climate [255], average soil type for the central Ohio region [260] and data on regionally specific agricultural management practices. [15] Data obtained from WinEPIC simulations and used in the superstructure model is as follows: yield of grain and lignocellulosic biomass, carbon sequestered in and removed from the soil, fuel use, amount of surface water runoff, amount of nitrate in the runoff and nitrogen emissions from the soil. Data on carbon dioxide emitted via crop respiration [1] was also included in the superstructure model. Emissions of nitrous oxide and nitrogen oxides was calculated from fuel use data obtained from WinEPIC and from emissions factors in GREET 2014. [30]

The life cycles of all inputs to the agricultural activities (seeds, fertilizers, pesticides, and so on) were modeled using the EEIO model within the P2P modeling framework: that is, all inputs to the value chain activities were modeled as upstream
cutoff flows. Were the life cycles of agricultural inputs also modeled at the value chain scale, great care would need to be taken that each input’s life cycle has the same degree of completeness and accuracy. Keeping all inputs as upstream cutoffs ensures that the system boundary for each activity model is roughly the same. Sufficient data could not be found to account for farming equipment and labor inputs for all agricultural activities, thus these inputs were neglected. The manufacture, installation and maintenance of both wind turbines and solar panels was also modeled at the economy scale using cost data for each of these activities. This was again done to ensure that every land use option was modeled with approximately the same life cycle boundary; attempting to model the complete life cycle of wind turbines or solar panels at the value chain scale would inevitably lead to truncation error, and could give those land use options an unfair advantage due to under-representing their life cycle impacts.

Reforestation with six tree species native to Ohio was modeled using iTree, a software suite that models tree growth and calculates various ecosystem services for different forest ecosystems. [16] The same soil and climate data for central Ohio used to simulate the agricultural activities was used in the tree growth simulation. Data on carbon sequestered per tree and tree crown area was obtained from iTree for each of the six species (white oak, Scots pine, American elm, spruce, birch and Eastern hemlock). To avoid overcrowding the trees, a 2 meter buffer zone between trees was added.

Table 7.9 lists the sources of data used to build the P2P model for this case study. Prices for commodity chemicals and some fertilizers were obtained from [165]. Fuel and energy prices were obtained from the Energy Information Administration. [2, 5,
Prices for inputs that could not be found within these sources were obtained from online retailers. Where possible, prices were obtained for the year 2002; any prices not already in 2002 levels were converted using producer price index data from the US Bureau of Labor Statistics.  

Biomass conversion processes were modeled at the equipment scale. Although the P2P framework is capable of using fundamental process models with unit operation design variables as was done in Section 7.3, in this case study the process scale was modeled with linear models derived from plant design and economics studies in the literature. Table 7.9 lists the sources of data used to build each biomass conversion model. All inputs to the equipment scale processes except for the biomass feedstocks were modeled equipment-economy upstream cutoffs, as was done for inputs

### Table 7.9: Summary of data sources for farming and biomass conversion processes.

<table>
<thead>
<tr>
<th>Model</th>
<th>Source(s) of model data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn farming</td>
<td>[15, 48]</td>
</tr>
<tr>
<td>Corn-soybean farming</td>
<td>[15, 48]</td>
</tr>
<tr>
<td>Switchgrass farming</td>
<td>[33, 48, 93]</td>
</tr>
<tr>
<td>Wind turbines</td>
<td>[90, 135]</td>
</tr>
<tr>
<td>PV modules</td>
<td>[85, 218, 313]</td>
</tr>
<tr>
<td>Corn grain fermentation</td>
<td>[25, 206]</td>
</tr>
<tr>
<td>Soybean biodiesel</td>
<td>[30, 35, 67, 128, 257]</td>
</tr>
<tr>
<td>Corn stover biochemical</td>
<td>[25, 155, 206]</td>
</tr>
<tr>
<td>Switchgrass biochemical</td>
<td>[25, 155, 206]</td>
</tr>
<tr>
<td>Corn stover pyrolysis</td>
<td>[166, 238, 280]</td>
</tr>
<tr>
<td>Switchgrass pyrolysis</td>
<td>[166, 238, 280]</td>
</tr>
<tr>
<td>Corn stover combustion</td>
<td>[30, 34]</td>
</tr>
<tr>
<td>Switchgrass combustion</td>
<td>[30, 34]</td>
</tr>
</tbody>
</table>
to the value chain activities. Chemical process equipment was also included as an equipment-economy upstream cutoff flow, using the total installed equipment cost for each conversion process.

Because the EEIO model used in this case study represented the 2002 US economy, disaggregation was only necessary for those value chain activities and equipment scale processes that were commercially active at that time. The continuous corn and corn-soybean rotation cropping systems were removed from the economy, as were the corn grain ethanol and soybean biodiesel processes. The switchgrass cropping systems and all other equipment scale processes were not removed from the economy. Production, installation and maintenance of wind turbines and solar panels was modeled at the economy scale, so no disaggregation was necessary. Disaggregation of the value chain scale was also unnecessary, as the biomass conversion processes did not overlap with any of the land use options.

The P2P model of the energy system represents twenty year’s continuous operation, with the restriction that the choice of land use options and biomass conversion processes do not change over time. When considering twenty year’s operation all at once rather than year by year, the size and complexity of the problem is greatly reduced without excluding any essential features of the model. At the economy scale, considering the full lifetime of the production system is less than realistic due to the static nature of the EEIO model. This case study implicitly assumes that the US economy as well as all market prices remain fixed in the 2002 state for the lifetime of the production system, which is questionable at best. However, accounting for temporal dynamics at the economy scale would require the use of a general equilibrium
or similar model at the economy scale, which is beyond the scope of this case study but is discussed in Section 8.6.

As this case study is still ongoing and further alterations to the model are extremely likely, the data and code used to generate results are not given in the Appendix but are available from the author on request, as are any and all updated versions of the model and case study results.

### 7.4.2 Optimization problem

#### Decision variables

In this case study, the decision variables dealing with the energy production pathway are all elements of the P2P scaling vector $s$. Value chain scaling factors determine which land use options to implement and how extensively, including which crop management practice to employ for agricultural options. Scaling factors for agricultural options represent the number of acres planted in each cropping system and are continuous variables. For the wind turbines and solar panels, scaling factors represented the number of each installed on the land. Realistically, the numbers of wind turbines and solar panels should be integer variables; however, due to the limitations of the solver used to optimize the model, the variables were left as continuous. This modeling decision is not expected to impact the optimal system designs significantly. Design options at the value chain scale are summarized in Table 7.10.

Equipment scale scaling factors determine which, if any, of the biomass conversion processes to implement, which determines the mix of end products and by-products. All decision variables at the equipment scale were continuous and restricted to values between 0 (process is not implemented) and 1 (process is implemented at its maximum
Table 7.10: Value chain scale decision variables determine the land use option and the crop management system for agricultural options.

<table>
<thead>
<tr>
<th>Value chain scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Switchgrass farming with 0 kg/acre N fertilizer</td>
</tr>
<tr>
<td>Switchgrass farming with 100 kg/acre N fertilizer</td>
</tr>
<tr>
<td>Continuous corn rotation, conventional till</td>
</tr>
<tr>
<td>Continuous corn rotation, no till</td>
</tr>
<tr>
<td>Corn-soybean rotation, conventional till</td>
</tr>
<tr>
<td>Corn-soybean rotation, no till</td>
</tr>
<tr>
<td>2 MW wind turbine</td>
</tr>
<tr>
<td>100 W solar panel</td>
</tr>
</tbody>
</table>

possible capacity). Design options at the equipment scale are summarized in Table 7.11.

The model contained six decision variables dealing with the reforested land area. Each decision variable represents the number of trees planted that were of a particular species. No decision variables related to the regional watershed were included in the model.

Objective functions

The energy production system was optimized under five separate objective functions, all of which were maximized: net present value (MM$) of the entire energy system, total energy produced (gasoline gallon equivalents, GGE), fraction of nitrate runoff that is mitigated by the watershed, and fraction of nitrogen emissions mitigated by the farmland. An attempt was made at using the fraction of carbon dioxide emissions mitigated by the combined farmland and reforested land, but no feasible
Table 7.11: Equipment scale decision variables determine which biomass conversion process is implemented and which mix of end products and by-products is produced.

<table>
<thead>
<tr>
<th>Equipment scale</th>
<th>Corn stover</th>
<th>Switchgrass</th>
<th>Corn stover</th>
<th>Switchgrass</th>
<th>Corn grain</th>
<th>Soybeans</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biochemical (ethanol,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>electricity)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fast pyrolysis (bio-oil,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>electricity)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Combustion (electricity)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fermentation (ethanol)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Soybean biodiesel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

solution for that objective function could be obtained using the current solver. All objective functions are based on the system’s 20 year operating period.

The net present value objective function includes the entire energy system: land use options (value chain scale), biomass conversion processes (equipment scale) and reforested land. Net present value of the land use options excludes the cost of purchasing farmland and equipment, as well as the sale of primary biomass products that are converted to fuels or electricity. Farmland and equipment costs are assumed to be approximately the same for all agricultural activities, and as the energy system is being designed as a whole, only revenue from products sold outside the system is included in the economic objective. Included in the land use option net present values are the cost of all material and fuel inputs to the agricultural activities, the purchase and installation costs of wind turbines and solar panels, and revenue from sale of
biomass by-products except for switchgrass and corn stover, which were assumed to have no monetary value. In 2015 there is not yet a widespread market for either of these products; it is therefore reasonable to assume that in 2002, the year in which this model is based, there was also no market and switchgrass and stover had no market value except after conversion to energy. At the equipment scale, the net present value objective function [229] accounts for capital costs for the biomass conversion processes, both fixed and variable operating costs, depreciation and income taxes, and revenue from sales of by-products where relevant. The purchase of land on which to build the process(es) is excluded, because it is assumed to be approximately the same for all processes. Finally, the net present value of the reforested land includes only the cost of establishing the reforested area; ongoing maintenance and management costs as well as the initial purchase cost of land are excluded.

Because the net present value objective function includes all stages of energy production, it can be stated as the sum of the net present values of each individual stage:

$$Z_{NPV} = \sum s NPV(s) - C_{trees} \cdot \left( A_{trees} \hat{s}_{trees} \right)$$

In Equation (7.6), $NPV$ is a vector of net present value per acre (agricultural activities) or unit (wind turbines, solar panels) of land use options. NPV is a vector of net present value functions for the maximum-capacity biomass conversion processes; each element of NPV is non-linearly dependent on elements of $s$. $C_{trees}$ is the cost of establishing one acre of reforested land, and $A_{trees}$ is the area occupied by each tree, including the buffer area. The quantity $A_{trees} \hat{s}_{trees}$ thus represents the number of acres occupied by trees of all species, which is multiplied by the cost per acre of reforestation. Because the reforestation was assumed to take place all at once, at the
beginning of the energy system’s lifetime, no discounting factors were applied as they were in calculating the land use option and biomass conversion process net present values.

The net energy objective function includes only the energy produced as a final product:

\[ Z_{\text{energy}} = \mathbf{f}_{\text{energy}} \cdot \mathbf{GGE} \]  

(7.7)

where \( \mathbf{f}_{\text{energy}} \) is the last five elements of the P2P product balance, defined as

\[ \mathbf{f} = \mathbf{Xs} \]  

(7.8)

Note that Equation (7.8) is not a constraint but rather the calculation of \( \mathbf{f} \). Constraints are placed on \( \mathbf{f} \) to impose mass and energy balances on the P2P model, and these constraints are presented later in the section. \( \mathbf{f}_{\text{energy}} \) is a vector of fuel and electricity production by wind turbines, solar panels, and all biomass conversion processes. In Equation (7.7), \( \mathbf{GGE} \) is a vector of factors for converting MJ of energy products (the units of \( \mathbf{f}_{\text{energy}} \)) to gasoline gallon equivalents, such that all energy products are being measured in equivalent units:

\[ \mathbf{GGE} = \begin{bmatrix} 8.4 \times 10^{-3} & 0.68 & 1.06 & 1.55 & 8.4 \times 10^{-3} \end{bmatrix} \]  

(7.9)

The order of factors in \( \mathbf{GGE} \) is electricity (MJ), ethanol, biodiesel, crude bio-oil and electricity. Electricity appears twice because it is a product both of the value chain and of the equipment scale. Data to calculate \( \mathbf{GGE} \) was obtained from [30].

Both of the environmental objective functions are stated as mitigation capacity divided by required mitigation, or in other words, ecosystem service supply (mitigation) divided by ecosystem service demand (emissions). The objective function for
nitratenitrate runoff is stated as follows:

\[ Z_{\text{NO}_3} = \frac{\text{TMDL}}{\mathbf{b}_{\text{NO}_3} \cdot \mathbf{s}} \]  

(7.10)

where TMDL is the Total Maximum Daily Load of nitrification potential for the local watershed [87]; this value was converted to kg nitrate equivalents to match the units of nitrate runoff. \( \mathbf{b}_{\text{NO}_3} \) is a vector of kg nitrate in surface and sub-surface runoff per acre or unit of each land use option. For wind turbines and solar panels, \( \mathbf{b}_{\text{NO}_3} \) was assumed to be zero because no nitrogen containing fertilizer is applied.

For nitrogen emissions, the objective function is similar to Equation (7.10):

\[ Z_N = \frac{\mathbf{b}_{\text{N fixation}} \cdot \mathbf{s}}{\mathbf{b}_{\text{N emissions}} \cdot \mathbf{s}} \]  

(7.11)

where \( \mathbf{b}_{\text{N fixation}} \) and \( \mathbf{b}_{\text{N emissions}} \) are vectors of nitrogen fixation in the soil and nitrogen emissions to air, respectively, per acre or unit of each land use option. These values were assumed to be zero for both wind turbines and solar panels.

**Constraints**

The decision variables \( \mathbf{s} \) are constrained by the P2P balance equations on production and consumption. For the economy scale scaling factors \( \mathbf{s} \) these balance equations are

\[
\begin{bmatrix}
I - A^* & -\mathbf{X}_u & -\mathbf{X}_E^E
\end{bmatrix}
\mathbf{s} = \mathbf{0}
\]  

(7.12)

Equation (7.12) states that no commodities may leave the P2P system or, in other words, economic activity is limited to that necessary to provide inputs to the smaller scales.

At the value chain scale, any biomass product may leave the system by being sold as a by-product rather than being converted to fuel or electricity. The resulting
constraints on the value chain scale scaling factors are

\[
\begin{bmatrix} -A_d & X & -X_u^V \end{bmatrix} \bar{s} \geq 0
\]  

(7.13)

Similarly, at the equipment scale, the balance constraints are all inequalities to account for the different combinations of end products that may be produced:

\[
\begin{bmatrix} -A^E_d & -X^V_u & X \end{bmatrix} \bar{s} \geq 0
\]  

(7.14)

The area of farmland used by the energy system was constrained to be between 5,000 and 10,000 acres:

\[
\begin{align*}
\bar{s} \cdot L & \geq 5,000 \\
\bar{s} \cdot L & \leq 10,000
\end{align*}
\]  

(7.15)  

(7.16)

where the vector \(L\) contains the amount of land in acres required by each land use option, as follows,

\[
L = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.1633 & 1.73 \times 10^{-4} \end{bmatrix}
\]  

(7.17)

Each agricultural land use option represented in the value chain activity models occupies 1 acre of land, each wind turbine occupies 0.1633 acres (the spacing requirement for turbines is captured in Equation (7.24)), and each PV module occupies 0.7 m² or 1.73×10^{-4} acres.

A constraint was also placed on the carbon dioxide emissions and mitigation capacity of the farmland and reforested area, in order to model the decision to reforest as a means of reducing net environmental impacts. Without this constraint, the optimal energy system designs would never involve reforestation, as additional monetary
and intangible benefits provided by the reforested area were not quantified. The constraint is stated as

\[ b_{trees, CO_2 seq} s_{trees} + b_{CO_2 seq} s - 0.5 (b_{CO_2 ems} s + b_{CO_2 ems} s) = 0 \] (7.18)

and requires that 50% of the carbon dioxide emissions produced by the value chain and equipment scales be mitigated by the combined sequestration capacity of the agricultural activities and the reforested area.

Net present value was constrained to be greater than or equal to zero:

\[ Z_{NPV} \geq 0 \] (7.19)

for all objective functions except for energy production. An optimal and feasible solution could not be found that maximized energy production while satisfying the NPV constraint, so it was removed from the model for the energetic objective function optimization only.

The final constraints restrict scaling factors to allowable values,

\[ s \geq 0 \]
(7.20)
\[ s \geq 0 \]
(7.21)
\[ s \geq 0 \]
(7.22)
\[ s \leq 1 \]
(7.23)
\[ s_{turbine} \leq 500.0 \]
(7.24)
\[ s_{pv} \leq 57812156.0 \]
(7.25)
\[ s_{ag. options} \leq 10000.0 \]
(7.26)

Equation (7.24) constrains the number of wind turbines to be 500 or fewer to allow for sufficient spacing between turbines.
Table 7.12: Maximum energy design for the renewable energy production system.

<table>
<thead>
<tr>
<th>Acres/Units</th>
<th>Land use option</th>
</tr>
</thead>
<tbody>
<tr>
<td>9,918</td>
<td>Continuous corn, conventional till</td>
</tr>
<tr>
<td>500</td>
<td>2 MW wind turbines</td>
</tr>
<tr>
<td></td>
<td>Corn grain ethanol (35% capacity)</td>
</tr>
<tr>
<td></td>
<td>Stover pyrolysis (99% capacity)</td>
</tr>
<tr>
<td></td>
<td>126 acres of white oak trees</td>
</tr>
</tbody>
</table>

7.4.3 Results and discussion

The model given in Equations (7.12) - (7.23) was optimized separately under the four objective functions, Equations (7.6) - (7.11), yielding four unique production system designs. Tables 7.12 - 7.15 give details of each optimal energy pathway, and Table 7.16 gives the net present value and energy production of the four designs. Figure 7.20 gives the emissions production and mitigation capacity for the four designs.

The production system design that maximized energy production, shown in Table 7.12, utilized the entire 10,000 acres of cropland with the maximum allowable number of 2 MW wind turbines and the remaining land planted in continuous corn under conventional tillage. This design had by far the lowest NPV and the lowest overall ecological performance (see Figure 7.20) of the four optimal designs, indicating that simply designing for maximum energy efficiency on a land basis is neither economically nor ecologically feasible.

All 10,000 acres of farmland were planted in a corn-soybean rotation managed with a no-till practice for the maximum net present value system design, shown in Table 7.13. Of the three agricultural products, only soybeans were converted to
Table 7.13: Maximum net present value design for the renewable energy production system.

<table>
<thead>
<tr>
<th>Acres/Units</th>
<th>Land use option</th>
</tr>
</thead>
<tbody>
<tr>
<td>10,000</td>
<td>Corn-soybean rotation, no till</td>
</tr>
<tr>
<td></td>
<td>Soybean biodiesel (100% capacity)</td>
</tr>
<tr>
<td></td>
<td>103 acres of white oak trees</td>
</tr>
</tbody>
</table>

energy; corn grain was sold as a by-product and corn stover was disposed of. As seen in Table 7.16, the maximum NPV design produces much less energy than the maximum energy system, as expected, and even produces less energy than one of the ecologically optimal system designs, which was not expected. It is likely that soybean biodiesel is the economically optimal biomass conversion process due to its production of relatively high-value by-products such as glycerin. These byproducts add significantly to the plant’s revenue stream, although they do so without increasing the energy output of the system.

Maximizing nitrate mitigation produced a design, shown in Table 7.14, that used only 9,277 acres of farmland, planted in a continuous corn cropping system under a no-till practice. Once again, corn grain was sold as an agricultural by-product; the corn stover was converted to crude bio-oil and electricity via fast pyrolysis. This design had the minimum allowable NPV of $0 over the twenty-year lifetime of the energy system, which unsurprisingly indicates a strong tradeoff between this particular ecological objective (nitrate runoff) and the economic objective. However, the maximum nitrate runoff mitigation design did produce three times as much energy on a GGE basis than the maximum NPV design, indicating that while there are tradeoffs between
Table 7.14: Maximum nitrate runoff mitigation design for the renewable energy production system.

<table>
<thead>
<tr>
<th>Acres/Units</th>
<th>Land use option</th>
</tr>
</thead>
<tbody>
<tr>
<td>9,277</td>
<td>Continuous corn, no till</td>
</tr>
<tr>
<td></td>
<td>Stover pyrolysis (47% capacity)</td>
</tr>
<tr>
<td></td>
<td>168 acres of white oak trees</td>
</tr>
</tbody>
</table>

Table 7.15: Maximum nitrogen emissions mitigation design for the renewable energy production system.

<table>
<thead>
<tr>
<th>Acres/Units</th>
<th>Land use option</th>
</tr>
</thead>
<tbody>
<tr>
<td>10,000</td>
<td>Corn-soybean rotation, no till</td>
</tr>
<tr>
<td></td>
<td>Soybean biodiesel (77% capacity)</td>
</tr>
<tr>
<td></td>
<td>103 acres of white oak trees</td>
</tr>
</tbody>
</table>

economic, energetic and ecological objectives, they are not universal and it may be possible to find designs that perform well in more than one set of objectives.

Designing for maximum nitrogen emissions mitigation again resulted in the corn-soybean rotation managed with a no-till practice being planted over the entire 10,000 acres of farmland, as shown in Table 7.15. Soybean biodiesel was again selected as the optimal biomass conversion process, with corn grain and a small amount of soybeans being sold as an agricultural by-product and stover being disposed of. The net present value of this system was $0 just as it was for the other ecologically optimal system design, so the existence of a strong tradeoff between economic and ecological objectives has been demonstrated twice with these results.
Table 7.16: Net present values and energy production of the four optimal energy pathways.

<table>
<thead>
<tr>
<th>Pathway</th>
<th>NPV (MM$)</th>
<th>Energy (billion GGE)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max. NPV</td>
<td>1.4</td>
<td>1.0</td>
</tr>
<tr>
<td>Max. Energy</td>
<td>-241.0</td>
<td>17.4</td>
</tr>
<tr>
<td>Max. NO\textsubscript{3} Mitigation</td>
<td>0.0</td>
<td>4.2</td>
</tr>
<tr>
<td>Max. N\textsubscript{2}O\textsubscript{4} NO\textsubscript{x} Mitigation</td>
<td>0.0</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Figure 7.20 compares the ecosystem service demand and supply across the four energy systems. Once again the energy maximizing design performs poorly overall, with significantly higher demand for CO\textsubscript{2} and nitrate mitigation and no more supply than found in the other three system designs. The other three designs are fairly comparable in terms of these three ecological criteria, indicating that the tradeoffs between economics and ecological objectives, and between ecological objectives, are less severe than the tradeoff between the energetic and other objectives.

7.4.4 Findings

The results of this case study come with a general caveat: the superstructure model optimized to produce these energy system designs represent agricultural practices in central Ohio. These results should not be generalized to energy systems in other geographic regions, as agriculture is highly spatially variable; a renewable energy production system that is optimal in Ohio may not be feasible in, for example, Arizona.
Figure 7.20: Ecosystem service supply and demand values for the four optimal energy system designs.
For this case study, there is a clear if unsurprising tradeoff between the economic and ecological objectives, and between the energetic and economic objectives. Somewhat unexpectedly, there was a less consistent tradeoff between the energetic and ecological objectives, indicating that with careful decision making it may be possible to realize an energy production system that is ecologically sustainable but still produces significant amounts of energy.

While corn grain was produced in all four of the optimal designs, it was only once, in the maximum energy production system, converted to ethanol; in the other three designs, corn grain was sold as an agricultural by-product. These results suggest a possible alternative to the current system of producing corn for fuel: by implementing multi-functional agricultural activities or exploring second-generation biofuels, the food vs. fuel debate may be somewhat mitigated. However, further and more complete study is needed before these conclusions can be generalized. In particular, the widescale implementation of any new biofuels system, such as soybean biodiesel, will inevitably lead to global changes in current agricultural practices such as an increase in soybean planting and a decrease in other crops that may outweigh the initial benefits of changes to the agricultural activities.
Chapter 8: Equilibrium modeling extensions to the P2P framework

8.1 Introduction

The P2P framework of Chapter 6 combines engineering, life cycle and economic models to represent a system operating at steady state. In Chapter 7, the framework was utilized within an optimization formulation to make small scale engineering decisions, based on the environmental impacts of those decisions at a large scale. Another potential category of applications involves modeling interactions between macro scale economic systems and smaller scale engineering systems, which is made possible by the multiscale and multidisciplinary nature of the P2P framework. Engineering-economic interactions are difficult or impossible to capture using either conventional engineering or economic models: engineering models, which may occasionally include the value chain scale, do not currently extend to the economy scale, and economic models likewise do not extend to the scale at which engineering decisions are made. However, the economic model within the existing P2P framework is a static EEIO model that cannot capture market effects, such as changes in prices, in the level of final demand and in the structure of the economy.
Market effects have already been incorporated into sustainability analyses in the field of consequential LCA. Consequential studies extend the typical static life cycle inventory model with an economy scale partial equilibrium model of relevant markets (economic sectors). As a result, consequential life cycle models can capture both physical and economic consequences of decisions made within the life cycle – regardless of whether those consequences manifest within the life cycle or within the surrounding economy. For instance, modeling global land use change caused by increasing biofuel production is done with a consequential life cycle model that includes a partial equilibrium model. [254] Replacing the static EEIO model in the existing P2P framework with a partial equilibrium model will enable engineering design decisions based on these types of physical and economic consequences. This concept can also be extended to general equilibrium models, which unlike partial equilibrium models capture the entire economy, albeit at a highly aggregated level. Replacing the EEIO model with a general equilibrium model in the P2P framework will allow the aforementioned market effects – changes in market prices, shifts in economy scale production technologies, and changes in final demand, among others – to be modeled endogenously, or as a consequence of relatively small scale design decisions.

Incorporating equilibrium models into the P2P framework enables a further category of applications, one in which the interactions of interest are “top down” (economy influencing the engineering system) rather than “bottom up” (engineering system influencing the economy, described in the previous paragraph). General equilibrium models are commonly used to quantify and analyze the effects of economic policies, including taxes and government regulations; see for instance [253] and [276], among
many others. However, as discussed above, such models do not extend to an engineering scale, although some hybrid equilibrium models have been developed that incorporate value chain scale models. [153] A general equilibrium model within the P2P framework will allow the effects of economic and other macro-scale policies to be modeled and then propagated down to the scale at which design decisions are made. The policy can then be evaluated and designed based on the effects on decision makers at multiple scales.

This chapter presents several methods for incorporating economy scale equilibrium models into the P2P framework, with the following general objectives.

1. Model “top-down” effects of macro-economic events on decisions made at the value chain and equipment scales

2. Model “bottom-up” effects of value chain and equipment scale decisions on the surrounding economy

Section 8.2 describes how the effects of a macro-economic policy on value chain and equipment scale decisions can be captured in the P2P framework, and Section 8.3 applies this procedure to optimize an ethanol plant under several tax scenarios. Section 8.4 gives an overview of potential applications and insight obtainable from incorporating a partial equilibrium model into the P2P framework. Section 8.5 demonstrates a method for including fundamental engineering knowledge in nested production functions used in general equilibrium models. Section 8.6 applies the method of Section 8.5 to hybrid general equilibrium models and qualitatively develops an equilibrium-model-based version of the existing P2P framework.
8.2 Modeling short term effects of a macro-economic environmental tax policy

Choi, Bakshi and Haab [70] developed an input-output based procedure for modeling an economy in the short term after a macro-economic tax policy, specifically a carbon price, is implemented. This “pseudo-equilibrium” procedure models the tax as an economy-wide increase in value added and applies the Leontief cost-push model [209] to calculate endogenous changes in commodity prices. This price change and price elasticity of demand data are used to calculate the post-tax final demand vector, which is then used in the demand pull model (the standard input-output model of Section 2.3) to calculate the post-tax sector output vector and total environmental interventions for each sector. The result of the pseudo-equilibrium procedure is an EEIO model representing monetary exchanges within the economy, final demand by commodity and emissions by sector, immediately after the tax policy is implemented. The post-tax EEIO model generated by the procedure simply replaces the original pre-tax EEIO model in the P2P framework; no changes to the structure of the framework are necessary.

From the cost-push model, the pseudo-equilibrium procedure generates a vector of price changes for each commodity in the economy. These price changes, although endogenous to the economy scale, are assumed to be exogenous to the equipment and value chain scales, in that the smaller scales have no influence on the price change and can only adjust to the new prices. This is implemented in the P2P framework by using the vector of price changes to adjust the market prices of the equipment and value chain scale products to their post-tax level. The economy scale changes in commodity prices induced by the tax policy are thereby propagated to the smaller
scales, where they will influence any engineering decisions made based on economic criteria.

Tax induced changes in economy scale emissions are calculated in the pseudo-equilibrium procedure from price elasticity of demand and the demand-pull model. While emissions generated at the equipment and value chain scales are unaffected by the tax policy, the emissions associated with the production of value chain and equipment-economy upstream cutoffs may either increase or decrease. The changes in economy scale emissions are also expected to influence small scale engineering decisions, if decisions are made based on life cycle emissions or on a combination of life cycle emissions and economic criteria.

Incorporating the results of the pseudo-equilibrium procedure into the P2P framework thus allows the effect of macro-economic events to be modeled at the economy scale and, from there, propagated down to the scale at which engineering decisions are made. The insight gained by combining the pseudo-equilibrium procedure with the P2P framework can be used to design economic policies according to the desired effect on decisions made at the smaller scales. As an example, a carbon price, emissions tax or increase in the price of water can be modeled, and assuming that decision makers at the smaller scales will continue to behave optimally or in some predictable manner, the net economy-wide change in environmental impacts or other criteria can be calculated. This type of analysis will verify that environmental policies have the desired effect on industrial decision makers. Alternatively, the pseudo-equilibrium/P2P approach can be used as a form of risk management for decision makers at the smaller scales, by applying different macro-economic events and evaluating the feasibility and optimality of current decisions under the effects of the various events.
Despite its advantages, the pseudo-equilibrium procedure does not accomplish everything in terms of incorporating market effects into the P2P framework. Because the EEIO model upon which the procedure is based does not capture change over time, the implementation of an economic policy is modeled as a sudden price shock to the economy. The implementation of any new tax policy and especially an environmental tax policy is in reality likely to be anticipated well in advance. Producers will take preemptive action to minimize the risk of losing profits and customers, which could involve changes in the production technology or in the supply chain – neither of which can be modeled using the input-output based pseudo-equilibrium procedure. Instead, the only action allowable under the pseudo-equilibrium procedure is for producers in the economy to pass on 100\% of the tax-induced production cost increase to consumers of final demand, which is unlikely even in the event of a true unexpected price shock. Moreover, the pseudo-equilibrium procedure can only capture the top-down effects described in Section 8.1. Bottom-up effects, or the influence of smaller scale decisions on economy scale prices, activity and emissions, cannot be captured using the pseudo-equilibrium procedure. Section 8.6 presents an approach for accounting for such feedback loops.

8.2.1 Pseudo-equilibrium procedure

The discussion that follows is adapted from [70]. Figure 8.1 gives a diagram of the pseudo-equilibrium procedure and its integration into the P2P model. The original P2P model represents the status quo system before any policy is implemented. At this point, the price of economic commodities can be calculated from the cost-push
Figure 8.1: The pseudo-equilibrium procedure produces an EEIO model representing an economy after a tax policy is applied. This EEIO model is then incorporated into the P2P framework in place of the original pre-tax EEIO model. Adapted from Figure 1 in [70].
Leontief model as [209]

\[ \mathbf{p}_0 = \left( \mathbf{I} - \mathbf{A}_0^T \right)^{-1} \mathbf{v}_0 \]  
\[ (8.1) \]

in which \( \mathbf{p}_0 \) is the vector of commodity prices, \( \mathbf{A}_0 \) is the direct requirements matrix and \( \mathbf{v}_0 \) is the vector of value added. The subscript 0 indicates the pre-tax or status quo economy.

Suppose an exogenous change in value added \( \mathbf{C} \), which may represent a tax, technology subsidy, wage increase or other event, is imposed on the economy. The cost-push model can again be applied, using the new value added vector \( \mathbf{v}_0 + \mathbf{C} \), to calculate new commodity prices:

\[ \mathbf{p}_1 = \left( \mathbf{I} - \mathbf{A}_0^T \right)^{-1} (\mathbf{v}_0 + \mathbf{C}) \]  
\[ (8.2) \]

Note that, because the direct requirements matrix \( \mathbf{A}_0 \) has not changed, the assumption is that production technologies have not changed anywhere in the economy. The change in commodity prices is of primary interest in this procedure, and is also calculated from the cost-push model using the change in value added \( \Delta \mathbf{k}_1 \):

\[ \Delta \mathbf{p}_1^\% = \left( \mathbf{I} - \mathbf{A}_0^T \right)^{-1} \Delta \mathbf{k}_1 \]  
\[ (8.3) \]

in which \( \Delta \mathbf{k}_1 \) is calculated from \( \mathbf{v}_0 \) and \( \mathbf{C} \) as

\[ \Delta \mathbf{k}_1 = \mathbf{v}_0(\mathbf{x})^{-1} \Delta \mathbf{v}^\% = \mathbf{v}_0(\mathbf{x})^{-1} \mathbf{C} \mathbf{v}_0^{-1} \]  
\[ (8.4) \]

\( \Delta \mathbf{p}_1^\% \) and the pre-tax make and use matrices \( \mathbf{V}_0 \) and \( \mathbf{U}_0 \) are now used to calculate the post-tax make and use matrices, \( \mathbf{V}_1 \) and \( \mathbf{U}_1 \), as follows:

\[ \mathbf{U}_1 = \left( \mathbf{U}_0^T \left( \mathbf{I} + \hat{\mathbf{p}}_1^\% \right) \right)^T \]  
\[ (8.5) \]

\[ \mathbf{V}_1 = \mathbf{V}_0 \left( \mathbf{I} + \hat{\mathbf{p}}_1^\% \right) \]  
\[ (8.6) \]
The post-tax direct requirements matrix, $\overline{A}_1$, is calculated from $U_1$ and $V_1$ using Equation (2.30):

$$\overline{A}_1 = U_1 \left( V_1^T \right)^{-1} \quad (8.7)$$

Next, $\Delta \overline{p}_1^\%$ and price elasticity of demand data, $\overline{\epsilon}_d$, are combined to calculate the post-tax final demand. The price change is first applied to the original final demand vector $\overline{f}_0$ to calculate an interim final demand, $\overline{f}_{0.5}$:

$$\overline{f}_{0.5} = \left( I + \Delta \overline{p}_1^\% \right) \overline{f}_0 \quad (8.8)$$

The post-tax final demand $\overline{f}_1$ is then calculated from the interim final demand and price elasticity data, assuming that price elasticities are given as negative values:

$$\overline{f}_1 = \left( I + \overline{\epsilon}_d \Delta \overline{p}_1^\% \right) \overline{f}_{0.5} \quad (8.9)$$

Combining Equations (8.8) and (8.9) yields the complete equation for calculating post-tax final demand from pre-tax final demand:

$$\overline{f}_1 = \left( I + \overline{\epsilon}_d \Delta \overline{p}_1^\% \right) \left( I + \Delta \overline{p}_1^\% \right) \overline{f}_0 \quad (8.10)$$

Once the post-tax final demand is known, the demand-pull model is applied to calculate the post-tax sector output vector $\overline{x}_1$, from which the post-tax emissions information is calculated. $\overline{x}_1$ is calculated simply as

$$\overline{x}_1 = (I - \overline{A}_1)^{-1} \overline{f}_1 \quad (8.11)$$

where $\overline{A}_1$ is given in Equation (8.7) and $\overline{f}_1$ is given in Equation (8.10). Post-tax total emissions are calculated from $\overline{x}_1$ as

$$\overline{R}_1 = \overline{B}_1 \overline{x}_1 \quad (8.12)$$
where $\bar{B}_1$, the post-tax emissions factors, are calculated from $\Delta \bar{p}_1^{\%}$ and the pre-tax emissions factors $\bar{B}_0$ as

$$\bar{B}_1 = \bar{B}_0 \left( \mathbf{I} + \Delta \bar{p}_1^{\%} \right)^{-1} \quad (8.13)$$

Python code that implements the pseudo-equilibrium procedure is given in Appendix E.3.

### 8.2.2 Propagating economy scale effects to the value chain and equipment scales

Imposing $\mathcal{C}$ on the economy causes changes in product prices at the smaller scales as well as commodity price changes. Post-tax value chain and equipment scale product prices, $p_1$ and $p_1$, are approximated using the original prices and the element of $\Delta \bar{p}_1^{\%}$ that corresponds to each product’s parent commodity:

$$p_1 = p_0^T \left( \mathbf{I} + \Delta \bar{p}_1^{\%} \mathbf{P}_F \right) \quad (8.14)$$

$$p_1 = p_0^T \left( \mathbf{I} + \Delta \bar{p}_1^{\%} \mathbf{P}_E \right) \quad (8.15)$$

The product permutation matrices $\mathbf{P}_F$ and $\mathbf{P}_E$ are used to connect the economy scale price change information with the equipment and value chain scale product prices. In Equation (8.14) and (8.15), $\mathbf{I}$ and $\mathbf{I}$ are identity matrices with as many rows and columns as there are value chain scale products and equipment scale products, respectively.

A key assumption in Equations (8.14) and (8.15) is that the change in a commodity price at the economy scale is the same change in price that will be seen for individual products at the smaller scales. For instance, the $\Delta \bar{p}_1^{\%}$ for the commodity product of the Other basic organic chemical manufacturing is assumed to apply to, among other products, urea, fuel ethanol and glycerin. The validity of this assumption
is questionable at best, as the markets for the various products constituent to any
given commodity are likely to respond quite differently to a tax policy. This issue is
discussed further, and ways of altering the P2P/pseudo-equilibrium model to make
the price changes more accurate are proposed, in Section 9.2.5.

8.2.3 Incorporating the post-tax EEIO model into the P2P
framework

Equations (6.16), (6.17), (6.29) and (6.30) are now applied to disaggregate the
post-tax EEIO model. Equations (6.22) and (6.23) are applied if necessary to dis-ag-
aggregate the value chain model.

A P2P transactions matrix representing the post-tax system can now be stated as

\[
\mathbf{X}_1 = \begin{bmatrix}
I - \mathbf{A}_1^* & -\mathbf{X}_{1u} & -\mathbf{X}_{1u}^E \\
-\mathbf{A}_{1d} & \mathbf{X}^* & -\mathbf{X}_d^V \\
-\mathbf{A}_{1d}^E & -\mathbf{X}_d^V & \mathbf{X}
\end{bmatrix}
\]  

(8.16)

and a post-tax P2P interventions matrix as

\[
\mathbf{B}_1 = \begin{bmatrix}
\mathbf{B}_1^* & \mathbf{B}^* & \mathbf{B}
\end{bmatrix}
\]  

(8.17)

Dependence on the equipment scale variables \{z\} has been dropped from Equations
(8.16) and (8.17) for clarity. Matrices with a subscript 1 indicate that elements of that
matrix have been affected by the policy, either by the change in commodity prices,
the change in final demand or the change in sector output. Note that in Equation
(8.16), \(\mathbf{A}_1^*\) is a commodity-commodity direct requirements matrix; originally in [70],
the EEIO model used was industry-industry (sector-sector). \(\mathbf{X}_{1u}\) and \(\mathbf{X}_{1u}^E\) are affected
by the commodity price change, because the product prices used to convert physical
to monetary flows have been adjusted to reflect the new prices. \(\mathbf{A}_{1d}\) and \(\mathbf{A}_{1d}^E\) are
affected by the sector output change, because non-zero elements are normalized by
the total output of the disaggregated destination sectors, which is reflected in the $\mathbf{V}_1$. The total sector output after the price change and after disaggregation, $\mathbf{x}'_1$, normalizes the downstream cutoff flows. $\mathbf{B}_1'$ is affected by both the change in final demand, used to calculate post-tax total emissions, and the change in sector output, used to calculate post-tax emissions factors.

Optimization problems analogous to the SED problem presented in Section 6.4 can now be formulated using the post-tax P2P model. The economic objective function,

$$Z_s = Z (\{z\})$$

is unchanged in form from Section 6.4, but is now based on the post-tax market prices. Similarly, the environmental objective function is unchanged in form from Section 6.4:

$$Z_{\text{env},r} = \mathbf{s} \cdot \mathbf{b}_r (\{z\})$$

but is again based on post-tax environmental interventions data. The P2P product balance constraints for remain as

$$\begin{bmatrix} \mathbf{I} - \mathbf{A}_1^* (\{z\}) & -\mathbf{X}_{1u} (\{z\}) & -\mathbf{X}_{1u}^E (\{z\}) \\ -\mathbf{A}_{1d} (\{z\}) & \mathbf{X}^* (\{z\}) & -\mathbf{X}_{d}^V (\{z\}) \\ -\mathbf{A}_{1d}^E (\{z\}) & -\mathbf{X}_{d}^V (\{z\}) & \mathbf{X} (\{z\}) \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{s} \\ \mathbf{s} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_1 \\ \mathbf{f}_1 \end{bmatrix}$$

Finally, the fundamental equipment scale models are unchanged:

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

8.3 Corn ethanol plant design under a carbon dioxide emissions tax

The P2P/pseudo-equilibrium framework described in the previous section was combined with the corn ethanol plant model of Section 7.3, in order to optimize the
plant for (a) maximum revenue and (b) minimum life cycle CO₂ emissions under three tax scenarios. In the first scenario, no tax was applied and the P2P model was built from the pre-tax EEIO model and market prices. This is the “status quo” scenario. The second scenario, the “equipment scale tax” scenario, represents a conventional engineering approach to modeling an emissions tax. A $50 per short ton CO₂ tax is applied only to the ethanol plant itself as an additional cost of emitting. [42, 115, 187] The pre-tax EEIO model and market prices are used to build the P2P model, such that the only difference between the optimization formulations of the status quo and equipment scale tax scenarios is in the economic objective function. Finally, the third tax scenario, “economy scale tax,” involves the same $50 per short ton CO₂ emissions tax applied to the entire P2P system. Under this scenario, the P2P model is built with the post-tax EEIO model, economy scale emissions factors and prices. The ethanol plant has an additional cost of emitting under this scenario as well as under the equipment scale tax scenario. Both the economic and environmental objective functions change between the equipment scale and economy scale tax scenarios: the price change and cost of emitting affects all terms in the economic objective, and the post-tax economy scale emissions factors affect the environmental objective. The optimal plant designs are therefore expected to change, at least between the equipment and economy scale tax scenarios, for both the economic and environmental objective functions. Between the status quo and equipment scale tax scenarios, only the economically optimal design is expected to change and only then if the additional cost of emitting is sufficient to force the plant design to a new optimum. The environmentally optimal plant design is not expected to change between the status quo and
Table 8.1: Prices of ethanol plant inputs and outputs under the status quo scenario (pre-tax) and under the economy-scale tax scenario (post-tax).

<table>
<thead>
<tr>
<th>Input</th>
<th>Pre-tax price ($/kg or $/kJ)</th>
<th>Post-tax price ($/kg or $/kJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn grain</td>
<td>0.133</td>
<td>0.144</td>
</tr>
<tr>
<td>Natural gas</td>
<td>0.833</td>
<td>0.860</td>
</tr>
<tr>
<td>Coal</td>
<td>0.094</td>
<td>0.099</td>
</tr>
<tr>
<td>Electricity</td>
<td>0.072</td>
<td>0.107</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>3.324</td>
<td>3.587</td>
</tr>
<tr>
<td>α-amylase</td>
<td>3.324</td>
<td>3.587</td>
</tr>
<tr>
<td>Yeast</td>
<td>6.648</td>
<td>7.175</td>
</tr>
<tr>
<td>Urea</td>
<td>0.133</td>
<td>0.143</td>
</tr>
<tr>
<td>Corn grits</td>
<td>0.133</td>
<td>0.144</td>
</tr>
<tr>
<td>Water</td>
<td>$5.280 \times 10^{-6}$</td>
<td>$5.425 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Outputs</th>
<th>Pre-tax price ($/kg)</th>
<th>Post-tax price ($/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>0.750</td>
<td>0.813</td>
</tr>
<tr>
<td>DDGS</td>
<td>0.126</td>
<td>0.134</td>
</tr>
<tr>
<td>CO₂ (cost)</td>
<td>0.0</td>
<td>0.055</td>
</tr>
</tbody>
</table>

The optimization formulation of this case study is very similar to that of Section 7.3; the only major differences are the addition of economic objective functions, and the updating of the economy scale model from 2002 to 2007. In this case study, three economic objective functions are defined, each of which represents simple profits (excluding capital and fixed operating costs) under one tax scenario. Under the equipment scale tax scenarios, as the same P2P model and thus the same life cycle emissions are used under both scenarios.

8.3.1 Optimization formulation

The optimization formulation of this case study is very similar to that of Section 7.3; the only major differences are the addition of economic objective functions, and the updating of the economy scale model from 2002 to 2007. In this case study, three economic objective functions are defined, each of which represents simple profits (excluding capital and fixed operating costs) under one tax scenario. Under the
status quo tax scenario, in which there is no emissions tax at either the equipment or the economy scale, the profit objective function is based on the pre-tax market prices given in Table 8.1 and there is no additional cost of emitting. Under the equipment scale tax scenario, the profit objective function includes an additional cost of emitting equivalent to $0.055 per kg CO$_2$ but the prices remain at their pre-tax levels. Under the economy scale tax scenario, there is an additional cost of emitting and the emissions tax has caused prices of all the plant inputs and outputs to change; the profit objective function for this scenario is thus based on the post-tax market prices given in Table 8.1.

The environmental objective function, life cycle CO$_2$ emissions, is given in Equation (7.2) and did not change form under the different tax scenarios.

Price elasticity of demand data generated for the 2007 economy from the GTAP database [145] was used to implement the pseudo-equilibrium procedure. Because the elasticity data represented 2007, the 2002 EEIO model used in Section 7.3 was replaced with the 2007 benchmark input-output model of the US economy. [286] Emissions data for the 2007 economy was obtained from [39]. The pre-tax prices in Table 8.1 also represent 2007 levels; sources for pre-tax prices are given in Table 8.2. Where prices were not available at 2007 levels, producer price index data from the US Bureau of Labor Statistics was used to convert prices from other years to 2007. [287]
Table 8.2: Sources for pre-tax 2007 market prices.

<table>
<thead>
<tr>
<th>Product</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuels (all)</td>
<td>[5, 7–10]</td>
</tr>
<tr>
<td>Electricity</td>
<td>[2]</td>
</tr>
<tr>
<td>Fertilizer</td>
<td>[4]</td>
</tr>
<tr>
<td>Herbicide and insecticide (approx.)</td>
<td>[6]</td>
</tr>
<tr>
<td>Corn seed</td>
<td>[14]</td>
</tr>
<tr>
<td>Corn grits</td>
<td>[3]</td>
</tr>
<tr>
<td>α-amylase</td>
<td>[206]</td>
</tr>
<tr>
<td>Gluco-amylase</td>
<td>[206]</td>
</tr>
<tr>
<td>Yeast</td>
<td>[206]</td>
</tr>
<tr>
<td>Urea</td>
<td>[206]</td>
</tr>
<tr>
<td>Water (approx.)</td>
<td>[46]</td>
</tr>
</tbody>
</table>

8.3.2 Results and discussion

Optimizing for minimum life cycle CO$_2$ emissions and for maximum simple profits produced different optimal plant designs, shown in Table 8.3, but these two designs were unaffected by the three tax scenarios.

There are two potential reasons for the tax scenarios failing to influence the plant design. First, and most likely, is that combining the pseudo-equilibrium procedure with the P2P framework is not a flexible and accurate enough modeling strategy to capture the true effects of a macro-economic event. Several simplifying assumptions were necessary to apply the pseudo-equilibrium procedure, including the assumption of fixed production technologies at the economy scale and the assumption that price changes at the commodity level apply without alteration to all smaller scale products that belong to each commodity. In reality, even a relatively small magnitude emissions tax is likely to induce some changes in production technologies, and the
Table 8.3: Values of unit operation design variables for the economically and environmentally optimal plant designs under all three tax scenarios. Differences between the two designs are indicated in bold.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
<th>Optimal values</th>
<th>Minimum CO₂</th>
<th>Maximum Profit</th>
</tr>
</thead>
<tbody>
<tr>
<td>z₁</td>
<td>kg/s</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>z₂</td>
<td>kg/s</td>
<td>1.04</td>
<td>0.90</td>
<td></td>
</tr>
<tr>
<td>z₃</td>
<td>°C</td>
<td>120.0</td>
<td>300.0</td>
<td></td>
</tr>
<tr>
<td>z₄</td>
<td>kg/s</td>
<td>8.15</td>
<td>8.31</td>
<td></td>
</tr>
<tr>
<td>z₅</td>
<td>kg/s</td>
<td>0.086</td>
<td>0.086</td>
<td></td>
</tr>
<tr>
<td>z₆</td>
<td>°C</td>
<td>25.0</td>
<td>25.0</td>
<td></td>
</tr>
<tr>
<td>z₇</td>
<td>-</td>
<td>0.92</td>
<td>0.92</td>
<td></td>
</tr>
<tr>
<td>z₈</td>
<td>-</td>
<td>1.0</td>
<td>0.97</td>
<td></td>
</tr>
<tr>
<td>z₉</td>
<td>-</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>z₁₀</td>
<td>°C</td>
<td>94.6</td>
<td>94.6</td>
<td></td>
</tr>
<tr>
<td>z₁₁</td>
<td>-</td>
<td>0.20</td>
<td>0.20</td>
<td></td>
</tr>
<tr>
<td>z₁₂</td>
<td>-</td>
<td>0.14</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>z₁₃</td>
<td>-</td>
<td>0.37</td>
<td>0.37</td>
<td></td>
</tr>
<tr>
<td>z₁₄</td>
<td>-</td>
<td>0.001</td>
<td>0.001</td>
<td></td>
</tr>
<tr>
<td>z₁₅</td>
<td>-</td>
<td>0.08</td>
<td>0.08</td>
<td></td>
</tr>
</tbody>
</table>
Figure 8.2: The plant designs for minimum CO$_2$ emissions and for maximum simple profit were identical under all three tax scenarios, although the profit and emissions magnitudes were affected by the tax policies.

resulting changes in market prices are unlikely to be consistent for all products belonging to a particular commodity. The results of this case study indicate the need for incorporating more detailed and potentially more accurate economy scale models into the P2P framework, including the partial, general and hybrid equilibrium models discussed later in this chapter.

The second potential explanation for the results is that the emissions tax was of such a small magnitude that it could not affect the plant design. A sensitivity analysis comparing the effects of $100 and $150 per short ton CO$_2$ taxes is currently in progress, to test this theory.
8.4 Partial equilibrium models in process and supply chain design

Extending the existing P2P framework with the pseudo-equilibrium procedure allows top-down price effects to be captured, but does not allow for top-down quantity effects, for example changes in the available supply of inputs to the engineering system. Bottom-up effects also cannot be captured, due to the static nature of the pre- and post-tax EEIO models. While incorporating bottom-up price effects must be done using computable general equilibrium models at the economy scale (Section 8.6), a partial equilibrium (PE) model at the economy scale allows for top-down price and quantity effects and bottom-up quantity effects to be captured. This section focuses on adapting the P2P approach to incorporate PE models, while the next two sections discuss methods for combining the P2P approach with CGE models.

A P2P/PE modeling framework is expected to be most useful for the design and analysis of relatively small-scale engineering systems, particularly those that involve new production technologies. Due to the limited scope of PE models, they are not suitable for modeling and analyzing technologies expected to have a significant impact on the entire economy. Rather, the P2P/PE framework should be applied to problems analogous to supply chain design and analysis, where it is of interest to examine the interactions between the production technology implemented in the supply chain, and processes upstream (and potentially downstream) of that technology.

A previous study looked at an application of this type [296] by combining a PE model of forestry product sectors [173] (harvest, intermediate production and final production) with a simplified engineering scale model of a wood-to-2-methyltetrahydrofuran (MTHF) process. The objective was to capture interactions over time between the
forestry market and the wood-to-MTHF conversion process. Because the wood-to-
MTHF conversion process represented a new technology that was not previously
active in the economy, implementing the process increased feedstock demand and
affected prices and production levels throughout the PE model. The price of wood
feedstock to the wood-to-MTHF process was passed to the engineering scale model
and used to optimize the process’ net present value. Time dynamics of the system
were captured using discrete time periods, with each period involving new parame-
ters for the PE model. [173] The general procedure used in [296] is easily adaptable
to more detailed models at the engineering scale such as the process model used in
Section 7.3.

Another potential application of the P2P/PE modeling framework, not related
to engineering design, is consequential LCA. The P2P/PE framework is capable of
capturing changes at the engineering scale, changes at the economy scale (including a change in commodity supply, demand or price), and interactions between the
two scales. Assuming that the PE model used contains time dynamics, it is also
possible to capture different trajectories that the engineering-economic system takes
over time, either due to a different initial point or due to some change imposed at
a particular time step. Time dynamics and scale interaction effects are two insights
possible with the P2P/PE modeling framework that cannot be captured using the
existing P2P framework; the P2P/pseudo-equilibrium approach also cannot capture
time dynamics, and captures only top-down scale interactions due to price changes.
8.5 Incorporating engineering models into nested production functions

The Cobb-Douglas and CES production functions of Equations (2.35) and (2.37) were one-level production functions that related the proportions of various inputs to the production of one output. Each production function carries with it assumptions about how inputs can be combined to produce a particular output: for instance, the CES production function is based on the assumption that each pair of inputs can substitute for each other at the same rate. \[261\] For many production technologies, a single production function may not be able to represent the relationship between the various inputs with sufficient accuracy. Greater flexibility in modeling production technologies, and to some extent greater accuracy, can be achieved by nesting production functions for different inputs. \[251\]

The structure of a generic two-level nested production function for capital \(C\), labor \(L\) and energy \(E\) is

\[
X = f(C, L, E(C, L))
\]

Output \(X\) is then produced from all three inputs, and the energy input \(E\) also has a production function associated with it that describes how \(E\) is produced from capital and labor. Suppose that production of \(X\) can be represented with a CES production function, and production of \(E\) can be represented with a Cobb-Douglas production function. Then Equation (8.22) is re-stated as

\[
X = \left(\alpha_C^{1/\sigma} C^{(\sigma-1)/\sigma} + \alpha_L^{1/\sigma} L^{(\sigma-1)/\sigma} + \alpha_E^{1/\sigma} E(C, L)^{\alpha_{E,C} \sigma^{(\sigma-1)/\sigma}} + \alpha_{E,E}^{1/\sigma} E(C, L)^{\alpha_{E,E} \sigma^{(\sigma-1)/\sigma}}\right)^{\sigma/(\sigma-1)} \tag{8.23}
\]

\[
E(C, L) = A_E^{\alpha_{E,E}} C^{\alpha_{E,C}} L^{\alpha_{E,L}}
\]
The nesting of production functions is not limited to two levels, but can be done for as many levels as there are inputs with production functions.

Nested production functions are routinely used in equilibrium analysis for the reasons stated above. [289] An additional benefit of nesting production functions is that the resulting production technologies are modeled in greater detail than is possible with one-level production functions. Nested functions therefore allow for including several production technologies that produce the same output in an equilibrium model, and the choice between technologies is made as part of finding the equilibrium point. [51, 207]

Equation (8.23) combined a CES and a Cobb-Douglas production function, but it is also possible to nest Leontief production functions, either within a CES function, within a Cobb-Douglas function or as part of a multi-level production function that combines all three forms. A Leontief production function is stated as [86]

\[ X = \min(a_1Y_1, a_2Y_2, \ldots, a_NY_N) \] (8.24)

in which \( Y_i \) are inputs to the production of \( X \) and \( a_i \) are technical coefficients. The Leontief production function is the basis of input-output analysis and is also analogous to the input-output vectors used to represent life cycle processes and equipment scale processes in the P2P framework.

Using a Leontief production function as part of a multi-level production function creates an opportunity for integration with engineering models. As was done in the P2P framework, the exact form of the production function can be calculated from fundamental models at the unit operation level. Alternatively, the production function can be derived from plant level data, if detail at the unit operation level is not required. Integrating engineering and economic models in this fashion preserves
Figure 8.3: Nested production functions are used to model discrete choices between production technologies in hybrid equilibrium models. Adapted from Figures 1 and 2 in [233].

the mathematical properties of the nested (economic) production function that allows it to be utilized in a partial or general equilibrium model, while adding additional detail and increasing the accuracy of the function. Figures 8.3 and 8.4 illustrate the integration of engineering models with a nested production function.

8.6 Extending hybrid equilibrium models to the engineering scale

Top-down effects, such as the price change captured by the P2P/pseudo-equilibrium approach, are relatively straightforward to model and do not require significant modifications to the existing engineering and equilibrium models. Bottom-up quantity
Figure 8.4: If a technology can be modeled with a Leontief production function, then it can be linked to the P2P approach. Adapted from Figure 4 in [233].

effects, such as those discussed in Section 8.4, require a true equilibrium model but can still be captured without substantial changes to existing models. However, capturing bottom-up *price* effects, for instance commodity prices changes induced from the engineering scale up, require some adjustments to the equilibrium model assumptions. Producers in the economy are commonly assumed to be price-takers, implying that an individual producer (firm) has no control over commodity prices. Producers being price-takers also ties in with markets being perfectly competitive: in a perfectly competitive market, monopolies do not exist and no one producer has any control over market prices. To allow the engineering system to influence the economic system, the price-taker assumption must be relaxed at the engineering scale only, such that the engineering system is a price-setter and the economic system consists of price-takers.

In contrast to the existing P2P framework which includes both models in a single optimization problem, integrating engineering and equilibrium models is more efficiently accomplished using an iterative calculation procedure, as follows.

**Step 1** Calibrate equilibrium model to baseline prices and quantities.
• Optimize the engineering system for zero NPV under baseline prices for inputs.

• Find the selling price of the commodity produced by the engineering system, \( e \): This is the break-even price for the engineering system.

**Step 2** Treat the new selling price of commodity \( e \) as a price shock to the economy.

• Find the new equilibrium point, consisting of new production quantities for all commodities and new prices for all commodities except \( e \).

• Pass these prices to the engineering scale.

• Optimize the engineering system for zero NPV under these prices.

• Find new selling price of commodity \( e \).

**Step 3** Repeat Step 2 until convergence, at which the prices and production quantities of all commodities, including \( e \), are stable.

**Step 4** Update the equilibrium model with the new baseline data (final demand, production capacity, etc.) for the next time step.

**Step 5** Repeat Steps 1 - 3 for this time step.

**Step 6** Repeat Steps 4 - 5 for all time steps being simulated.

A similar procedure was used in [296], with a partial equilibrium model at the economy scale.

The research opportunities implied by integrating engineering and hybrid equilibrium models are many and varied. In general, because the level of detail in a typical CGE and hybrid equilibrium model is likely to be much less than in a typical IO model...
(on the order of dozens of sectors in CGE instead of hundreds in IO), the additional insight gained from using an equilibrium model is expected to be most significant for large scale engineering systems. Small case studies such as the corn ethanol plant of Section 7.3 are not expected to benefit significantly from the P2P/equilibrium approach: the feedback effects between the system and the economy will be quite small, and the lack of economy scale detail means that even the type of insight obtained using the existing P2P framework - namely, that increasing energy consumption and decreasing corn grits consumption was an environmentally optimal choice - may not be obtainable. Even if similar insights are gained, the increased effort required to complete a case study may outweigh the benefits for small scale problems.

The P2P/equilibrium approach allows for macro-economic policy modeling, and for policy design applications in which taxes, subsidies and regulations are imposed according to the effect they have on the combined engineering and economy scales. Similarly, production technologies and capacities modeled at the engineering scale can be chosen and developed over time while taking into account the macro-economic effects of such changes. Further applications are discussed in Section 9.2.6.
Chapter 9: Conclusions and future work

9.1 Conclusions

Sustainable design and assessment methods, regardless of the system to which they are applied, must incorporate a holistic perspective and must be theoretically sound. The holistic perspective is essential to identify and potentially prevent harmful externalities of the system of interest. Such externalities are not limited to environmental impacts, but may also be social, economic or technological impacts. All externalities, regardless of their exact nature, have the potential to cause feedback effects on the system of interest – in particular negative feedback effects. The combination of externalities and feedback effects, if not accounted for during the design process or as part of an assessment, can lead to decisions made within the system of interest having effects very different from what was intended. Decisions that appear optimal, for an economic, environmental or other criteria, become sub-optimal or even perverse when both externalities and feedback effects are taken into account.

One difficulty of accounting for externalities and the subsequent feedback effects, that may explain why they are so rarely accounted for in practice, is the increased complexity of the system under study. In design activities, taking a holistic perspective means considering a larger design problem with more decision variables and
potentially much greater uncertainty. Assessment activities are also complicated by a holistic perspective. These complexities are difficult to address using techniques developed within a single discipline: fundamental chemical engineering models are suited to represent physical processes, material properties and other relatively small-scale quantities, but are not well suited to represent the economic system within which a given chemical plant operates. Likewise, economic models can represent large-scale economic systems involving complex exchanges of goods, money, capital and labor, but cannot capture technological details at the supply chain and plant scales. Life cycle assessment, a modeling and assessment methodology developed specifically for holistic analyses, contains some technological details but reduces all processes to simple, linearized models. The ultimate conclusion is that, in order to address the additional complexity of sustainability-oriented design and assessment, modeling techniques from previously disparate disciplines must be integrated and applied to the same problem. By doing so, the various shortcomings of individual models are to a large extent mitigated by the combined strengths of the integrated approach.

This dissertation proposed two novel methodologies for sustainability assessment, both of which combined mathematical and statistical modeling techniques with life cycle assessment. Chapter 4 discussed the application of regression and model cross-validation to a streamlined LCA (SLCA) procedure. Whereas conventional SLCA procedures attempt to minimize the amount of inventory data to gather, regression streamlining is a method for extracting useful inventory information from data already gathered. The core concept is that, once inventory data is known for a set of products with similar characteristics, that data is used to build regression models for
predicting inventory information for other products with the same or similar characteristics. Using a statistical model-building technique provides not only quantitative streamlined inventory information for the new products, but also estimates of the error incurred by using the streamlined inventory rather than performing a full-scale LCA. Conventional SLCA methods can often provide quantitative streamlined inventories, but to date no other SLCA method provides streamlining error estimates as well.

The second sustainability assessment method presented in this dissertation addresses multi-functionality in life cycles. Multi-functionality is currently dealt with by using system expansion or partitioning allocation to remove technological and environmental flows attributable to the by-product(s) from the inventory. However, linear model theory provides the insight that calculating a life cycle inventory for a multi-functional life cycle is an ill-posed problem with infinite, equally valid solutions (inventories) that vary widely with allocation decisions. Applying partitioning allocation within a comparative LCA study has been shown to produce several sets of often contradictory results, in which the life cycle with the lowest impacts is determined not by inventory data but by the choice of allocation method: a situation in which the results are not robust to allocation. Chapter 5 presented the Comprehensive Allocation Investigation Strategy (CAIS), a method for calculating the multi-functional inventory as a function of allocation decisions and extracting useful information from that function. The CAIS can be used to detect robust and non-robust life cycle comparisons, and in the case that a comparison is not robust can be used to provide more detailed information on the effects of allocation decisions.
Another primary contribution of this dissertation is the “process-to-planet” (P2P) techno-economic modeling framework, which as presented in Chapter 6 integrates fundamental engineering models, standard process LCA models and an economic input-output model. The resulting model is both comprehensive, with a national scale analysis boundary, and detailed, with data and models at the process and unit operation levels. As shown in Chapter 7, the P2P framework within an optimization formulation can be applied to a variety of sustainable engineering design problems. The demonstration problem of Section 7.2 and the corn ethanol plant case study of Section 7.3 both showed that the more comprehensive analysis boundary of the P2P framework results in environmentally superior engineering designs, compared to conventional sustainable engineering design methods which rely on a narrower, process LCA-based analysis boundary. The framework is also general enough to be applied to life cycle assessment, including both attributional and consequential LCA; in this context, the P2P framework results in a life cycle model that is more comprehensive than process based LCA and more detailed than conventional hybrid LCA.

Because the P2P framework extends to the scale of macro-economic systems, it creates further opportunities for integrating engineering models with other, more flexible models at the economy scale, such as partial and computable general equilibrium problems. Chapter 8 discussed several methods for combining equilibrium models with the existing P2P framework. Such an integration creates a unique opportunity for modeling interactions between engineering and economic systems. Potential applications include, but are not limited to, determining the best new production technology to implement for a particular commodity, based on what effect that new
technology will have on the supply, demand and price of that and other commodi-
ties; designing a plant or supply chain under a carbon tax, subsidy or other macro-
economic change; and capturing the effects of large-scale shifts in technology such
as a shift from fossil-based to bio-based chemical feedstocks. In general, integrat-
ing equilibrium models with the P2P framework extends the potential applications
to not only bottom-up, engineering system-oriented design and assessment problems
but also top-down, economic policy-oriented problems.

9.2 Future work

9.2.1 Multi-functionality in life cycle inventories

The CAIS systematically parameterizes an allocated inventory and provides ex-
tensive information on the effects of allocation on the inventory, but it does not solve
the ill-posed allocation problem. A complete, mathematically valid solution to allo-
cation requires the addition of data external to the original inventories. The external
data is used to impose a new relationship or relationships between the variables $s$ and $w$, creating additional equations in Equation (2.1). Ideally, after incorporating exter-
nal data, the problem will no longer be under-determined and will have one unique
solution. Partitioning allocation relies on data from the original inventories and so
does not adequately solve the problem, as discussed in Section 5.3. Work is needed
on what type of external data is best and how to guarantee that the newly well-posed
problem will have a solution. One possibility is to use the method of Cherubini et al
[69] and derive partitioning weights from system expansion data, which is external to
the original life cycle. If the endless regression problem can be resolved, this may be
the most straightforward way to find a valid solution to the allocation problem.
Another issue to be addressed is how to compare life cycles that have few or no multi-functional processes in common. This situation can be addressed by treating inventory functions as constants over any allocation weights that do not appear in the function, as was done for corn stover gasification and the ethanol process allocation weight. Results of the CAIS can thereby be analyzed and interpreted just as they would be for life cycles that share a common allocation space.

Finally, additional work is also needed on ways of incorporating uncertainty in inventory data into the CAIS. With the addition of uncertainty information and particularly of probability distributions for inventory data, the differences between preferred products can be determined to be statistically significant or insignificant. Such information could be used to identify zones in allocation weight space in which products are statistically equivalent; these zones would be analogous to preference boundaries but could potentially cover a large portion of the possible weight combinations. For instance, consider a case where several processes have similar inventory functions. If confidence regions were calculated for each inventory function, it is possible that differences in the functions would not be statistically significant, in which case all processes would be equally preferred and allocation decisions would be irrelevant.

9.2.2 Boundary selection and aggregation in the P2P framework

The existing P2P framework removes some of the need for defining a specific analysis boundary, through its inclusion of a national-scale economy. However, there remain boundary decisions to be made in deciding which portions of the life cycle are modeled at the equipment and value chain scales, and which remain at the economy
scale. As shown in the corn ethanol case study of Section 7.3, choosing to model life cycle process at the value chain versus economy scales can have a significant impact on the optimal design. In the original P2P model of Section 7.3, the rule of thumb applied was that every life cycle process for which value chain scale data was available was modeled at the value chain: this results in a more detailed and specific model, but resulted in fewer upstream, indirect contributions from the economy scale being captured. Modeling more of the life cycle at the economy scale, as done in the alternative P2P model of Section 7.3, makes for a more comprehensive model that contains less detail and potentially contains much greater uncertainty. Some systematic method of deciding which stages to model in detail and which to capture using the EEIO model is needed. One possibility for developing such a method is adapting already established hybrid LCA methods for drawing the system boundary between the process analysis and EEIO portions of the life cycle. \[147\]

Another boundary and inventory data related issue is that of modeling the different production technologies in a given stage. In optimizing the life cycle, the design decisions must be based on differences in the production technologies themselves, not in any differences in the level of detail in individual technology models. For instance, if technology A has 20 inputs, only 14 of which are modeled, it may appear superior to technology B which also has 20 inputs, if all 20 of technology B’s outputs are included in the model. This may prove problematic when data from many different sources are used to model different technologies, as the level of detail and completeness will not necessarily be equivalent across all data sources.
9.2.3 Use of a global input-output model in the P2P framework

The existing P2P modeling framework, like conventional SED methods, does not account for the economic and environmental effects of international trade. Global supply chains, with manufacturing and processing stages located all over the world, have become extremely common. This gives rise to a situation in which one nation’s consumption results in another nation’s or, more likely, several other nation’s emissions. Neglecting such international interactions can lead to systematic under-representation of environmental interventions, as supply chain stages located outside the national boundary are not captured. Another consequence is inaccurate intervention accounting caused by products produced internationally, possibly using widely different production technology, being modeled as domestic purchases from domestic technology. [283]

Two options exist for expanding the P2P framework to a global model: incorporating a second economy scale that captures the “rest of world” (RoW) economy, and replacing the national economy scale model with a global multi-regional input-output model. Neither options requires alteration to the existing value chain and equipment scale models, save for the addition of upstream and downstream cutoff flows that connect to RoW sectors.

Incorporating a RoW economy model in addition to the domestic or national scale model is done as follows (dependence on equipment scale variables is not shown, for
Disaggregation is only necessary for the domestic economy model, unless there are system components at the value chain or equipment scales that are not part of the domestic economy. In quantifying upstream cutoffs that come from the RoW model ($X_u$, $X_{RoW}^u$ and $X_{RoW}^d$), the product prices used must reflect market prices in the nation(s) of origin rather than domestic purchase prices. [65]

The second option for the global P2P framework is replacing the national scale economy model with an environmentally-extended global multi-regional input-output (EE-GMRIO) model. Such models capture both international trade and the effects of globally variable technology and associated environmental interventions. [191] Each region in an EE-GMRIO represents either an individual nation or a block of nations, with blocks usually determined by geographic proximity. Commodity exchanges within each region (domestic exchanges) are represented with direct requirements sub-matrices arranged on the diagonal of the EE-GMRIO direct requirements matrix:

$$\overline{A}^W = \begin{bmatrix} \overline{A}_1 & \overline{A}_{12} & \overline{A}_{13} \\ \overline{A}_{21} & \overline{A}_2 & \overline{A}_{23} \\ \overline{A}_{31} & \overline{A}_{32} & \overline{A}_3 \end{bmatrix}$$

(9.2)

$\overline{A}_1$, $\overline{A}_2$ and $\overline{A}_3$ are the domestic direct requirements matrices, while $\overline{A}_{n_1,n_2}$ contain commodity flows from nation $n_1$ to $n_2$. $\overline{A}_{21}$, for instance, represents commodities that are exported by nation 2 to be imported by nation 1.
Assuming that $\overline{A}^W$ is available, it is incorporated into the P2P framework as follows.

$$
\overline{X}^W = \begin{bmatrix}
\mathbf{I}^W - \overline{A}^W & -X^W_u & -X^W_u \\
-A_d^W & \mathbf{X}^* & -X^V_u \\
-A_d^W & -A_d^V & \mathbf{X}
\end{bmatrix}
$$

(9.3)

As in Equation (9.1), disaggregation is not necessary for those regions of the EE-GMrio model representing nations other than the one in which the value chain and equipment scale components are located, and product prices for upstream cutoffs must be matched to the nation of origin for each product.

Extending the P2P framework to the global scale using input-output models is, methodologically speaking, a trivial exercise; however, due to the increased scope of the economy scale model, implementing the global P2P model is likely to be more of a challenge compared to the national P2P model. The amount of data required to build a RoW or EE-GMrio model is many times greater than for a national scale EEIO model, and the global models are likely to have higher uncertainty than national models because data must be aggregated from a variety of different sources with different formats and various degrees of reliability. Several EE-GMrio models have already been developed and verified. Details on several such models are given in Table 9.1.

Supply chain analysis involves modeling a pre-determined supply chain with a fixed structure and deducing information from the model, including the identification of environmental “hot spots,” or sources of intense pollution, in the supply chain. [23, 24] Applying the global P2P framework to supply chain analysis extends the supply chain to include contributions from other nations, allowing insight into how industrial activity in one nation causes both industrial activity and environmental
Table 9.1: Partial list of currently available EE-GMRIO models suitable for use in the P2P modeling framework (adapted from Table 1 in [282].)

<table>
<thead>
<tr>
<th>Model</th>
<th>No. of nations</th>
<th>Dimensions $(I \times J)$</th>
<th>Environmental data</th>
</tr>
</thead>
<tbody>
<tr>
<td>EXIOPOL [281]</td>
<td>43 + RoW</td>
<td>$120 \times 129$</td>
<td>Emissions, energy, resources</td>
</tr>
<tr>
<td>GTAP-MRIO [228]</td>
<td>129</td>
<td>$57 \times 57$</td>
<td>GWP, land use, energy</td>
</tr>
<tr>
<td>EORA [190]</td>
<td>150</td>
<td>20 - 500 (square)</td>
<td>Various</td>
</tr>
</tbody>
</table>

impacts in other nations. In addition, the EE-GMRIO model enables analysis of a system’s dependence on imported products; such dependence can be included in the P2P optimization problem either as a constraint (keep imported products below X% of total input flows) or as an objective (minimize total use of imported products).

### 9.2.4 Renewable energy production system design

The results of the renewable energy case study presented in Section 7.4 are still preliminary, and much work can still be done that will add value to the case study and to the general approach to energy systems design. Only work that is currently in progress or planned is discussed here.

One of the novel aspects of the case study was its inclusion of both ecosystem service demand, namely pollutant production, and ecosystem service supply, the capacity of agro- and other ecosystems to mitigate those pollutants. What remains to be done is to compare, in a quantitative manner, the results of the same design problem performed without considering ecosystem service supply with the results when both demand and supply are considered. In the case that ecosystem service supply is
not considered, the equivalent ecological objective function would simply be ecosystem service demand, which would be minimized to find the optimal design(s). It is expected that, when only ecosystem service demand is included in the objective function, the resulting designs will in fact be less sustainable (higher net environmental impacts) than when the balance between demand and supply is optimized. The effects on system net present value and total energy production are not as easy to predict, but it is expected that at least there will be different degrees of tradeoff between the three objective functions for the two sets of system designs.

Additional future work on this case study includes alterations and improvements to the model superstructure. The current model iteration does not treat by-product disposal as a decision variable. Biomass fast pyrolysis produces bio-char and ash as well as bio-oil, and biomass combustion produces ash in addition to electricity. The production of ash was neglected entirely in the current model, and bio-char was assumed to be combusted for electricity generation that was used to meet the pyrolysis plants’ parasitic energy generation. Bio-char can instead be sold as a soil amendment, and ash can be sold for use in building roads or as a soil amendment. Different end uses for the by-products have different economic and environmental characteristics. Bio-char combustion requires more capital and produces more direct emissions, but reduces production costs and provides revenue from electricity sales. On the other hand, selling the bio-char as a soil amendment also provides revenue, requires less capital up front, reduces direct emissions and potentially reduces life cycle emissions through displacement of chemical soil amendments. It is not obvious which by-product decision provides the most benefits, and it is extremely likely that the
disposal decision will change when the system is optimized under different objective functions.

Currently the planting of trees for carbon sequestration is modeled in a rather simplistic manner, with interactions between trees being neglected and the provisioning of ecosystem services in addition to CO₂ sequestration being neglected. In future iterations of the model, multiple services provided by forest ecosystem will be considered, with the first being air purification via NOₓ removal. By considering the provisioning of multiple ecosystem services, it will be possible to select an optimal mix of tree species rather than the single species selected in the current set of results. Reforesting with a mix of species will not only provide more benefits to the energy system, it is also a more ecologically sound strategy and will provide greater biodiversity and a better habitat for native wildlife. Additional future work on the reforestation modeling include accounting for and potentially designing for the provisioning of ecosystem services that do not directly benefit the energy system, such as soil erosion prevention and groundwater replenishment.

Finally, the case study in its current and future iterations is a highly multi-objective problem and should be analyzed with multi-objective optimization methods rather than the single-objective method used currently. The ϵ-constraint method will be applied to locate system designs that lie on the Pareto curve, which represent the best possible combinations of objective functions. Pareto designs cannot improve in one objective function without deteriorating in another. It was apparent even from the results in Section 7.4 that trade-offs exist between the various objective functions. Finding the Pareto curve will provide more insight into these trade-offs and potentially allow for a best-compromise production system design to be located.
9.2.5 Pseudo-equilibrium procedure and the P2P framework

As discussed in Section 8.3, a sensitivity analysis is currently in progress to test the effect of a higher magnitude emissions tax on equipment scale design decisions. However, the pseudo-equilibrium procedure, while informative when applied at the macro-economic scale, does not provide any more detailed information about the effects of economic events on smaller scales. A small amount of detail can be gained by applying the procedure to an EEIO model at the detailed, or most disaggregated, level, but the resulting commodity price changes will still be at a more aggregated level than is needed to accurately model price changes at either the value chain or the equipment scales. By modifying assumptions made within the post-tax model, it may be possible to capture the effects of the emissions tax in greater detail. This would involve applying a variant of the existing pseudo-equilibrium procedure at the value chain scale, thereby calculating price changes for value chain scale products specifically. The economy scale price changes would then be applied only to products modeled as upstream flows from the economy scale; the change in all other product prices would be calculated at a more detailed level.

9.2.6 Process to planet equilibrium modeling

Quantitative work on combining the P2P framework with partial and general equilibrium models remains to be done. This includes the development of a general, systematic methodology for building a P2P/equilibrium framework, much like the existing P2P framework methodology of Chapter 6. In addition to the mathematical development, code for implementing the P2P/equilibrium framework will be developed and demonstrated with application to a toy problem. The toy problem will also
serve as a proof of concept and a demonstration of the insight obtainable through this approach.

Eventually, the P2P/equilibrium framework will be applied to large scale engineering systems such as the ones examined in [101] and [314]. Using the same engineering scale models, the P2P/equilibrium framework will be used to connect the engineering scale with a hybrid equilibrium model, thereby capturing the feedback effects over time, as the supply chains are implemented and grow in capacity, and also in space, as the supply chains affect the local and national economy.
Appendix A: Emissions inventories for the iADs life cycle assessment

Tables A.1 and A.2 contain the emissions inventories calculated from openLCA. Tables A.3 and A.4 contain the emissions inventories calculated from Eco-LCA. For each emissions, the tiered hybrid inventory is equal to the sum of the process based and Eco-LCA inventories.
Table A.1: Process based emissions inventory for nine configurations of the iADs production system and three conventional products for comparison (1 of 2).

<table>
<thead>
<tr>
<th>End Product</th>
<th>Feedstock</th>
<th>kg CO₂</th>
<th>kg VOCs</th>
<th>kg CO</th>
<th>kg PM2.5</th>
<th>kg PM10</th>
<th>kg CH₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNG</td>
<td>Miscanthus</td>
<td>10.1833</td>
<td>5.8198×10⁻³</td>
<td>1.4275×10⁻¹</td>
<td>3.9237×10⁻⁴</td>
<td>4.9473×10⁻⁶</td>
<td>6.2695×10⁻³</td>
</tr>
<tr>
<td>CNG</td>
<td>Corn stover</td>
<td>5.6711</td>
<td>3.2215×10⁻³</td>
<td>7.9117×10⁻²</td>
<td>2.1854×10⁻⁴</td>
<td>4.5102×10⁻⁶</td>
<td>3.4754×10⁻³</td>
</tr>
<tr>
<td>CNG</td>
<td>Yard waste</td>
<td>10.3722</td>
<td>5.7885×10⁻⁶</td>
<td>1.4908×10⁻¹</td>
<td>4.0894×10⁻⁴</td>
<td>4.6272×10⁻⁶</td>
<td>6.4595×10⁻³</td>
</tr>
<tr>
<td>CNG</td>
<td>Fossil</td>
<td>163.4500</td>
<td>1.7787×10⁻²</td>
<td>5.3572×10⁻²</td>
<td>2.9753×10⁻²</td>
<td>5.0218×10⁻²</td>
<td>2.7722×10⁻¹</td>
</tr>
<tr>
<td>Electricity</td>
<td>Miscanthus</td>
<td>40.6829</td>
<td>2.3151×10⁻²</td>
<td>5.6876×10⁻¹</td>
<td>1.5567×10⁻³</td>
<td>9.5077×10⁻⁷</td>
<td>2.4871×10⁻²</td>
</tr>
<tr>
<td>Electricity</td>
<td>Corn stover</td>
<td>41.6284</td>
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<td>1.5927×10⁻³</td>
<td>9.7322×10⁻⁷</td>
<td>2.5397×10⁻²</td>
</tr>
<tr>
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<td>Yard waste</td>
<td>43.3975</td>
<td>2.4701×10⁻²</td>
<td>6.0756×10⁻¹</td>
<td>1.6609×10⁻³</td>
<td>1.0889×10⁻⁶</td>
<td>2.6233×10⁻²</td>
</tr>
<tr>
<td>Electricity</td>
<td>U.S. Grid</td>
<td>10.4170</td>
<td>1.0653×10⁻²</td>
<td>3.3857×10⁻²</td>
<td>1.1592×10⁻³</td>
<td>1.7061×10⁻³</td>
<td>2.6977×10⁻¹</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Miscanthus</td>
<td>0.0487</td>
<td>2.7881×10⁻⁵</td>
<td>6.8403×10⁻⁴</td>
<td>1.8825×10⁻⁶</td>
<td>3.3930×10⁻⁸</td>
<td>3.0081×10⁻⁵</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Corn stover</td>
<td>0.0487</td>
<td>2.7836×10⁻⁵</td>
<td>6.8374×10⁻⁴</td>
<td>1.8818×10⁻⁶</td>
<td>3.3930×10⁻⁸</td>
<td>3.0012×10⁻⁵</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Yard waste</td>
<td>0.0507</td>
<td>2.9061×10⁻⁵</td>
<td>7.1385×10⁻⁴</td>
<td>1.9620×10⁻⁶</td>
<td>3.3981×10⁻⁸</td>
<td>3.0994×10⁻⁵</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Soybean</td>
<td>-55.7686</td>
<td>2.2931×10⁻²</td>
<td>5.3939×10⁻²</td>
<td>3.5117×10⁻³</td>
<td>4.1894×10⁻³</td>
<td>3.3341×10⁻²</td>
</tr>
</tbody>
</table>
Table A.2: Process based emissions inventory for nine configurations of the iADs production system and three conventional products for comparison (2 of 2).

<table>
<thead>
<tr>
<th>End Product</th>
<th>Feedstock</th>
<th>kg NO&lt;sub&gt;x&lt;/sub&gt;</th>
<th>kg N&lt;sub&gt;2&lt;/sub&gt;O</th>
<th>kg SO&lt;sub&gt;x&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNG</td>
<td>Miscanthus</td>
<td>6.8298×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>2.1701×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>1.0997×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>CNG</td>
<td>Corn stover</td>
<td>3.7926×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>1.2024×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>6.7135×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
<tr>
<td>CNG</td>
<td>Yard waste</td>
<td>7.1183×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>2.2658×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>9.4214×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
<tr>
<td>CNG</td>
<td>Fossil</td>
<td>2.0458×10&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>2.5733×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>4.2235×10&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>Electricity</td>
<td>Miscanthus</td>
<td>2.7139×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>8.6411×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.5014×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>Electricity</td>
<td>Corn stover</td>
<td>2.7757×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>8.8451×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.3446×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>Electricity</td>
<td>Yard waste</td>
<td>2.8954×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>9.2349×10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>2.4256×10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>Electricity</td>
<td>U.S. Grid</td>
<td>4.5709×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>1.5430×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>2.1078×10&lt;sup&gt;-2&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Miscanthus</td>
<td>3.2741×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>1.0390×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>6.2466×10&lt;sup&gt;-7&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Corn stover</td>
<td>3.2720×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>1.0390×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>5.4712×10&lt;sup&gt;-7&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Yard waste</td>
<td>3.4126×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>1.0848×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>5.5216×10&lt;sup&gt;-7&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Soybean</td>
<td>4.3023×10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>6.0025×10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>3.2862×10&lt;sup&gt;-2&lt;/sup&gt;</td>
</tr>
</tbody>
</table>
Table A.3: EEIO emissions inventory, calculated using Eco-LCA, for nine configurations of the iADs production system and three conventional products for comparison (1 of 2). Eco-LCA does not calculate PM2.5 emissions, thus those values are marked nan.

<table>
<thead>
<tr>
<th>End Product</th>
<th>Feedstock</th>
<th>kg CO₂</th>
<th>kg VOCs</th>
<th>kg CO</th>
<th>kg PM2.5</th>
<th>kg PM10</th>
<th>kg CH₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNG</td>
<td>Miscanthus</td>
<td>4.9900 × 10⁻³</td>
<td>2.6200 × 10⁻⁵</td>
<td>1.4200 × 10⁻⁴</td>
<td>nan</td>
<td>1.8000 × 10⁻⁵</td>
<td>2.0700 × 10⁻⁵</td>
</tr>
<tr>
<td>CNG</td>
<td>Corn stover</td>
<td>2.7600 × 10⁻³</td>
<td>1.0100 × 10⁻⁵</td>
<td>4.8200 × 10⁻⁵</td>
<td>nan</td>
<td>5.5100 × 10⁻⁶</td>
<td>1.1000 × 10⁻⁵</td>
</tr>
<tr>
<td>CNG</td>
<td>Yard waste</td>
<td>1.6296 × 10⁻²</td>
<td>1.1944 × 10⁻⁵</td>
<td>5.0945 × 10⁻⁵</td>
<td>nan</td>
<td>5.0477 × 10⁻⁶</td>
<td>3.3895 × 10⁻⁵</td>
</tr>
<tr>
<td>CNG</td>
<td>Fossil</td>
<td>2.1420 × 10⁻⁴</td>
<td>1.1490 × 10⁻⁶</td>
<td>6.5910 × 10⁻⁷</td>
<td>nan</td>
<td>3.8980 × 10⁻⁸</td>
<td>6.1510 × 10⁻⁵</td>
</tr>
<tr>
<td>Electricity</td>
<td>Miscanthus</td>
<td>2.1304 × 10⁻²</td>
<td>1.1083 × 10⁻⁴</td>
<td>5.9162 × 10⁻⁴</td>
<td>nan</td>
<td>7.4639 × 10⁻⁵</td>
<td>8.8898 × 10⁻⁵</td>
</tr>
<tr>
<td>Electricity</td>
<td>Corn stover</td>
<td>2.2599 × 10⁻²</td>
<td>1.9310 × 10⁻⁴</td>
<td>1.5774 × 10⁻³</td>
<td>nan</td>
<td>1.9900 × 10⁻⁴</td>
<td>1.0774 × 10⁻⁴</td>
</tr>
<tr>
<td>Electricity</td>
<td>Yard waste</td>
<td>8.4052 × 10⁻²</td>
<td>5.9594 × 10⁻⁵</td>
<td>2.5685 × 10⁻⁴</td>
<td>nan</td>
<td>2.5625 × 10⁻⁵</td>
<td>1.7337 × 10⁻⁴</td>
</tr>
<tr>
<td>Electricity</td>
<td>U.S. Grid</td>
<td>7.0030 × 10⁻³</td>
<td>3.7570 × 10⁻⁵</td>
<td>2.1540 × 10⁻⁵</td>
<td>nan</td>
<td>1.2740 × 10⁻⁶</td>
<td>2.0100 × 10⁻³</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Miscanthus</td>
<td>5.9223 × 10⁻⁵</td>
<td>2.7279 × 10⁻⁷</td>
<td>9.9740 × 10⁻⁷</td>
<td>nan</td>
<td>1.3535 × 10⁻⁷</td>
<td>1.0346 × 10⁻⁶</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Corn stover</td>
<td>8.3572 × 10⁻⁴</td>
<td>3.1376 × 10⁻⁶</td>
<td>1.2510 × 10⁻⁵</td>
<td>nan</td>
<td>1.1458 × 10⁻⁶</td>
<td>3.3907 × 10⁻⁶</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Yard waste</td>
<td>8.5415 × 10⁻⁴</td>
<td>2.8749 × 10⁻⁶</td>
<td>9.3304 × 10⁻⁶</td>
<td>nan</td>
<td>7.1722 × 10⁻⁷</td>
<td>3.3945 × 10⁻⁶</td>
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<tr>
<td>Liquid HC fuel</td>
<td>Soybean</td>
<td>8.2080 × 10⁻³</td>
<td>4.4040 × 10⁻⁵</td>
<td>2.5250 × 10⁻⁵</td>
<td>nan</td>
<td>1.4930 × 10⁻⁶</td>
<td>2.3560 × 10⁻³</td>
</tr>
</tbody>
</table>
Table A.4: EEIO emissions inventory, calculated using Eco-LCA, for nine configurations of the iADs production system and three conventional products for comparison (2 of 2).

<table>
<thead>
<tr>
<th>End Product</th>
<th>Feedstock</th>
<th>kg NO&lt;sub&gt;x&lt;/sub&gt;</th>
<th>kg N&lt;sub&gt;2&lt;/sub&gt;O</th>
<th>kg SO&lt;sub&gt;x&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNG</td>
<td>Miscanthus</td>
<td>1.5100×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>4.8700×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>1.4900×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
<tr>
<td>CNG</td>
<td>Corn stover</td>
<td>1.2800×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>7.8200×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>7.8800×10&lt;sup&gt;-6&lt;/sup&gt;</td>
</tr>
<tr>
<td>CNG</td>
<td>Yard waste</td>
<td>2.1481×10&lt;sup&gt;-5&lt;/sup&gt;</td>
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</tr>
<tr>
<td>CNG</td>
<td>Fossil</td>
<td>3.1740×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>2.5030×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>3.9900×10&lt;sup&gt;-7&lt;/sup&gt;</td>
</tr>
<tr>
<td>Electricity</td>
<td>Miscanthus</td>
<td>6.6503×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>2.2606×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>6.3161×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
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<td>Corn stover</td>
<td>1.0493×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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</tr>
<tr>
<td>Electricity</td>
<td>Yard waste</td>
<td>1.0994×10&lt;sup&gt;-4&lt;/sup&gt;</td>
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</tr>
<tr>
<td>Electricity</td>
<td>U.S. Grid</td>
<td>1.0370×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>8.1830×10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>1.3040×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Miscanthus</td>
<td>1.3000×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>2.4293×10&lt;sup&gt;-8&lt;/sup&gt;</td>
<td>1.7773×10&lt;sup&gt;-7&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Corn stover</td>
<td>2.0515×10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>1.1570×10&lt;sup&gt;-7&lt;/sup&gt;</td>
<td>2.4105×10&lt;sup&gt;-6&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Yard waste</td>
<td>2.0172×10&lt;sup&gt;-6&lt;/sup&gt;</td>
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<td>2.4658×10&lt;sup&gt;-6&lt;/sup&gt;</td>
</tr>
<tr>
<td>Liquid HC fuel</td>
<td>Soybean</td>
<td>1.2160×10&lt;sup&gt;-5&lt;/sup&gt;</td>
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<td>1.5280×10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
</tbody>
</table>
Appendix B: Regression streamlining implementation and case study data

Both the packaging and material data sets and all R code files are available electronically from the author on request.

B.1 Packaging data set

Data set obtained from [109].
Table B.1: Data set used in packaging case study (1 of 4)

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<th>nox.atm</th>
<th>n2o.atm</th>
<th>hc.atm</th>
<th>sox.atm</th>
<th>co.atm</th>
<th>ch4.atm</th>
<th>co2.fossil.atm</th>
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</thead>
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<td>336.00</td>
<td>45.30</td>
<td>34417.00</td>
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<td>box</td>
<td>259.80</td>
<td>61.40</td>
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<td>226.00</td>
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<td>226.00</td>
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<td>257.00</td>
<td>335.00</td>
<td>37.70</td>
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<td>227.00</td>
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<td>34738.00</td>
</tr>
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<td>55.80</td>
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</tr>
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<td>102.00</td>
<td>296.00</td>
<td>261.00</td>
<td>57.80</td>
<td>44336.00</td>
</tr>
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B.2 Packaging case study R code

```r
## Read in data
packaging.data = as.data.frame(read.csv("packaging.csv",header=TRUE))
# attach(package.data)
library(gtools) ##Contains the "ask" function
library(calibrate) ## Need this library for the textxy function ##
library(cvTools) ##for MSPE calculation
library(quantreg) ## for LAD regression
library(lars) ## LASSO via LARS
library(pls) ## for PCR, PLSR
library(ggplot2) ## for plotting
library(GGally) #for scatterplot matrix
library(RColorBrewer)

# multiplot function from r-cookbook.com
multiplot <- function(..., plotlist=NULL, file, cols=1, layout=NULL) {
  require(grid)

  # Make a list from the ... arguments and plotlist
  plots <- c(list(...), plotlist)
  numPlots = length(plots)

  # If layout is NULL, then use 'cols' to determine layout
  if (is.null(layout)) {
    # Make the panel
    # ncol: Number of columns of plots
    # nrow: Number of rows needed, calculated from # of cols
    layout <- matrix(seq(1, cols * ceiling(numPlots/cols)),
                     ncol = cols, nrow = ceiling(numPlots/cols))
  }

  if (numPlots==1) {
    print(plots[[1]])
  } else {
    # Set up the page
    grid.newpage()
    pushViewport(viewport(layout = grid.layout(nrow(layout),
                                             ncol(layout))))

    # Make each plot, in the correct location
    ```
for (i in 1:numPlots) {
    # Get the i,j matrix positions of the regions that contain
    # this subplot
    matchidx <- as.data.frame(which(layout == i, arr.ind = TRUE))
    print(plots[[i]], vp = viewport(layout.pos.row = matchidx$\text{row}
        , layout.pos.col = matchidx$\text{col}\n    )
}
}

# Define function to calculate MSE normalized by variance of data
# for OLS models
mse.norm = function(aov.model, data) (sum(residuals(aov.model)^2)/
    aov.model$\text{df}/\text{var}(data)

package.data = data.frame(subset(packaging.data,
    select = c(total.energy,
        co2.total.atm, co.atm,
        ch4.atm, sox.atm, nox.atm,
        n2o.atm, hc.atm,
        particulates.atm,
        ammonia.atm, pb.atm,
        hg.atm, hg.wtr, cadm.wtr,
        dis.slds.wtr, sus.slds.wtr,
        cod.wtr, ccl4.atm,
        total.solid.waste)))

package.data.log = log(package.data)

package.data.plot = data.frame(CED = package.data$total.energy,
    CO2 = package.data$co2.total.atm,
    CO = package.data$co.atm,
    CH4 = package.data$ch4.atm,
    SOx = package.data$sox.atm,
    NOx= package.data$nox.atm,
    N2O = package.data$n2o.atm)

corr.matrix = ggpairs(package.data.plot, columns=1:4,
    params=list(corSize=6,labelSize=9))
corr.matrix.2 = ggpairs(package.data.plot, columns=c(1,5:7),
    params=list(corSize=6,labelSize=9))
a = ggplot(package.data.plot, aes(x=CED, y=CO2)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

b = ggplot(package.data.plot, aes(x=CED, y=CO)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

c = ggplot(package.data.plot, aes(x=CED, y=CH4)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

d = ggplot(package.data.plot, aes(x=CED, y=SOx)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

e = ggplot(package.data.plot, aes(x=CED, y=NOx)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

f = ggplot(package.data.plot, aes(x=CED, y=N2O)) +
geom_point(size=3) +
geom_smooth(method=lm, se=FALSE, lwd=1.3) +
theme(axis.text.x = element_text(size=14),
      axis.text.y = element_text(size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16))

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sampleregplot = multiplot(a,b,c)
sampleregplot.2 = multiplot(d,e,f)

ahist = ggplot(package.data.plot, aes(x=CED)) + geom_histogram() +
  xlab("CED") + ylab("Frequency") +
  theme(axis.text.x = element_text(size=14),
        axis.text.y = element_text(size=14),
        axis.title.x = element_text(colour="#990000", size=16),
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bhist = ggplot(package.data, aes(x=total.energy)) +
  geom_histogram() +
  xlab("CED") + ylab("Frequency") +
  theme(axis.text.x = element_text(size=14),
        axis.text.y = element_text(size=14),
        axis.title.x = element_text(colour="#990000", size=16),
        axis.title.y = element_text(colour="#990000", size=16))

co.mod = lm(co.atm ~ total.energy, data = package.data); 
co2.mod = lm(co2.total.atm ~ total.energy, data = package.data); 
ch4.mod = lm(ch4.atm ~ total.energy, data = package.data);

co.mod.log = lm(co.atm ~ total.energy, data = package.data.log); 
co2.mod.log = lm(co2.total.atm ~ total.energy, 
                data = package.data.log); 
ch4.mod.log = lm(ch4.atm ~ total.energy, data = package.data.log);

r.sq = data.frame(CO = summary(co.mod)$r.squared, 
                  CO2 = summary(co2.mod)$r.squared, 
                  CH4 = summary(ch4.mod)$r.squared)

r.sq.log = data.frame(CO = summary(co.mod.log)$r.squared, 
                      CO2 = summary(co2.mod.log)$r.squared, 
                      CH4 = summary(ch4.mod.log)$r.squared)

################

# Create vectors of all values to be bootstrapped ##
mse.train = data.frame(co.atm = rep(0,length(package.data[,1]))), 
                  co2.atm = rep(0,length(package.data[,1])), 
                  ch4.atm = rep(0,length(package.data[,1])), 
                  sox.atm = rep(0,length(package.data[,1])), 
                  nox.atm = rep(0,length(package.data[,1])), 
                  n2o.atm = rep(0,length(package.data[,1])), 
                  solid.waste = rep(0,length(package.data[,1])), 

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COD = rep(0,length(package.data[,1])),
dis.slds = rep(0,length(package.data[,1])),
sus.slds = rep(0,length(package.data[,1])),
parts = rep(0,length(package.data[,1])),
hc.atm = rep(0,length(package.data[,1])),
pb.atm = rep(0,length(package.data[,1])),
hg.atm = rep(0,length(package.data[,1])),
ccl4.atm = rep(0,length(package.data[,1])),
amm.atm = rep(0,length(package.data[,1])),
hg.wtr = rep(0,length(package.data[,1])),
cadm.wtr = rep(0,length(package.data[,1])))

pct.err.train = mse.train
pct.err.test = mse.train
mse.train.log = mse.train
pct.err.train.log = mse.train
pct.err.test.log = mse.train

## Perform leave-one-out cross-validation for models built using
## the specified predictor variable ##

for(i in 1:length(package.data[,1])) {
  training.data = package.data[-i,] ;
  testing.data = package.data[i,] ;

  ## Create a multitude of models ~ CED ##
  co.model = lm(co.atm ~ total.energy, data = training.data) ;
  co2.model = lm(co2.total.atm ~ total.energy,
               data = training.data) ;
  ch4.model = lm(ch4.atm ~ total.energy, data = training.data) ;
  sox.model = lm(sox.atm ~ total.energy, data = training.data) ;
  nox.model = lm(nox.atm ~ total.energy, data = training.data) ;
  n2o.model = lm(n2o.atm ~ total.energy, data = training.data) ;
  solid.waste.model = lm(total.solid.waste ~ total.energy,
                         data=training.data);
  COD.model = lm(cod.wtr ~ total.energy, data=training.data);
  dissolids.model = lm(dis.slds.wtr ~ total.energy,
                       data=training.data);
  sussolids.model = lm(sus.slds.wtr ~ total.energy,
                       data=training.data);
}

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particulates.model = lm(particulates.atm ~ total.energy,
               data=training.data);
hc.model = lm(hc.atm ~ total.energy, data=training.data);
pb.atm.model = lm(pb.atm ~ total.energy, data=training.data);
hg.atm.model = lm(hg.atm ~ total.energy, data=training.data);
ccl4.atm.model = lm(ccl4.atm ~ total.energy, data=training.data);
ammonia.atm.model = lm(ammonia.atm ~ total.energy,
               data=training.data);
hg.wtr.model = lm(hg.wtr ~ total.energy, data=training.data);
cadm.wtr.model = lm(cadm.wtr ~ total.energy, data=training.data);

## CO ~ CED ##
co.model.predicted.values.testing = co.model$coef[1] +
   testing.data$total.energy*co.model$coef[2];

## CO2 ~ CED ##
co2.model.predicted.values.testing = co.model$coef[1] +
   testing.data$total.energy*co2.model$coef[2];

## CH4 ~ CED ##
ch4.model.predicted.values.testing = ch4.model$coef[1] +
   testing.data$total.energy*ch4.model$coef[2];

## SOx ~ CED ##
sox.model.predicted.values.testing = sox.model$coef[1] +
   testing.data$total.energy*sox.model$coef[2];

## NOx ~ CED ##
nox.model.predicted.values.testing = nox.model$coef[1] +
   testing.data$total.energy*nox.model$coef[2];

## N2O ~ CED ##
n2o.model.predicted.values.testing = n2o.model$coef[1] +
   testing.data$total.energy*n2o.model$coef[2];

## Total solid waste ~ CED ##
solid.waste.model.predicted.values.testing =
   solid.waste.model$coef[1] +
   testing.data$total.energy*solid.waste.model$coef[2];

## COD ~ CED ##
COD.model.predicted.values.testing = COD.model$coef[1] +
   testing.data$total.energy*COD.model$coef[2];
## Dissolved solids ~ CED ##
dissolids.model.predicted.values.testing =
    dissolids.model$coef[1] +
    testing.data$total.energy*dissolids.model$coef[2];

## Suspended solids ~ CED ##
sussolids.model.predicted.values.testing =
    sussolids.model$coef[1] +
    testing.data$total.energy*sussolids.model$coef[2];

## Air particulates ~ CED ##
particulates.model.predicted.values.testing =
    particulates.model$coef[1] +
    testing.data$total.energy*particulates.model$coef[2];

## Hydrocarbons ~ CED ##
hc.model.predicted.values.testing = hc.model$coef[1] +
    testing.data$total.energy*hc.model$coef[2];

## Lead (atm) ~ CF ##
pb.atm.model.predicted.values.testing = pb.atm.model$coef[1] +
    testing.data$total.energy*pb.atm.model$coef[2];

## Mercury (atm) ~ CED ##
hg.atm.model.predicted.values.testing = hg.atm.model$coef[1] +
    testing.data$total.energy*hg.atm.model$coef[2];

## CCl4 (atm) ~ CED ##
ccl4.atm.model.predicted.values.testing = ccl4.atm.model$coef[1] +
    testing.data$total.energy*ccl4.atm.model$coef[2];

## Ammonia (atm) ~ CED ##
ammonia.atm.model.predicted.values.testing =
    ammonia.atm.model$coef[1] +
    testing.data$total.energy*ammonia.atm.model$coef[2];

## Mercury (wtr) ~ CED ## FLAG FOR CAUTION
hg.wtr.model.predicted.values.testing = hg.wtr.model$coef[1] +
    testing.data$total.energy*hg.wtr.model$coef[2];

## Cadmium (wtr) ~ CED ##
cadm.wtr.model.predicted.values.testing = cadm.wtr.model$coef[1] +
testing.data$total.energy*cadm.wtr.model$coef[2];

mse.train$co.atm[i] = mse.norm(co.model, training.data$co.atm);
pct.err.train$co.atm[i] = 100*sum(abs(training.data$co.atm - co.model$fitted)/training.data$co.atm)/25;
pct.err.test$co.atm[i] = 100*sum(abs(testing.data$co.atm - co.model.predicted.values.testing)/testing.data$co.atm);

mse.train$co2.atm[i] = mse.norm(co2.model, training.data$co2.total.atm);
pct.err.train$co2.atm[i] = 100*sum(abs(training.data$co2.total.atm - co2.model$fitted)/training.data$co2.total.atm)/25;
pct.err.test$co2.atm[i] = 100*sum(abs(testing.data$co2.total.atm - co2.model.predicted.values.testing)/testing.data$co2.total.atm);

mse.train$ch4.atm[i] = mse.norm(ch4.model, training.data$ch4.atm);
pct.err.train$ch4.atm[i] = 100*sum(abs(training.data$ch4.atm - ch4.model$fitted)/training.data$ch4.atm)/25;
pct.err.test$ch4.atm[i] = 100*sum(abs(testing.data$ch4.atm - ch4.model.predicted.values.testing)/testing.data$ch4.atm);

mse.train$sox.atm[i] = mse.norm(sox.model, training.data$sox.atm);
pct.err.train$sox.atm[i] = 100*sum(abs(training.data$sox.atm - sox.model$fitted)/training.data$sox.atm)/25;
pct.err.test$sox.atm[i] = 100*sum(abs(testing.data$sox.atm - sox.model.predicted.values.testing)/testing.data$sox.atm);

mse.train$nox.atm[i] = mse.norm(nox.model, training.data$nox.atm);
pct.err.train$nox.atm[i] = 100*sum(abs(training.data$nox.atm - nox.model$fitted)/training.data$nox.atm)/25;
pct.err.test$nox.atm[i] = 100*sum(abs(testing.data$nox.atm - nox.model.predicted.values.testing)/testing.data$nox.atm);

mse.train$n2o.atm[i] = mse.norm(n2o.model, training.data$n2o.atm);
pct.err.train$n2o.atm[i] = 100*sum(abs(training.data$n2o.atm - n2o.model$fitted)/training.data$n2o.atm)/25;
pct.err.test$n2o.atm[i] = 100*sum(abs(testing.data$n2o.atm - n2o.model.predicted.values.testing)/testing.data$n2o.atm);

mse.train$solid.waste[i] = mse.norm(solid.waste.model, training.data$total.solid.waste);
pct.err.train$solid.waste[i] = 100*sum(abs(
    training.data$total.solid.waste - solid.waste.model$fitted)/
    training.data$total.solid.waste)/25;
pct.err.test$solid.waste[i] = 100*sum(abs(
    testing.data$total.solid.waste -
    solid.waste.model.predicted.values.testing)/
    testing.data$total.solid.waste)/1;

mse.train$COD[i] = mse.norm(COD.model, training.data$cod.wtr);
pct.err.train$COD[i] = 100*sum(abs(training.data$cod.wtr -
    COD.model$fitted)/training.data$cod.wtr)/25;
pct.err.test$COD[i] = 100*sum(abs(testing.data$cod.wtr -
    COD.model.predicted.values.testing)/
    testing.data$cod.wtr)/1;

mse.train$dis.slds[i] = mse.norm(dissolids.model,
    training.data$dis.slds.wtr);
pct.err.train$dis.slds[i] = 100*sum(abs(
    training.data$dis.slds.wtr - dissolids.model$fitted)/
    training.data$dis.slds.wtr)/25;
pct.err.test$dis.slds[i] = 100*sum(abs(testing.data$dis.slds.wtr -
    dissolids.model.predicted.values.testing)/
    testing.data$dis.slds.wtr)/1;

mse.train$sus.slds[i] = mse.norm(sussolids.model,
    training.data$sus.slds.wtr);
pct.err.train$sus.slds[i] = 100*sum(abs(
    training.data$sus.slds.wtr - sussolids.model$fitted)/
    training.data$sus.slds.wtr)/25;
pct.err.test$sus.slds[i] = 100*sum(abs(testing.data$sus.slds.wtr -
    sussolids.model.predicted.values.testing)/
    testing.data$sus.slds.wtr)/1;

mse.train$parts[i] = mse.norm(particulates.model,
    training.data$particulates.atm);
pct.err.train$parts[i] = 100*sum(abs(
    training.data$particulates.atm - particulates.model$fitted)/
    training.data$particulates.atm)/25;
pct.err.test$parts[i] = 100*sum(abs(
    testing.data$particulates.atm -
    particulates.model.predicted.values.testing)/
    testing.data$particulates.atm)/1;

mse.train$hc.atm[i] = mse.norm(hc.model, training.data$hc.atm);
pct.err.train$hc.atm[i] = 100*sum(abs(
    training.data$hc.atm - hc.model$fitted)/
    training.data$hc.atm)/25;
pct.err.test$hc.atm[i] = 100*sum(abs(
    testing.data$hc.atm - hc.model.predicted.values.testing)/
    testing.data$hc.atm)/1;

mse.train$pb.atm[i] = mse.norm(pb.atm.model, training.data$pb.atm);
pct.err.train$pb.atm[i] = 100*sum(abs(
    training.data$pb.atm - pb.atm.model$fitted)/
    training.data$pb.atm)/25;
pct.err.test$pb.atm[i] = 100*sum(
    abs(testing.data$pb.atm -
        pb.atm.model.predicted.values.testing)/
    testing.data$pb.atm)/1;

mse.train$hg.atm[i] = mse.norm(hg.atm.model, training.data$hg.atm);
pct.err.train$hg.atm[i] = 100*sum(abs(
    training.data$hg.atm - hg.atm.model$fitted)/
    training.data$hg.atm)/25;
pct.err.test$hg.atm[i] = 100*sum(abs(
    testing.data$hg.atm - hg.atm.model.predicted.values.testing)/
    testing.data$hg.atm)/1;

mse.train$ccl4.atm[i] = mse.norm(ccl4.atm.model,
    training.data$ccl4.atm);
pct.err.train$ccl4.atm[i] = 100*sum(abs(
    training.data$ccl4.atm - ccl4.atm.model$fitted)/
    training.data$ccl4.atm)/25;
pct.err.test$ccl4.atm[i] = 100*sum(abs(
    testing.data$ccl4.atm - ccl4.atm.model.predicted.values.testing)/
    testing.data$ccl4.atm)/1;

mse.train$amm.atm[i] = mse.norm(ammonia.atm.model,
    training.data$ammonia.atm);
pct.err.train$amm.atm[i] = 100*sum(abs(
    training.data$ammonia.atm - ammonia.atm.model$fitted)/
    training.data$ammonia.atm)/25;
pct.err.test$amm.atm[i] = 100*sum(abs(
    testing.data$ammonia.atm - ammonia.atm.model.predicted.values.testing)/
    testing.data$ammonia.atm)/1;
mse.train$hg.wtr[i] = mse.norm(hg.wtr.model,
   training.data$hg.wtr);
pct.err.train$hg.wtr[i] = 100*sum(abs(
   training.data$hg.wtr - hg.wtr.model$fitted)/
   training.data$hg.wtr)/25;
pct.err.test$hg.wtr[i] = 100*sum(abs(
   testing.data$hg.wtr - hg.wtr.model.predicted.values.testing)/
   testing.data$hg.wtr)/1;

mse.train$cadm.wtr[i] = mse.norm(cadm.wtr.model,
   training.data$cadm.wtr);
pct.err.train$cadm.wtr[i] = 100*sum(abs(
   training.data$cadm.wtr - cadm.wtr.model$fitted)/
   training.data$cadm.wtr)/25;
pct.err.test$cadm.wtr[i] = 100*sum(abs(
   testing.data$cadm.wtr -
   cadm.wtr.model.predicted.values.testing)/
   testing.data$cadm.wtr)/1;

## Same calculations with the log transform
training.data.log = package.data.log[-i,] ;

## Create a multitude of models ~ log(CED) ##
co.model.log = lm(co.atm ~ total.energy,
   data = training.data.log) ;
co2.model.log = lm(co2.total.atm ~ total.energy,
   data = training.data.log) ;
ch4.model.log = lm(ch4.atm ~ total.energy,
   data = training.data.log) ;
sox.model.log = lm(sox.atm ~ total.energy,
   data = training.data.log) ;
nox.model.log = lm(nox.atm ~ total.energy,
   data = training.data.log) ;
n2o.model.log = lm(n2o.atm ~ total.energy,
   data = training.data.log) ;
solid.waste.model.log = lm(total.solid.waste ~ total.energy,
   data=training.data.log);
COD.model.log = lm(cod.wtr ~ total.energy,
   data=training.data.log);
dissolids.model.log = lm(dis.slds.wtr ~ total.energy,
   data=training.data.log);
sussolids.model.log = lm(sus.slds.wtr ~ total.energy,
particulates.model.log = lm(particulates.atm ~ total.energy,
data=training.data.log);

hc.model.log = lm(hc.atm ~ total.energy,
data=training.data.log);

pb.atm.model.log = lm(pb.atm ~ total.energy,
data=training.data.log);

hg.atm.model.log = lm(hg.atm ~ total.energy,
data=training.data.log);

ccl4.atm.model.log = lm(ccl4.atm ~ total.energy,
data=training.data.log);

ammonia.atm.model.log = lm(ammonia.atm ~ total.energy,
data=training.data.log);

hg.wtr.model.log = lm(hg.wtr ~ total.energy,
data=training.data.log);

cadm.wtr.model.log = lm(cadm.wtr ~ total.energy,
data=training.data.log);

## CO ~ CED ##
co.model.predicted.values.testing.log =
exp(co.model.log$coef[1])*
testing.data$total.energy^co.model.log$coef[2];

## CO2 ~ CED ##
co2.model.predicted.values.testing.log =
exp(co2.model.log$coef[1])*
testing.data$total.energy^co2.model.log$coef[2];

## CH4 ~ CED ##
ch4.model.predicted.values.testing.log =
exp(ch4.model.log$coef[1])*
testing.data$total.energy^ch4.model.log$coef[2];

## SOx ~ CED ##
sox.model.predicted.values.testing.log =
exp(sox.model.log$coef[1])*
testing.data$total.energy^sox.model.log$coef[2];

## NOx ~ CED ##
nox.model.predicted.values.testing.log =
exp(nox.model.log$coef[1])*
testing.data$total.energy^nox.model.log$coef[2];
## N2O ~ CED ##
n2o.model.predicted.values.testing.log =
\exp(n2o.model.log$coef[1])*
\text{testing.data$total.energy}^{n2o.model.log$coef[2]};

## Total solid waste ~ CED ##
solid.waste.model.predicted.values.testing.log =
\exp(solid.waste.model.log$coef[1])*
\text{testing.data$total.energy}^{solid.waste.model.log$coef[2]};

## COD ~ CED ##
COD.model.predicted.values.testing.log =
\exp(COD.model.log$coef[1])*
\text{testing.data$total.energy}^{COD.model.log$coef[2]};

## Dissolved solids ~ CED ##
dissolids.model.predicted.values.testing.log =
\exp(dissolids.model.log$coef[1])*
\text{testing.data$total.energy}^{dissolids.model.log$coef[2]};

## Suspended solids ~ CED ##
sussolids.model.predicted.values.testing.log =
\exp(sussolids.model.log$coef[1])*
\text{testing.data$total.energy}^{sussolids.model.log$coef[2]};

## Air particulates ~ CED ##
particulates.model.predicted.values.testing.log =
\exp(particulates.model.log$coef[1])*
\text{testing.data$total.energy}^{particulates.model.log$coef[2]};

## Hydrocarbons ~ CED ##
hc.model.predicted.values.testing.log =
\exp(hc.model.log$coef[1])*
\text{testing.data$total.energy}^{hc.model.log$coef[2]};

## Lead (atm) ~ CF ##
pb.atm.model.predicted.values.testing.log =
\exp(pb.atm.model.log$coef[1])*
\text{testing.data$total.energy}^{pb.atm.model.log$coef[2]};

## Mercury (atm) ~ CED ##
hg.atm.model.predicted.values.testing.log =
\exp(hg.atm.model.log$coef[1])*
\text{testing.data$total.energy}^{hg.atm.model.log$coef[2]};
testing.data$total.energy^hg.atm.model.log$coef[2];

## CCl4 (atm) ~ CED ##
ccl4.atm.model.predicted.values.testing.log =
exp(ccl4.atm.model.log$coef[1])*testing.data$total.energy^ccl4.atm.model.log$coef[2];

## Ammonia (atm) ~ CED ##
ammonia.atm.model.predicted.values.testing.log =
exp(ammonia.atm.model.log$coef[1])*testing.data$total.energy^ammonia.atm.model.log$coef[2];

## Mercury (wtr) ~ CED ##  FLAG FOR CAUTION
hg.wtr.model.predicted.values.testing.log =
exp(hg.wtr.model.log$coef[1])*testing.data$total.energy^hg.wtr.model.log$coef[2];

## Cadmium (wtr) ~ CED ##
cadm.wtr.model.predicted.values.testing.log =
exp(cadm.wtr.model.log$coef[1])*testing.data$total.energy^cadm.wtr.model.log$coef[2];

mse.train.log$co.atm[i] = mse.norm(co.model.log,
    training.data.log$co.atm);
pct.err.train.log$co.atm[i] = 100*sum(abs(
    training.data$co.atm - exp(co.model.log$fitted))/
    training.data$co.atm)/25;
pct.err.test.log$co.atm[i] = 100*sum(abs(
    testing.data$co.atm - co.model.predicted.values.testing.log)/
    testing.data$co.atm);

mse.train.log$co2.atm[i] = mse.norm(co2.model.log,
    training.data.log$co2.total.atm);
pct.err.train.log$co2.atm[i] = 100*sum(abs(
    training.data$co2.total.atm - exp(co2.model.log$fitted))/
    training.data$co2.total.atm)/25;
pct.err.test.log$co2.atm[i] = 100*sum(abs(
    testing.data$co2.total.atm -
    co2.model.predicted.values.testing.log)/
    testing.data$co2.total.atm);

mse.train.log$ch4.atm[i] = mse.norm(ch4.model.log,
    training.data.log$ch4.atm);
pct.err.train.log$ch4.atm[i] = 100*sum(abs(
    training.data$ch4.atm - exp(ch4.model.log$fitted))/
    training.data$ch4.atm)/25;
pct.err.test.log$ch4.atm[i] = 100*sum(abs(
    testing.data$ch4.atm - ch4.model.predicted.values.testing.log)/
    testing.data$ch4.atm);

mse.train.log$sox.atm[i] = mse.norm(sox.model.log,
    training.data.log$sox.atm);
pct.err.train.log$sox.atm[i] = 100*sum(abs(
    training.data$sox.atm - exp(sox.model.log$fitted))/
    training.data$sox.atm)/25;
pct.err.test.log$sox.atm[i] = 100*sum(abs(
    testing.data$sox.atm - sox.model.predicted.values.testing.log)/
    testing.data$sox.atm);

mse.train.log$nox.atm[i] = mse.norm(nox.model.log,
    training.data.log$nox.atm);
pct.err.train.log$nox.atm[i] = 100*sum(abs(
    training.data$nox.atm - exp(nox.model.log$fitted))/
    training.data$nox.atm)/25;
pct.err.test.log$nox.atm[i] = 100*sum(abs(
    testing.data$nox.atm - nox.model.predicted.values.testing.log)/
    testing.data$nox.atm);

mse.train.log$n2o.atm[i] = mse.norm(n2o.model.log,
    training.data.log$n2o.atm);
pct.err.train.log$n2o.atm[i] = 100*sum(abs(
    training.data$n2o.atm - exp(n2o.model.log$fitted))/
    training.data$n2o.atm)/25;
pct.err.test.log$n2o.atm[i] = 100*sum(abs(
    testing.data$n2o.atm - n2o.model.predicted.values.testing.log)/
    testing.data$n2o.atm);

mse.train.log$solid.waste[i] = mse.norm(solid.waste.model.log,
    training.data.log$total.solid.waste);
pct.err.train.log$solid.waste[i] = 100*sum(abs(
    training.data$total.solid.waste - exp(solid.waste.model.log$fitted))/
    training.data$total.solid.waste)/25;
pct.err.test.log$solid.waste[i] = 100*sum(abs(
    testing.data$total.solid.waste - solid.waste.model.predicted.values.testing.log)/
    testing.data$total.solid.waste);
testing.data$total.solid.waste)/1;

mse.train.log$COD[i] = mse.norm(COD.model.log, 
                        training.data.log$cod.wtr);

pct.err.train.log$COD[i] = 100*sum(abs(
   training.data$cod.wtr - exp(COD.model.log$fitted))/
   training.data$cod.wtr)/25;

pct.err.test.log$COD[i] = 100*sum(abs(
   testing.data$cod.wtr - COD.model.predicted.values.testing.log)/
   testing.data$cod.wtr)/1;

mse.train.log$dis.slds[i] = mse.norm(dissolids.model.log, 
                        training.data.log$dis.slds.wtr);

pct.err.train.log$dis.slds[i] = 100*sum(abs(
   training.data$dis.slds.wtr - exp(dissolids.model.log$fitted))/
   training.data$dis.slds.wtr)/25;

pct.err.test.log$dis.slds[i] = 100*sum(abs(
   testing.data$dis.slds.wtr - 
   dissolids.model.predicted.values.testing.log)/
   testing.data$dis.slds.wtr)/1;

mse.train.log$sus.slds[i] = mse.norm(sussolids.model.log, 
                        training.data.log$sus.slds.wtr);

pct.err.train.log$sus.slds[i] = 100*sum(abs(
   training.data$sus.slds.wtr - exp(sussolids.model.log$fitted))/
   training.data$sus.slds.wtr)/25;

pct.err.test.log$sus.slds[i] = 100*sum(abs(
   testing.data$sus.slds.wtr - 
   sussolids.model.predicted.values.testing.log)/
   testing.data$sus.slds.wtr)/1;

mse.train.log$parts[i] = mse.norm(particulates.model.log, 
                        training.data.log$particulates.atm);

pct.err.train.log$parts[i] = 100*sum(abs(
   training.data$particulates.atm - 
   exp(particulates.model.log$fitted))/
   training.data$particulates.atm)/25;

pct.err.test.log$parts[i] = 100*sum(abs(
   testing.data$particulates.atm - 
   particulates.model.predicted.values.testing.log)/
   testing.data$particulates.atm)/1;

mse.train.log$hc.atm[i] = mse.norm(hc.model.log,
pct.err.train.log$hc.atm[i] = 100*sum(abs(
    training.data$hc.atm - exp(hc.model.log$fitted))/
    training.data$hc.atm)/25;

pct.err.test.log$hc.atm[i] = 100*sum(abs(
    testing.data$hc.atm - hc.model.predicted.values.testing.log)/
    testing.data$hc.atm)/1;

mse.train.log$pb.atm[i] = mse.norm(pb.atm.model.log,
    training.data.log$pb.atm);

pct.err.train.log$pb.atm[i] = 100*sum(abs(
    training.data$pb.atm - exp(pb.atm.model.log$fitted))/
    training.data$pb.atm)/25;

pct.err.test.log$pb.atm[i] = 100*sum(abs(
    testing.data$pb.atm - pb.atm.model.predicted.values.testing.log)/
    testing.data$pb.atm)/1;

mse.train.log$hg.atm[i] = mse.norm(hg.atm.model.log,
    training.data.log$hg.atm);

pct.err.train.log$hg.atm[i] = 100*sum(abs(
    training.data$hg.atm - exp(hg.atm.model.log$fitted))/
    training.data$hg.atm)/25;

pct.err.test.log$hg.atm[i] = 100*sum(abs(
    testing.data$hg.atm -
    hg.atm.model.predicted.values.testing.log)/
    testing.data$hg.atm)/1;

mse.train.log$ccl4.atm[i] = mse.norm(ccl4.atm.model.log,
    training.data.log$ccl4.atm);

pct.err.train.log$ccl4.atm[i] = 100*sum(abs(
    training.data$ccl4.atm - exp(ccl4.atm.model.log$fitted))/
    training.data$ccl4.atm)/25;

pct.err.test.log$ccl4.atm[i] = 100*sum(abs(
    testing.data$ccl4.atm -
    ccl4.atm.model.predicted.values.testing.log)/
    testing.data$ccl4.atm)/1;

mse.train.log$amm.atm[i] = mse.norm(ammonia.atm.model.log,
    training.data.log$ammonia.atm);

pct.err.train.log$amm.atm[i] = 100*sum(abs(
    training.data$ammonia.atm - exp(ammonia.atm.model.log$fitted))/
    training.data$ammonia.atm)/25;

pct.err.test.log$amm.atm[i] = 100*sum(abs(
    testing.data$ammonia.atm -
    ammonia.atm.model.predicted.values.testing.log)/
    training.data$ammonia.atm)/25;
pct.err.test.log$amm.atm[i] = 100*sum(abs(
    testing.data$ammonia.atm -
    ammonia.atm.model.predicted.values.testing.log)/
    testing.data$ammonia.atm)/1;

mse.train.log$hg.wtr[i] = mse.norm(hg.wtr.model.log,
    training.data.log$hg.wtr);

pct.err.train.log$hg.wtr[i] = 100*sum(abs(
    training.data$hg.wtr -
    exp(hg.wtr.model.log$fitted))/
    training.data$hg.wtr)/25;

pct.err.test.log$hg.wtr[i] = 100*sum(abs(
    testing.data$hg.wtr -
    hg.wtr.model.predicted.values.testing.log)/
    testing.data$hg.wtr)/1;

mse.train.log$cadm.wtr[i] = mse.norm(cadm.wtr.model.log,
    training.data.log$cadm.wtr);

pct.err.train.log$cadm.wtr[i] = 100*sum(abs(
    training.data$cadm.wtr - exp(cadm.wtr.model.log$fitted))/
    training.data$cadm.wtr)/25;

pct.err.test.log$cadm.wtr[i] = 100*sum(abs(
    testing.data$cadm.wtr -
    cadm.wtr.model.predicted.values.testing.log)/
    testing.data$cadm.wtr)/1;

}  
## Loop ends ##

# ANALYSIS OF BOOTSTRAP MODEL BUILDING 
# & VALIDATION
train = data.frame(Data = c(rep("Untransformed",
    length(package.data[1,])-1),
    rep("Transformed",
    length(package.data[1,])-1)),
    mse.mean = c(apply(mse.train, 2, mean),
    apply(mse.train.log, 2, mean)),
    mse.sd = c(apply(mse.train, 2, sd),
    apply(mse.train.log, 2, sd)),
    mse.med = c(apply(mse.train,2,median),
    apply(mse.train.log,2,median)),
    mse.q.25 = c(apply(mse.train,2,quantile,prob=0.25),
    apply(mse.train.log,2,quantile,prob=0.25)),

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mse.q.975 = c(apply(mse.train, 2, quantile, prob=0.75),
apply(mse.train.log, 2, quantile, prob=0.75)),
pct.err.mean = c(apply(pct.err.train, 2, mean),
apply(pct.err.train.log, 2, mean)),
pct.err.sd = c(apply(pct.err.train, 2, sd),
apply(pct.err.train.log, 2, sd)),
pct.err.med = c(apply(pct.err.train, 2, median),
apply(pct.err.train.log, 2, median)),
pct.err.q.25 = c(apply(pct.err.train, 2, quantile, prob=0.25),
apply(pct.err.train.log, 2, quantile, prob=0.25)),
pct.err.q.975 = c(apply(pct.err.train, 2, quantile, prob=0.75),
apply(pct.err.train.log, 2, quantile, prob=0.75)))

names = rep(names(mse.train), 2)

test = data.frame(Data = c(rep("Untransformed",
length(package.data[,1])-1),
rep("Transformed",
length(package.data[,1])-1)),
pct.err.mean = c(apply(pct.err.test, 2, mean),
apply(pct.err.test.log, 2, mean)),
pct.err.sd = c(apply(pct.err.test, 2, sd),
apply(pct.err.test.log, 2, sd)),
pct.err.med = c(apply(pct.err.test, 2, median),
apply(pct.err.test.log, 2, median)),
pct.err.q.25 = c(apply(pct.err.test, 2, quantile, prob=0.25),
apply(pct.err.test.log, 2, quantile, prob=0.25)),
pct.err.q.975 = c(apply(pct.err.test, 2, quantile, prob=0.75),
apply(pct.err.test.log, 2, quantile, prob=0.75)))

## MSE plot - median, 2.5% and 97.5% quantiles - training data
dodge = position_dodge(width=0.9)
mse.q = ggplot(train, aes(x=names, y=mse.med, fill=Data)) +

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```r
geom_bar(stat='identity', position=dodge) +
geom_errorbar(aes(ymin=mse.q.25, ymax=mse.q.975), width=.25,
position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("Normalized MSE") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
axis.title.x = element_text(colour="#990000", size=16),
axis.title.y = element_text(colour="#990000", size=16),
legend.title = element_text(colour="#990000", size = 14),
legend.background = element_rect(fill="gray90", size=.5))

## % error plot - median, 2.5% and 97.5% quantiles - training data
pct.err.train.q = ggplot(train, aes(x=names, y=pmin(pct.err.med,75),
fill=Data)) +
geom_bar(stat='identity', position=dodge) +
geom_errorbar(aes(ymin=pct.err.q.25, ymax=pmin(pct.err.q.975,75)),
width=0.25, position=dodge) +
ylim(0,75) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
axis.title.x = element_text(colour="#990000", size=16),
axis.title.y = element_text(colour="#990000", size=16),
legend.title = element_text(colour="#990000", size = 14),
legend.background = element_rect(fill="gray90", size=.5))

## % error plot - median, 2.5% and 97.5% quantiles - training data
pct.err.train.mean = ggplot(train, aes(x=names, y=pct.err.mean,
fill=Data)) +
geom_bar(stat='identity', position=dodge) +
geom_errorbar(aes(ymin=pmax(rep(0,36),pct.err.mean - pct.err.sd),
ymax=pmin(pct.err.mean + pct.err.sd, rep(200,36))), width=0.25,
position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylim(0,200) +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
axis.title.x = element_text(colour="#990000", size=16),
axis.title.y = element_text(colour="#990000", size=16),
```
## % error plot - median, 2.5% and 97.5% quantiles - testing data
pct.err.test.q = ggplot(test, aes(x=names, y=pct.err.med, fill=Data)) +
geom_bar(stat='identity', position=dodge) +
ylim(0,75) +
geom_errorbar(aes(ymin=pct.err.q.25,
                   ymax=pmin(pct.err.q.975,75)),
              width=0.25, position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16),
      legend.title = element_text(colour="#990000", size = 14),
      legend.background = element_rect(fill="gray90", size=.5))

## % error plot - mean +/- 1 sd - testing data
pct.err.test.mean = ggplot(test, aes(x=names, y=pct.err.mean, fill=Data)) +
geom_bar(stat='identity', position=dodge) +
ylim(0,200) +
geom_errorbar(aes(ymin=pmax(rep(0,36),
                   pct.err.mean - pct.err.sd),
               ymax=pmin(pct.err.mean + pct.err.sd,
                      rep(200,36))), width=0.25,
            position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16),
      legend.title = element_text(colour="#990000", size = 14),
      legend.background = element_rect(fill="gray90", size=.5))
B.3 Materials data set

Data set is taken from [246].
Table B.5: Data set used in materials case study (1 of 2)

<table>
<thead>
<tr>
<th>material.num</th>
<th>material.name</th>
<th>material.class</th>
<th>prim.energy</th>
<th>co2.atm</th>
<th>nox.atm</th>
<th>sox.atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>nonferrous.8</td>
<td>metal</td>
<td>375</td>
<td>20</td>
<td>10</td>
<td>658</td>
</tr>
<tr>
<td>2</td>
<td>nonferrous.5</td>
<td>metal</td>
<td>171</td>
<td>10</td>
<td>20</td>
<td>65</td>
</tr>
<tr>
<td>3</td>
<td>ferrous.ni.g5</td>
<td>metal</td>
<td>65</td>
<td>4.1</td>
<td>3</td>
<td>152</td>
</tr>
<tr>
<td>4</td>
<td>ferrous.ni.l5</td>
<td>metal</td>
<td>28</td>
<td>1.5</td>
<td>4.4</td>
<td>26</td>
</tr>
<tr>
<td>5</td>
<td>ferrous.ni.0</td>
<td>metal</td>
<td>27</td>
<td>1.3</td>
<td>4.4</td>
<td>9.5</td>
</tr>
<tr>
<td>6</td>
<td>composites</td>
<td>composites</td>
<td>200</td>
<td>12</td>
<td>36</td>
<td>23</td>
</tr>
<tr>
<td>7</td>
<td>glasses</td>
<td>glasses</td>
<td>13</td>
<td>0.76</td>
<td>2.3</td>
<td>2.3</td>
</tr>
<tr>
<td>8</td>
<td>por.ceramics</td>
<td>por.ceramics</td>
<td>5.8</td>
<td>0.41</td>
<td>1.5</td>
<td>0.94</td>
</tr>
<tr>
<td>9</td>
<td>thermo.epoxy</td>
<td>polymers</td>
<td>180</td>
<td>3.5</td>
<td>26</td>
<td>11</td>
</tr>
<tr>
<td>10</td>
<td>thermoplastics</td>
<td>polymers</td>
<td>80</td>
<td>3.3</td>
<td>16</td>
<td>18</td>
</tr>
<tr>
<td>11</td>
<td>termo.pur.foam</td>
<td>polymers</td>
<td>96</td>
<td>4.5</td>
<td>20</td>
<td>51</td>
</tr>
<tr>
<td>12</td>
<td>rubbers</td>
<td>elastomers</td>
<td>97</td>
<td>1.7</td>
<td>10</td>
<td>15</td>
</tr>
<tr>
<td>13</td>
<td>wood.hi</td>
<td>woods</td>
<td>13</td>
<td>0.88</td>
<td>7.7</td>
<td>7.5</td>
</tr>
<tr>
<td>14</td>
<td>wood.mi</td>
<td>woods</td>
<td>14</td>
<td>1</td>
<td>9.6</td>
<td>9.5</td>
</tr>
<tr>
<td>15</td>
<td>wood.li</td>
<td>woods</td>
<td>9.3</td>
<td>0.65</td>
<td>5.2</td>
<td>5.1</td>
</tr>
<tr>
<td>16</td>
<td>cardboards</td>
<td>woods</td>
<td>18</td>
<td>0.56</td>
<td>2.1</td>
<td>3.7</td>
</tr>
<tr>
<td>17</td>
<td>papers</td>
<td>woods</td>
<td>25</td>
<td>0.64</td>
<td>3.9</td>
<td>5.1</td>
</tr>
</tbody>
</table>
Table B.6: Data set used in materials case study (2 of 2)

<table>
<thead>
<tr>
<th>material.num</th>
<th>ch4.atm</th>
<th>ni.atm</th>
<th>dust.atm</th>
<th>bod.wtr</th>
<th>land.change</th>
<th>eco99</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.4</td>
<td>0.26</td>
<td>2.9</td>
<td>0.39</td>
<td>0.089</td>
<td>2.5</td>
</tr>
<tr>
<td>2</td>
<td>9.7</td>
<td>2.8</td>
<td>5.9</td>
<td>1.3</td>
<td>0.19</td>
<td>0.56</td>
</tr>
<tr>
<td>3</td>
<td>0.22</td>
<td>0.038</td>
<td>1.2</td>
<td>0.2</td>
<td>0.052</td>
<td>0.45</td>
</tr>
<tr>
<td>4</td>
<td>0.19</td>
<td>0.034</td>
<td>0.94</td>
<td>0.09</td>
<td>0.059</td>
<td>0.15</td>
</tr>
<tr>
<td>5</td>
<td>1.1</td>
<td>0.79</td>
<td>0.56</td>
<td>15</td>
<td>0.06</td>
<td>0.077</td>
</tr>
<tr>
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<td>1.5</td>
<td>20</td>
<td>0.11</td>
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<tr>
<td>7</td>
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<td>0.41</td>
<td>1.2</td>
<td>0.5</td>
<td>0.00015</td>
<td>0.057</td>
</tr>
<tr>
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<td>1.9</td>
<td>0.11</td>
<td>0.015</td>
<td>0.028</td>
</tr>
<tr>
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<td>37</td>
<td>0.0002</td>
<td>8.5</td>
<td>616</td>
<td>0.033</td>
<td>0.76</td>
</tr>
<tr>
<td>10</td>
<td>13</td>
<td>1.3</td>
<td>3.2</td>
<td>352</td>
<td>0.04</td>
<td>0.36</td>
</tr>
<tr>
<td>11</td>
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<td>3.3</td>
<td>3.6</td>
<td>857</td>
<td>0.091</td>
<td>0.43</td>
</tr>
<tr>
<td>12</td>
<td>5</td>
<td>8.7</td>
<td>1.4</td>
<td>30</td>
<td>0.027</td>
<td>0.31</td>
</tr>
<tr>
<td>13</td>
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<td>0.036</td>
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<td>0.69</td>
<td>4.8</td>
<td>12</td>
</tr>
<tr>
<td>14</td>
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<td>0.041</td>
<td>0.16</td>
<td>0.97</td>
<td>2</td>
<td>6.3</td>
</tr>
<tr>
<td>15</td>
<td>0.28</td>
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<td>0.12</td>
<td>0.79</td>
<td>0.027</td>
<td>0.58</td>
</tr>
<tr>
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<td>1.1</td>
<td>2700</td>
<td>0.00015</td>
<td>0.035</td>
</tr>
<tr>
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<td>1.2</td>
<td>1.9</td>
<td>3500</td>
<td>0.00015</td>
<td>0.066</td>
</tr>
</tbody>
</table>
B.4 Materials case study R code

```r
## Read in data
full.data = as.data.frame(read.csv("materials.csv",header=TRUE))

library(quantreg)
library(ggplot2)
library(scales) ## for LAD regression and plotting

# Define function to calculate MSE normalized by variance of data
# for OLS models
mse.norm = function(aov.model, data) (sum(residuals(aov.model)^2)/
               aov.model$df)/var(data)

materials.data = full.data[,4:length(full.data[1,])]
materials.data.log = log(materials.data)

corr.CED = data.frame(Data = c(rep("Normal",length(
    materials.data[1,])),rep("Log",length(materials.data[1,]))),
    R.sq = c(cor(materials.data)[,1],
             cor(materials.data.log)[,1]))

names.corr = c(colnames(materials.data),colnames(materials.data.data))

corr.plot = ggplot(corr.CED, aes(x=names.corr, y=R.sq, fill=Data)) +
  geom_bar(stat='identity',position='dodge') +
  scale_fill_hue(l=25) +
  ylab(expression(paste(R^2))) + xlab("Emissions") +
  theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
         axis.title.x = element_text(colour="#990000", size=16),
         axis.title.y = element_text(colour="#990000", size=16),
         legend.title = element_text(colour="#990000", size = 14),
         legend.background = element_rect(fill="gray90", size=.5))

mse.train = data.frame(co2.atm = rep(0,length(materials.data.data[1,])),
                        nox.atm = rep(0,length(materials.data.data[1,])),
                        sox.atm = rep(0,length(materials.data.data[1,])),
                        ch4.atm = rep(0,length(materials.data.data[1,])),
                        ni.atm = rep(0,length(materials.data.data[1,])),
                        dust.atm = rep(0,length(materials.data.data[1,])),
                        bod.wtr = rep(0,length(materials.data.data[1,])),
                        land.change = rep(0,length(materials.data.data[1,])))
```
eco99 = rep(0,length(materials.data[,1]))
pct.err.train = mse.train
pct.err.test = mse.train

mse.train.log = mse.train
pct.err.train.log = mse.train
pct.err.test.log = mse.train

for(i in 1:length(materials.data[,1])) {
  training.data = materials.data[-i,]
  testing.data = materials.data[i,]

  training.data.log = materials.data.log[-i,]

  co2.model = aov(co2.atm ~ prim.energy, data = training.data)
  nox.model = aov(nox.atm ~ prim.energy, data = training.data)
  sox.model = aov(sox.atm ~ prim.energy, data = training.data)
  ch4.model = aov(ch4.atm ~ prim.energy, data = training.data)
  ni.model = aov(ni.atm ~ prim.energy, data = training.data)
  dust.model = aov(dust.atm ~ prim.energy, data = training.data)
  bod.model = aov(bod.wtr ~ prim.energy, data = training.data)
  land.change.model = aov(land.change ~ prim.energy,
                          data = training.data)
  eco99.model = aov(eco99 ~ prim.energy, data = training.data)

  co2.model.log = aov(co2.atm ~ prim.energy,
                      data = training.data.log)
  nox.model.log = aov(nox.atm ~ prim.energy,
                      data = training.data.log)
  sox.model.log = aov(sox.atm ~ prim.energy,
                      data = training.data.log)
  ch4.model.log = aov(ch4.atm ~ prim.energy,
                      data = training.data.log)
  ni.model.log = aov(ni.atm ~ prim.energy,
                      data = training.data.log)
  dust.model.log = aov(dust.atm ~ prim.energy,
                      data = training.data.log)
  bod.model.log = aov(bod.wtr ~ prim.energy,
                      data = training.data.log)
  land.change.model.log = aov(land.change ~ prim.energy,
                            data = training.data.log)
  eco99.model.log = aov(eco99 ~ prim.energy,
                        data = training.data.log)
}
co2.model.pred = co2.model$coef[1] +
    testing.data$prim.energy*co2.model$coef[2];
nox.model.pred = nox.model$coef[1] +
    testing.data$prim.energy*nox.model$coef[2];
sox.model.pred = sox.model$coef[1] +
    testing.data$prim.energy*sox.model$coef[2];
ch4.model.pred = ch4.model$coef[1] +
    testing.data$prim.energy*ch4.model$coef[2];
ni.model.pred = ni.model$coef[1] +
    testing.data$prim.energy*ni.model$coef[2];
dust.model.pred = dust.model$coef[1] +
    testing.data$prim.energy*dust.model$coef[2];
bod.model.pred = bod.model$coef[1] +
    testing.data$prim.energy*bod.model$coef[2];
land.change.model.pred = land.change.model$coef[1] +
    testing.data$prim.energy*land.change.model$coef[2];
eco99.model.pred = eco99.model$coef[1] +
    testing.data$prim.energy*eco99.model$coef[2];

c02.model.pred.log = exp(co2.model.log$coef[1])*
    testing.data$prim.energy^co2.model.log$coef[2];
nox.model.pred.log = exp(nox.model.log$coef[1])*
    testing.data$prim.energy^nox.model.log$coef[2];
sox.model.pred.log = exp(sox.model.log$coef[1])*
    testing.data$prim.energy^sox.model.log$coef[2];
ch4.model.pred.log = exp(ch4.model.log$coef[1])*
    testing.data$prim.energy^ch4.model.log$coef[2];
ni.model.pred.log = exp(ni.model.log$coef[1])*
    testing.data$prim.energy^ni.model.log$coef[2];
dust.model.pred.log = exp(dust.model.log$coef[1])*
    testing.data$prim.energy^dust.model.log$coef[2];
bod.model.pred.log = exp(bod.model.log$coef[1])*
    testing.data$prim.energy^bod.model.log$coef[2];
land.change.model.pred.log = exp(land.change.model.log$coef[1])*
    testing.data$prim.energy^land.change.model.log$coef[2];
eco99.model.pred.log = exp(eco99.model.log$coef[1])*
    testing.data$prim.energy^eco99.model.log$coef[2];

mse.train$co2.atm[i] = mse.norm(co2.model, training.data$co2.atm);
pct.err.train$co2.atm[i] = 100*sum(abs(
    training.data$co2.atm - co2.model$fitted)/
    training.data$co2.atm)/17;

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pct.err.test$co2.atm[i] = 100*sum(abs(
    testing.data$co2.atm - co2.model.pred)/testing.data$co2.atm);

mse.train$nox.atm[i] = mse.norm(nox.model, training.data$nox.atm);
pct.err.train$nox.atm[i] = 100*sum(abs(
    training.data$nox.atm - nox.model$fitted)/
    training.data$nox.atm)/17;
pct.err.test$nox.atm[i] = 100*sum(abs(
    testing.data$nox.atm - nox.model.pred)/testing.data$nox.atm);

mse.train$sox.atm[i] = mse.norm(sox.model, training.data$sox.atm);
pct.err.train$sox.atm[i] = 100*sum(abs(
    training.data$sox.atm - sox.model$fitted)/
    training.data$sox.atm)/17;
pct.err.test$sox.atm[i] = 100*sum(abs(
    testing.data$sox.atm - sox.model.pred)/
    testing.data$sox.atm);

mse.train$ch4.atm[i] = mse.norm(ch4.model, training.data$ch4.atm);
pct.err.train$ch4.atm[i] = 100*sum(abs(
    training.data$ch4.atm - ch4.model$fitted)/
    training.data$ch4.atm)/17;
pct.err.test$ch4.atm[i] = 100*sum(abs(
    testing.data$ch4.atm - ch4.model.pred)/testing.data$ch4.atm);

mse.train$ni.atm[i] = mse.norm(ni.model, training.data$ni.atm);
pct.err.train$ni.atm[i] = 100*sum(abs(
    training.data$ni.atm - ni.model$fitted)/
    training.data$ni.atm)/17;
pct.err.test$ni.atm[i] = 100*sum(abs(
    testing.data$ni.atm - ni.model.pred)/testing.data$ni.atm);

mse.train$dust.atm[i] = mse.norm(dust.model, training.data$dust.atm);
pct.err.train$dust.atm[i] = 100*sum(abs(
    training.data$dust.atm - dust.model$fitted)/
    training.data$dust.atm)/17;
pct.err.test$dust.atm[i] = 100*sum(abs(
    testing.data$dust.atm - dust.model.pred)/testing.data$dust.atm);

mse.train$bod.wtr[i] = mse.norm(bod.model, training.data$bod.wtr);
pct.err.train$bod.wtr[i] = 100*sum(abs(
    training.data$bod.wtr - bod.model$fitted)/
    training.data$bod.wtr)/17;
pct.err.test$bod.wtr[i] = 100*sum(abs(
    testing.data$bod.wtr - bod.model.predict)/testing.data$bod.wtr)/17;
testing.data$bod.wtr - bod.model.pred)/testing.data$bod.wtr);

mse.train$land.change[i] = mse.norm(land.change.model,
   training.data$land.change);
pct.err.train$land.change[i] = 100*sum(abs(
   training.data$land.change - land.change.model$fitted)/
   training.data$land.change)/17;
pct.err.test$land.change[i] = 100*sum(abs(
   testing.data$land.change - land.change.model.pred)/
   testing.data$land.change);

mse.train$eco99[i] = mse.norm(eco99.model, training.data$eco99);
pct.err.train$eco99[i] = 100*sum(abs(
   training.data$eco99 - eco99.model$fitted)/training.data$eco99)/17;
pct.err.test$eco99[i] = 100*sum(abs(
   testing.data$eco99 - eco99.model.pred)/testing.data$eco99);

mse.train.log$co2.atm[i] = mse.norm(co2.model.log,
   training.data.log$co2.atm);
pct.err.train.log$co2.atm[i] = 100*sum(abs(
   training.data$co2.atm - exp(co2.model.log$fitted))/
   training.data$co2.atm)/17;
pct.err.test.log$co2.atm[i] = 100*sum(abs(
   testing.data$co2.atm - co2.model.pred.log)/
   testing.data$co2.atm);

mse.train.log$nox.atm[i] = mse.norm(nox.model.log,
   training.data.log$nox.atm);
pct.err.train.log$nox.atm[i] = 100*sum(abs(
   training.data$nox.atm - exp(nox.model.log$fitted))/
   training.data$nox.atm)/17;
pct.err.test.log$nox.atm[i] = 100*sum(abs(
   testing.data$nox.atm - nox.model.pred.log)/testing.data$nox.atm);

mse.train.log$sox.atm[i] = mse.norm(sox.model.log,
   training.data.log$sox.atm);
pct.err.train.log$sox.atm[i] = 100*sum(abs(
   training.data$sox.atm - exp(sox.model.log$fitted))/
   training.data$sox.atm)/17;
pct.err.test.log$sox.atm[i] = 100*sum(abs(
   testing.data$sox.atm - sox.model.pred.log)/testing.data$sox.atm);
mse.train.log$ch4.atm[i] = mse.norm(ch4.model.log, training.data.log$ch4.atm);
pct.err.train.log$ch4.atm[i] = 100*sum(abs(
    training.data$ch4.atm - exp(ch4.model.log$fitted))/
    training.data$ch4.atm)/17;
pct.err.test.log$ch4.atm[i] = 100*sum(abs(
    testing.data$ch4.atm - ch4.model.pred.log)/testing.data$ch4.atm);

mse.train.log$ni.atm[i] = mse.norm(ni.model.log, training.data.log$ni.atm);
pct.err.train.log$ni.atm[i] = 100*sum(abs(
    training.data$ni.atm - exp(ni.model.log$fitted))/
    training.data$ni.atm)/17;
pct.err.test.log$ni.atm[i] = 100*sum(abs(
    testing.data$ni.atm - ni.model.pred.log)/testing.data$ni.atm);

mse.train.log$dust.atm[i] = mse.norm(dust.model.log, training.data.log$dust.atm);
pct.err.train.log$dust.atm[i] = 100*sum(abs(
    training.data$dust.atm - exp(dust.model.log$fitted))/
    training.data$dust.atm)/17;
pct.err.test.log$dust.atm[i] = 100*sum(abs(
    testing.data$dust.atm - dust.model.pred.log)/testing.data$dust.atm);

mse.train.log$bod.wtr[i] = mse.norm(bod.model.log, training.data.log$bod.wtr);
pct.err.train.log$bod.wtr[i] = 100*sum(abs(
    training.data$bod.wtr - exp(bod.model.log$fitted))/
    training.data$bod.wtr)/17;
pct.err.test.log$bod.wtr[i] = 100*sum(abs(
    testing.data$bod.wtr - bod.model.pred.log)/testing.data$bod.wtr);

mse.train.log$land.change[i] = mse.norm(
    land.change.model.log, training.data.log$land.change);
pct.err.train.log$land.change[i] = 100*sum(abs(
    training.data$land.change - exp(land.change.model.log$fitted))/
    training.data$land.change)/17;
pct.err.test.log$land.change[i] = 100*sum(abs(
    testing.data$land.change - land.change.model.pred.log)/
    testing.data$land.change);
mse.train.log$eco99[i] = mse.norm(eco99.model.log,
    training.data.log$eco99);
pct.err.train.log$eco99[i] = 100*sum(abs(  
    training.data$eco99 - exp(eco99.model.log$fitted))  
    training.data$eco99)/17;
pct.err.test.log$eco99[i] = 100*sum(abs(  
    testing.data$eco99 - eco99.model.pred.log)/testing.data$eco99);

} ## LOOP ENDS ###

train = data.frame(Data = c(rep("Untransformed",
    length(materials.data[1,])-1),
    rep("Transformed",
    length(materials.data[1,])-1)),
    mse.mean = c(apply(mse.train, 2, mean),
        apply(mse.train.log, 2, mean)),
    mse.sd = c(apply(mse.train, 2, sd),
        apply(mse.train.log, 2, sd)),
    mse.med = c(apply(mse.train,2,median),
        apply(mse.train.log,2,median)),
    mse.q.25 = c(apply(mse.train,2,quantile,
        prob=0.25),
        apply(mse.train.log,2,quantile,
        prob=0.25)),
    mse.q.975 = c(apply(mse.train,2,quantile,
        prob=0.75),
        apply(mse.train.log,2,quantile,
        prob=0.75)),
    pct.err.mean = c(apply(pct.err.train, 2, mean),
        apply(pct.err.train.log, 2, mean)),
    pct.err.sd = c(apply(pct.err.train, 2, sd),
        apply(pct.err.train.log, 2, sd)),
    pct.err.med = c(apply(pct.err.train,2,median),
        apply(pct.err.train.log,2,median)),
    pct.err.q.25 = c(apply(pct.err.train,2,quantile,
        prob=0.25),
        apply(pct.err.train.log,2,quantile,
        prob=0.25)),
    pct.err.q.975 = c(apply(pct.err.train,2,quantile,
        prob=0.75),
        apply(pct.err.train.log,2,quantile,
        prob=0.75)),
names = rep(names(mse.train), 2)

test = data.frame(Data = c(rep("Untransformed",
   length(materials.data[1,]) - 1),
   rep("Transformed",
   length(materials.data[1,]) - 1)),
pct.err.mean = c(apply(pct.err.test, 2, mean),
   apply(pct.err.test.log, 2, mean)),
pct.err.sd = c(apply(pct.err.test, 2, sd),
   apply(pct.err.test.log, 2, sd)),
pct.err.med = c(apply(pct.err.test, 2, median),
   apply(pct.err.test.log, 2, median)),
pct.err.q.25 = c(apply(pct.err.test, 2,
   quantile, prob=0.25),
   apply(pct.err.test.log, 2,
   quantile, prob=0.25)),
pct.err.q.975 = c(apply(pct.err.test, 2,
   quantile, prob=0.75),
   apply(pct.err.test.log, 2,
   quantile, prob=0.75))

## MSE plot - median, 2.5% and 97.5% quantiles - training data
dodge = position_dodge(width=0.9)
mse.q = ggplot(train, aes(x=names, y=mse.med, fill=Data)) +
   geom_bar(stat='identity', position=dodge) +
   geom_errorbar(aes(ymin=mse.q.25, ymax=mse.q.975), width=.25,
   position=dodge) +
   scale_fill_hue(l=35) +
   geom_line() +
   ylab("Normalized MSE") + xlab("Emissions") +
   theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16),
      legend.title = element_text(colour="#990000", size = 14),
      legend.background = element_rect(fill="gray90", size=.5))

## % error plot - median, 2.5% and 97.5% quantiles - training data
pct.err.train.q = ggplot(train, aes(x=names,
   y=pmin(pct.err.med, 500),
   fill=Data)) +
   geom_bar(stat='identity', position=dodge) +
   geom_errorbar(aes(ymin=pct.err.q.25, ymax=pct.err.q.975), width=.25,
   position=dodge) +
   scale_fill_hue(l=35) +
   geom_line() +
   ylab("Normalized Error") + xlab("Emissions") +
   theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
      axis.title.x = element_text(colour="#990000", size=16),
      axis.title.y = element_text(colour="#990000", size=16),
      legend.title = element_text(colour="#990000", size = 14),
      legend.background = element_rect(fill="gray90", size=.5))
ylim(0,500) +
geom_errorbar(aes(ymin=pct.err.q.25, ymax=pmin(500,pct.err.q.975)),
    width=0.25, position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
    axis.title.x = element_text(colour="#990000", size=16),
    axis.title.y = element_text(colour="#990000", size=16),
    legend.title = element_text(colour="#990000", size = 14),
    legend.background = element_rect(fill="gray90", size=.5))

## % error plot - median, 2.5% and 97.5% quantiles - training data
pct.err.train.mean = ggplot(train, aes(x=names, y=pct.err.mean,
    fill=Data)) +
geom_bar(stat='identity', position=dodge) +
geom_errorbar(aes(ymin=pct.err.mean - pct.err.sd,
    ymax=pct.err.mean + pct.err.sd), width=0.25,
    position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
    axis.title.x = element_text(colour="#990000", size=16),
    axis.title.y = element_text(colour="#990000", size=16),
    legend.title = element_text(colour="#990000", size = 14),
    legend.background = element_rect(fill="gray90", size=.5))

## % error plot - median, 2.5% and 97.5% quantiles - testing data
pct.err.test.q = ggplot(test, aes(x=names, y=pmin(500,pct.err.med),
    fill=Data)) +
geom_bar(stat='identity', position=dodge) +
ylim(0,500) +
geom_errorbar(aes(ymin=pct.err.q.25, ymax=pmin(500,pct.err.q.975)),
    width=0.25, position=dodge) +
scale_fill_hue(l=35) +
geom_line() +
ylab("% Error") + xlab("Emissions") +
theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
    axis.title.x = element_text(colour="#990000", size=16),
    axis.title.y = element_text(colour="#990000", size=16),
## % error plot - mean +/- 1 sd - testing data

```r
pct.err.test.mean = ggplot(test, aes(x=names, y=pct.err.mean, fill=Data)) +
  geom_bar(stat='identity', position=dodge) +
  ylim(0,200) +
  geom_errorbar(aes(ymin=pct.err.mean - pct.err.sd, ymax=pct.err.mean + pct.err.sd),
                width=0.25, position=dodge) +
  scale_fill_hue(l=35) +
  geom_line() +
  ylab("% Error") + xlab("Emissions") +
  theme(axis.text.x = element_text(angle=90, vjust=0.5, size=14),
        axis.title.x = element_text(colour="#990000", size=16),
        axis.title.y = element_text(colour="#990000", size=16),
        legend.title = element_text(colour="#990000", size = 14),
        legend.background = element_rect(fill="gray90", size=.5))
```
Appendix C: CAIS implementation, inventory data and supplementary information

C.1 Details of the CAIS calculation procedure

Details of the CAIS calculations are given in this section, along with an illustrative example using the widget life cycle inventory presented in Chapter 2. Figure 5.2 summarizes the procedure. As in Chapter 5, the following assumptions apply throughout this section:

- $X$ is rectangular due to the presence of multi-functional processes, therefore $p > n$

- Each multi-functional process provides exactly one primary product and one by-product

- No product is produced by more than one process

The CAIS begins with locating multi-functional processes in the inventory. Multi-functional processes are identified using the make matrix $V$. Columns of $V$ that contain more than one non-zero element correspond to multi-functional processes.

In order to write $X$ as a function of allocation weights, $V$ and $U$ must be expanded to square matrices and $B$ must be expanded to a $r \times p$ matrix. $V$ is expanded by
diagonalizing a vector $\hat{x}_+$ that contains all of the positive entries in $X$:

$$V_* = \hat{x}_+$$  \hspace{1cm} (C.1)

where a hat, $\hat{x}_+$, denotes diagonalization of a vector. This operation is equivalent to moving all off-diagonal elements of $\mathbf{V}$ onto the diagonal, adding rows and columns as needed.

The same procedure is used to expand $\mathbf{U}$ to a $p \times p$ matrix and $\mathbf{B}$ to a $r \times p$ matrix. Columns that correspond to multi-functional processes, which are located with the original $\mathbf{V}$, are duplicated. Pseudo-code for this procedure follows.

Initialize counting variable $m$ to 1
for $i = 1..n$
    if ($V(:,i)$ has more than one non-zero element)
        Process $i$ is multi-functional
        $U*(,m) = U(:,i)$
        $U*(,m+1) = U(:,i)$
        $B*(,m) = B(:,i)$
        $B*(,m+1) = B(:,i)$
        $m = m + 2$
    elseif ($V(:,i)$ has exactly one non-zero element)
        Process $i$ is mono-functional
        $U*(,m) = U(:,i)$
        $B*(,m) = B(:,i)$
        $m = m + 1$
    end
end

The weights matrix $\mathbf{W}$ is used to write $V_*$, $U_*$ and $B_*$ as functions of allocation weights. A $1 \times p$ vector $\mathbf{w}$ with a 1 in every element corresponding to a mono-functional process and $[w_m, 1 - w_m]$ in each pair of elements corresponding to a multi-functional process $m$ is diagonalized to give $\mathbf{W}$:

$$\mathbf{W} = \hat{\mathbf{w}},$$  \hspace{1cm} (C.2)

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**w** is constructed automatically using the unexpanded **V** matrix to locate multi-functional processes as detailed in the pseudo-code below.

**Initialize counting variable m to 1**
for i = 1..p
    if(V(:,i) has more than one non-zero element)
        Process i is multi-functional
        w(i) = w_m
        w(i+1) = 1 - w_m
        m = m + 1
    elseif(V(:,i) has exactly one non-zero element)
        Process i is mono-functional
        w(i) = 1
end

**V**, **U**, **B**, and **W** are now used to calculate the technology matrix **X**(w) and intervention matrix **B**(w) as functions of the allocation weights.

\[
X(w) = V - UW \tag{C.3}
\]

\[
B(w) = BW \tag{C.4}
\]

Finally, the product inventory vector as a function of the allocation weights, **g**(w), is calculated by applying Equation (2.2) to **X**(w) and **B**(w), as follows.

\[
g(w) = B(w)X(w)^{-1}f \tag{C.5}
\]

**C.2 CAIS implementation in MATLAB**

% Throughout the code, "grain" refers to corn grain fermentation, "bio"% refers to corn stover hydrolysis and "thermo" refers to corn stover% gasification

product_names = {'Grain EtOH','Bio CellEtOH','Thermo CellEtOH'};
A_files = {'A_grain.txt','A_bio.txt','A_thermo.txt'};
B_files = {'B_grain.txt','B_bio.txt','B_thermo.txt'};
product_files = {'products_grain.txt','products_bio.txt'},
'products_thermo.txt'};
process_files = {'processes_grain.txt','processes_bio.txt',...
'processes_thermo.txt'};

ncompare = length(product_names);

inventories = cell(1, ncompare);

for i = 1:ncompare
    product = product_names{i};
    A = importdata(A_files{i});
    B_small = importdata(B_files{i});
    products = importnames(product_files{i});
    processes = importnames(process_files{i});

    f = [zeros(1, length(products)-1) 1];

    U_small = abs(A.*(A<0));
    V = diag(sum(A.*(A>0),2));
    dimU = size(U_small);
    B = B_small;

    locate_coproducts = estimable(product_names{i},
        A_files{i}, product_files{i},
        process_files{i});
    locate_coproducts = locate_coproducts{1};
    count = 1;
    for j = 1:dimU(2)
        if locate_coproducts(j)
            U(:,count) = U_small(:,j);
            U(:,count+1) = U_small(:,j);
            B(:,count) = B_small(:,j);
            B(:,count+1) = B_small(:,j);
            count = count + 2;
        else
            U(:,count) = U_small(:,j);
            B(:,count) = B_small(:,j);
            count = count + 1;
        end
    end
end

num_wts = length(find(locate_coproducts));
if num_wts == 1
    syms w_1 real
    wts = w_1;
elseif num_wts == 2
    syms w_1 w_2 real
    wts = [w_1 w_2];
elseif num_wts == 3
    syms w_1 w_2 w_3 real
    wts = [w_1 w_2 w_3];
elseif num_wts == 4
    syms w_1 w_2 w_3 w_4 real
    wts = [w_1 w_2 w_3 w_4];
elseif num_wts == 5
    syms w_1 w_2 w_3 w_4 w_5 real
    wts = [w_1 w_2 w_3 w_4 w_5];
end

wt_names = [0 w_1 0];
count = 1;
wtcount = 1;

for j = 1:length(locate_coproducts)
    if locate_coproducts(j) == 1;
        wt_names(count) = wts(wtcount);
        wt_names(count + 1) = 1 - wts(wtcount);
        count = count + 2;
        wtcount = wtcount + 1;
    elseif locate_coproducts(j) == 0;
        wt_names(count) = 1;
        count = count + 1;
    end
end

wt_mat = diag(wt_names);
clear j count wtcount

A_wts = V’ - U*wt_mat;
B_wts = B*wt_mat;
A_wts_inv = inv(A_wts);
inventory_wts = B_wts*A_wts_inv;

inventories{i} = inventory_wts*f’;

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Table C.1: Widget final demand vector

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity (kWh)</td>
<td>0</td>
</tr>
<tr>
<td>Steel (kg)</td>
<td>0</td>
</tr>
<tr>
<td>Exp. Plastic (kg)</td>
<td>0</td>
</tr>
<tr>
<td>Thm. Plastic (kg)</td>
<td>0</td>
</tr>
<tr>
<td>Widget (units)</td>
<td>1</td>
</tr>
</tbody>
</table>

MATLAB code for generating the plots shown in Chapter 5 and in Section C.5 is available upon request.

C.3 Illustrative example: CAIS applied to the widget life cycle inventory

The CAIS procedure is demonstrated using the widget life cycle introduced in Section 2.2.3. The unallocated technology matrix is given in Table 2.4, the unallocated interventions matrix in Table 2.5 and the functional unit in Table C.1.

\[
V^* = \begin{bmatrix}
15 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 \\
0 & 0 & 1.5 & 0 & 0 \\
0 & 0 & 0 & 0.85 & 0 \\
0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\]  

(C.6)
\[
\mathbf{U}_* = \begin{bmatrix}
0 & 7 & 2 & 2 & 6 \\
0 & 0 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 1.5 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\mathbf{B}_* = \begin{bmatrix}
3 & 5 & 2.5 & 2.5 & 1.2 \\
0.8 & 1.3 & 1.5 & 1.5 & 0.4 \\
4.1 & 6.2 & 1.9 & 1.9 & 0.7 \\
15 & 8.7 & 4 & 4 & 0.5
\end{bmatrix}
\]

\[
\mathbf{W} = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & w & 0 & 0 \\
0 & 0 & 1-w & 0 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

\[
\mathbf{X}_*(w) = \begin{bmatrix}
15 & -7 & -2w & -2(1-w) & -6 \\
0 & 2 & 0 & 0 & -2 \\
0 & 0 & 1.5 & 0 & -1.5 \\
0 & 0 & 0 & 0.85 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

\[
\mathbf{B}_*(w) = \begin{bmatrix}
3 & 5 & 2.5w & 2.5(1-w) & 1.2 \\
0.8 & 1.3 & 1.5w & 1.5(1-w) & 0.4 \\
4.1 & 6.2 & 1.9w & 1.9(1-w) & 0.7 \\
15 & 8.7 & 4w & 4(1-w) & 0.5
\end{bmatrix}
\]

\[
\mathbf{g}_*(w) = \begin{bmatrix}
2.90w + 8.80 \\
1.61w + 2.39 \\
2.45w + 10.45 \\
6.00w + 22.20
\end{bmatrix}
\]

This example had only one process which required allocation, so the resulting product inventories are linear functions of the allocation weight. For larger systems with multiple instances of allocation, the product inventories will be higher-order nonlinear functions of the allocation weights.
C.4 Ethanol production pathway inventories

Tables C.2 - C.10 contain the inventory data used to create the bioethanol figures in the main paper and in the following sections. Data was taken from [41] and supplemented with data from [263] and [214].
### Table C.2: Technology matrix for corn grain fermentation life cycle (1 of 2)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>kg ammonium nitrate</td>
<td>1.17 × 10^{-1}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg phosphorus pentoxide</td>
<td>0</td>
<td>3.06 × 10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg potassium chloride</td>
<td>0</td>
<td>0</td>
<td>3.30 × 10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg lime</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>7.20 × 10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg agricultural chemical</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6.45 × 10^{-4}</td>
<td>0</td>
<td>6.64 × 10^{-1}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg corn seeds</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.86 × 10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>gal water</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>gal fuel</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>SCF natural gas</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.02 × 10^{2}</td>
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<tr>
<td>kWh electricity</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.89</td>
<td>0</td>
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<tr>
<td>kg steel</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg corn grain</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg dry corn stover</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg cement</td>
<td>0</td>
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<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>gal fuel</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>kg coal</td>
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<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>kg coal transported</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>L grain ethanol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg DDGS</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>L grain ethanol at pump</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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</tr>
</tbody>
</table>
Table C.3: Technology matrix for corn grain fermentation life cycle (2 of 2)

<table>
<thead>
<tr>
<th></th>
<th>Steel</th>
<th>Corn and cement pipeline</th>
<th>Coal</th>
<th>Rail</th>
<th>Fermentation bioethanol transport</th>
<th>Ethanol transport</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>prod.</td>
<td>stover prodn.</td>
<td>prodn.</td>
<td>transport</td>
<td>prodn.</td>
<td>prodn.</td>
</tr>
<tr>
<td>kg ammonium nitrate</td>
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<td>-0.116639926</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg phosphorus pentoxide</td>
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<td>-3.06×10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg potassium chloride</td>
<td>0</td>
<td>-3.30×10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg lime</td>
<td>0</td>
<td>-0.072031662</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg agricultural chemical</td>
<td>0</td>
<td>-6.45×10^{-4}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg corn seeds</td>
<td>0</td>
<td>-1.86×10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>gal water</td>
<td>0</td>
<td>-2.03×10^{1}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>gal fuel</td>
<td>0</td>
<td>-1.25×10^{-1}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>SCF natural gas</td>
<td>0</td>
<td>-4.79×10^{1}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kWh electricity</td>
<td>0</td>
<td>-2.88×10^{-2}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg steel</td>
<td>9.21×10^{-3}</td>
<td>-9.21×10^{-3}</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg corn grain</td>
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<td>2.381</td>
<td>0</td>
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</tr>
<tr>
<td>kg dry corn stover</td>
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<td>1.476</td>
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</tr>
<tr>
<td>kg cement</td>
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<td>0</td>
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</tr>
<tr>
<td>gal fuel</td>
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<td>0.184596756</td>
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</tr>
<tr>
<td>kg coal</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>1.256218845</td>
</tr>
<tr>
<td>kg coal transported</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.256218845</td>
</tr>
<tr>
<td>L grain ethanol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>kg DDGS</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>L grain ethanol at pump</td>
<td>0</td>
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<td>0</td>
<td>0</td>
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</tr>
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</table>
Table C.4: Intervention matrix for corn grain fermentation life cycle

<table>
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<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>kg CO₂</td>
<td>1.94×10⁻¹</td>
<td>4.77×10⁻²</td>
<td>1.22×10⁻²</td>
<td>6.49×10⁻²</td>
<td>6.80×10⁻³</td>
<td>0.00</td>
<td>7.41×10⁻¹</td>
<td>1.01×10⁻¹</td>
<td>2.37×10⁻¹</td>
<td>2.56</td>
</tr>
<tr>
<td>kg CO</td>
<td>6.37×10⁻⁴</td>
<td>2.42×10⁻⁴</td>
<td>3.40×10⁻⁵</td>
<td>1.34×10⁻⁵</td>
<td>5.77×10⁻⁵</td>
<td>0.00</td>
<td>2.28×10⁻³</td>
<td>4.23×10⁻⁴</td>
<td>1.86×10⁻³</td>
<td>1.42×10⁻³</td>
</tr>
<tr>
<td>kg CH₄</td>
<td>7.07×10⁻⁴</td>
<td>5.72×10⁻⁵</td>
<td>2.44×10⁻⁵</td>
<td>5.23×10⁻⁵</td>
<td>3.77×10⁻⁵</td>
<td>0.00</td>
<td>2.39×10⁻¹</td>
<td>2.22×10⁻³</td>
<td>1.67×10⁻²</td>
<td>4.18×10⁻³</td>
</tr>
<tr>
<td>kg NOₓ</td>
<td>5.81×10⁻⁴</td>
<td>4.93×10⁻⁵</td>
<td>1.55×10⁻⁵</td>
<td>2.10×10⁻⁵</td>
<td>4.30×10⁻⁵</td>
<td>0.00</td>
<td>1.10×10⁻³</td>
<td>1.73×10⁻⁴</td>
<td>8.89×10⁻⁴</td>
<td>6.55×10⁻³</td>
</tr>
<tr>
<td>kg N₂O</td>
<td>6.70×10⁻⁴</td>
<td>1.82×10⁻⁵</td>
<td>3.47×10⁻⁷</td>
<td>1.65×10⁻⁷</td>
<td>3.27×10⁻⁶</td>
<td>0.00</td>
<td>8.66×10⁻³</td>
<td>1.70×10⁻⁶</td>
<td>6.35×10⁻⁶</td>
<td>4.33×10⁻⁶</td>
</tr>
<tr>
<td>kg SO₂</td>
<td>2.92×10⁻⁴</td>
<td>3.41×10⁻⁵</td>
<td>3.60×10⁻⁵</td>
<td>2.80×10⁻⁵</td>
<td>3.95×10⁻⁵</td>
<td>0.00</td>
<td>1.38×10⁻³</td>
<td>2.97×10⁻⁴</td>
<td>1.26×10⁻³</td>
<td>1.38×10⁻²</td>
</tr>
<tr>
<td>kg coal</td>
<td>7.00×10⁻⁴</td>
<td>2.17×10⁻³</td>
<td>1.58×10⁻³</td>
<td>1.59×10⁻³</td>
<td>8.22×10⁻⁴</td>
<td>0.00</td>
<td>9.30×10⁻²</td>
<td>9.33×10⁻³</td>
<td>4.18×10⁻²</td>
<td>9.92×10⁻¹</td>
</tr>
<tr>
<td>kg crude oil</td>
<td>4.81×10⁻⁴</td>
<td>1.65×10⁻³</td>
<td>4.44×10⁻⁴</td>
<td>6.73×10⁻⁴</td>
<td>5.14×10⁻⁴</td>
<td>0.00</td>
<td>9.31×10⁻²</td>
<td>1.32×10⁻²</td>
<td>1.16×10⁻²</td>
<td>2.90×10⁻²</td>
</tr>
<tr>
<td>kg natural gas</td>
<td>7.42×10⁻²</td>
<td>1.65×10⁻²</td>
<td>3.27×10⁻³</td>
<td>4.29×10⁻³</td>
<td>1.41×10⁻³</td>
<td>0.00</td>
<td>1.08×10⁻¹</td>
<td>1.87×10⁻²</td>
<td>4.48×10⁻²</td>
<td>1.27×10⁻¹</td>
</tr>
<tr>
<td>kg water</td>
<td>2.34</td>
<td>5.75×10⁻¹</td>
<td>5.31×10⁻¹</td>
<td>5.15×10⁻¹</td>
<td>4.42×10⁻¹</td>
<td>0.00</td>
<td>3.14×10¹</td>
<td>3.09</td>
<td>1.36×10¹</td>
<td>5.58×10²</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Steel prod.</th>
<th>Corn and stover farming</th>
<th>Cement produ.</th>
<th>Pipeline transport</th>
<th>Coal prod.</th>
<th>Rail transport</th>
<th>Fermentation bioethanol produ.</th>
<th>Ethanol transport</th>
</tr>
</thead>
<tbody>
<tr>
<td>kg CO₂</td>
<td>...</td>
<td>7.27×10⁻³</td>
<td>8.00×10⁻⁵</td>
<td>6.25×10⁻⁶</td>
<td>2.30×10⁻²</td>
<td>9.96×10⁻³</td>
<td>1.56×10⁻²</td>
<td>8.71</td>
</tr>
<tr>
<td>kg CO</td>
<td>...</td>
<td>7.56×10⁻⁵</td>
<td>2.14×10⁻⁴</td>
<td>1.71×10⁻⁴</td>
<td>1.80×10⁻⁴</td>
<td>4.68×10⁻⁵</td>
<td>1.43×10⁻⁴</td>
<td>5.56×10⁻³</td>
</tr>
<tr>
<td>kg CH₄</td>
<td>...</td>
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<td>2.29×10⁻⁴</td>
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<td>8.66×10⁻⁶</td>
<td>3.09×10⁻⁵</td>
<td>5.92×10⁻³</td>
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<td>kg water</td>
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### Table C.5: Technology matrix for corn stover hydrolysis life cycle (1 of 2)

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<tr>
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<td>0</td>
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<td>0</td>
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<td>0</td>
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<tr>
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Table C.6: Technology matrix for corn stover hydrolysis (2 of 2)

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<th>Corn wet milling</th>
<th>Organic chemical</th>
<th>Misc. chemical</th>
<th>Pipeline transport</th>
<th>Hydrolysis bioethanol</th>
<th>Ethanol transport</th>
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Table C.7: Intervention matrix for corn stover hydrolysis life cycle

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<th></th>
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<td>4.23×10⁻¹</td>
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<td>9.97×10⁻²</td>
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<tr>
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<td>2.93×10⁻³</td>
<td>4.14×10⁻⁴</td>
<td>8.73×10⁻⁴</td>
<td>3.33×10⁻⁴</td>
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<td>2.98×10⁻⁴</td>
<td>7.75×10⁻⁴</td>
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<tr>
<td>kg CH₄</td>
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<td>2.97×10⁻⁴</td>
<td>3.41×10⁻⁴</td>
<td>2.18×10⁻⁴</td>
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<td>3.22×10⁻²</td>
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<tr>
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<tr>
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<td>4.39×10⁻⁴</td>
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<th>Hydrolysis bioethanol transport</th>
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Table C.9: Technology matrix for corn stover gasification life cycle (2 of 2)

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### Table C.10: Intervention matrix for corn stover gasification life cycle

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</tbody>
</table>
C.5  Detailed results of the ethanol comparison

C.5.1  Impact range plots

These plots are analogous to Figure 5.1 in Chapter 5, which showed how the magnitude of carbon dioxide emissions from each ethanol pathway varied due to allocation. Figures C.1 - C.9 show how the magnitudes of the other nine environmental impacts considered vary with allocation.

Figure C.1: Carbon monoxide emissions impact range plot.
Figure C.2: Methane emissions impact range plot.

Figure C.3: Coal consumption impact range plot.
Figure C.4: Nitrous oxide emissions impact range plot.

Figure C.5: Natural gas consumption impact range plot.
Figure C.6: Nitrogen oxide emissions impact range plot.

Figure C.7: Crude oil consumption impact range plot.
Figure C.8: Sulfur dioxide emissions impact range plot.

Figure C.9: Fresh water consumption impact range plot.
C.5.2 Preference plots showing impact magnitudes

Figure 5.4 in Chapter 5 shows preference plots for carbon dioxide and carbon monoxide emissions. These preference plots use color to show how the preferred pathway varies throughout the allocation space. The z-axis is used to show impact magnitudes as well.

Figure C.10: Methane emissions preference plot.
Figure C.11: Coal consumption preference plot.

Figure C.12: Nitrous oxide emissions preference plot.
Figure C.13: Natural gas consumption preference plot.

Figure C.14: Nitrogen oxides emissions preference plot.
Figure C.15: Crude oil consumption preference plot.

Figure C.16: Sulfur dioxide emissions preference plot.
Figure C.17: Fresh water consumption preference plot.
C.5.3 Preference plots without impact magnitudes

The same information displayed in the following plots was used to calculate the preference percentages given in Table 5.2 in Chapter 5. Figures C.18 - C.27 contain the same information as do Figures C.10 - C.17, but here the plots do not show impact magnitude.

Figure C.18: Carbon dioxide emissions preference plot.
Figure C.19: Carbon monoxide preference plot.

Figure C.20: Methane emissions preference plot.
Figure C.21: Coal consumption preference plot.

Figure C.22: Nitrous oxide emissions preference plot.
Figure C.23: Natural gas consumption preference plot.

Figure C.24: Nitrogen oxides emissions preference plot.
Figure C.25: Crude oil consumption preference plot.

Figure C.26: Sulfur dioxide emissions preference plot.
Figure C.27: Fresh water consumption preference plot.
C.6 1,3-propanediol inventory data

Tables C.11 - C.14 contain inventory data for fossil-based and biomass-based propanediol (PDO). Data is taken from the hybrid study performed in [285]. As the fossil-based PDO inventory did not require allocation, only the inventory vector is presented. The inventory vector for biomass-based PDO is shown in Eq. (C.13).

Table C.11: Technology matrix for fossil-based propanediol.

<table>
<thead>
<tr>
<th></th>
<th>Syngas production (kg)</th>
<th>EO production (kg)</th>
<th>PDO production (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Syngas (kg)</td>
<td>0.646</td>
<td>0</td>
<td>-0.646</td>
</tr>
<tr>
<td>EO (kg)</td>
<td>0</td>
<td>0.763</td>
<td>-0.763</td>
</tr>
<tr>
<td>PDO (kg)</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Table C.12: Technology matrix for biomass-based propanediol

<table>
<thead>
<tr>
<th></th>
<th>Corn farming and milling (kg)</th>
<th>Glucose production (kg)</th>
<th>PDO production (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starch (kg)</td>
<td>1.84</td>
<td>-1.84</td>
<td>0</td>
</tr>
<tr>
<td>Starch by-products (kg)</td>
<td>0.92</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose (kg)</td>
<td>0</td>
<td>1.96</td>
<td>-1.96</td>
</tr>
<tr>
<td>PDO (kg)</td>
<td>0</td>
<td>0</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Table C.13: Intervention matrix for biomass-based propanediol

<table>
<thead>
<tr>
<th></th>
<th>Corn farming and milling</th>
<th>Glucose production</th>
<th>PDO production</th>
</tr>
</thead>
<tbody>
<tr>
<td>g SO\textsubscript{x}</td>
<td>1.292</td>
<td>0.0153</td>
<td>1.895</td>
</tr>
<tr>
<td>g CO</td>
<td>2.886</td>
<td>0.0219</td>
<td>1.437</td>
</tr>
<tr>
<td>g NO\textsubscript{x}</td>
<td>12.461</td>
<td>8.274\times10\textsuperscript{-3}</td>
<td>2.077</td>
</tr>
<tr>
<td>g VOC</td>
<td>1.166</td>
<td>4.173\times10\textsuperscript{-3}</td>
<td>0.597</td>
</tr>
<tr>
<td>g Pb</td>
<td>5.00-05</td>
<td>0.000</td>
<td>4.50\times10\textsuperscript{-5}</td>
</tr>
<tr>
<td>g PM10</td>
<td>0.364</td>
<td>1.773\times10\textsuperscript{-3}</td>
<td>0.155</td>
</tr>
<tr>
<td>g CO\textsubscript{2}</td>
<td>909.465</td>
<td>8.730</td>
<td>1980.679</td>
</tr>
<tr>
<td>CH\textsubscript{4} (g CO\textsubscript{2}-eq)</td>
<td>105.187</td>
<td>0.702</td>
<td>138.281</td>
</tr>
<tr>
<td>N\textsubscript{2}O (g CO\textsubscript{2}-eq)</td>
<td>368.608</td>
<td>0.680</td>
<td>42.766</td>
</tr>
<tr>
<td>CFC (g CO\textsubscript{2}-eq)</td>
<td>3.990</td>
<td>0.056</td>
<td>4.799</td>
</tr>
<tr>
<td>Total Energy (MJ)</td>
<td>15.172</td>
<td>0.104</td>
<td>31.525</td>
</tr>
</tbody>
</table>

\[ \mathbf{g}_{\text{bio}}(w) = \begin{bmatrix} 1.292w_1 + 1.910 \\ 2.8869w_1 + 1.458 \\ 12.461w_1 + 2.085 \\ 1.166w_1 + 0.601 \\ 5.000 \times 10^{-5}w_1 + 4.500 \times 10^{-5} \\ 0.364w_1 + 0.157 \\ 909.465w_1 + 1.989 \times 10^3 \\ 105.187w_1 + 138.983 \\ 368.608w_1 + 43.446 \\ 3.990w_1 + 4.908 \\ 15.172w_1 + 31.629 \end{bmatrix} \]

\[ \text{g SO}_{x} \quad \text{g CO} \quad \text{g NO}_{x} \quad \text{g VOC} \quad \text{g Pb} \quad \text{g PM10} \quad \text{g CO}_{2} \quad \text{CH}_{4} \quad \text{N}_{2}O \quad \text{CFC} \quad \text{Total Energy (MJ)} \]
Table C.14: Inventory vector for fossil-based propanediol.

<table>
<thead>
<tr>
<th>Substance</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>g SO₂</td>
<td>28.097</td>
</tr>
<tr>
<td>g CO</td>
<td>6.555</td>
</tr>
<tr>
<td>g NOₓ</td>
<td>13.786</td>
</tr>
<tr>
<td>g VOC</td>
<td>6.320</td>
</tr>
<tr>
<td>g Pb</td>
<td>7.200 × 10⁻⁴</td>
</tr>
<tr>
<td>g PM10</td>
<td>0.885</td>
</tr>
<tr>
<td>g CO₂</td>
<td>4962.557</td>
</tr>
<tr>
<td>CH₄ (g CO₂-eq)</td>
<td>922.707</td>
</tr>
<tr>
<td>N₂O (g CO₂-eq)</td>
<td>338.228</td>
</tr>
<tr>
<td>CFC (g CO₂-eq)</td>
<td>328.000</td>
</tr>
<tr>
<td>Total Energy (MJ)</td>
<td>99.780</td>
</tr>
</tbody>
</table>
C.7 1,3-propanediol detailed results

For all interventions considered, fossil-based PDO had higher impacts than did biomass-based PDO.

Figure C.28: Fossil PDO inventory and biomass PDO inventory function for carbon monoxide emissions.
Figure C.29: Fossil PDO inventory and biomass PDO inventory function for carbon dioxide emissions.

Figure C.30: Fossil PDO inventory and biomass PDO inventory function for methane emissions.
Figure C.31: Fossil PDO inventory and biomass PDO inventory function for nitrogen oxide emissions.

Figure C.32: Fossil PDO inventory and biomass PDO inventory function for nitrous oxide emissions.
Figure C.33: Fossil PDO inventory and biomass PDO inventory function for sulfur oxide emissions.

Figure C.34: Fossil PDO inventory and biomass PDO inventory function for PM10 emissions.
Figure C.35: Fossil PDO inventory and biomass PDO inventory function for volatile organic carbon (VOC) emissions.

Figure C.36: Fossil PDO inventory and biomass PDO inventory function for chlorofluorocarbon (CFC) emissions.
Figure C.37: Fossil PDO inventory and biomass PDO inventory function for lead emissions.

Figure C.38: Fossil PDO inventory and biomass PDO inventory function for nonrenewable energy consumption.
Appendix D: P2P notation and implementation in Python

D.1 Notation

• A hat $\hat{\cdot}$ 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 multi-scale model: $\bar{X}$

• Bold lower-case symbols indicate vectors

• Bold upper-case symbols indicate matrices

• A superscript star $\star$ 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

• $i$: Producing sector (Section 2.3) or Commodity (elsewhere)

• $j$: Consuming sector (Section 2.3) 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

Table D.1: Symbol definitions

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description and Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{X}$</td>
<td>Transactions matrix used to derive EIO model ($$)</td>
</tr>
<tr>
<td>$\mathbf{v}$</td>
<td>Value added vector ($$)</td>
</tr>
<tr>
<td>$\mathbf{f}$</td>
<td>Final demand vector ($$)</td>
</tr>
<tr>
<td>$\mathbf{A}$</td>
<td>Industry-industry direct requirements matrix (this section); Commodity-commodity direct requirements matrix (elsewhere)</td>
</tr>
<tr>
<td>$\mathbf{x}$</td>
<td>Vector of total sector outputs ($$)</td>
</tr>
<tr>
<td>$\mathbf{I}$</td>
<td>Identity matrix with the same dimensions as $\mathbf{A}$</td>
</tr>
<tr>
<td>$(\mathbf{I} - \mathbf{A})^{-1}$</td>
<td>Total requirements matrix or Leontief inverse, before disaggregation</td>
</tr>
<tr>
<td>$\mathbf{B}$</td>
<td>Environmental interventions matrix containing data on $R$ environmental interventions (physical units)</td>
</tr>
<tr>
<td>$\mathbf{g}$</td>
<td>Inventory vector of $R$ total environmental interventions per sector</td>
</tr>
<tr>
<td>$\mathbf{U}$</td>
<td>Economy scale use table before disaggregation ($$)</td>
</tr>
<tr>
<td>$\mathbf{V}$</td>
<td>Economy scale make table before disaggregation ($$)</td>
</tr>
<tr>
<td>$\mathbf{A}_c$</td>
<td>Commodity-commodity direct requirements matrix</td>
</tr>
<tr>
<td>$\mathbf{q}$</td>
<td>Vector of total commodity outputs ($$)</td>
</tr>
<tr>
<td>$\mathbf{e}$</td>
<td>Commodity final demand vector ($$)</td>
</tr>
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</table>

Section 6.2

continued
Table D.1: Symbol definitions (continued)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$\bar{S}$</td>
<td>Economy scale component (sector) of a P2P system</td>
</tr>
<tr>
<td>$S$</td>
<td>Value chain scale component (activity) of a P2P system</td>
</tr>
<tr>
<td>$\mathcal{S}$</td>
<td>Equipment scale component (process of a P2P system)</td>
</tr>
</tbody>
</table>

**Section 6.2.1**

- $x_i$: Value chain activity model (physical units)
- $X$: Value chain technology matrix (physical units)
- $B$: Value chain scale interventions matrix containing data on $R$ environmental interventions (physical units)
- $h_n(z_n)$: One fundamental (unit operation) model associated process $n$
- $z_n$: Vector of unit operation variables in process $n$
- $x_n(z_n)$: Process input-output vector
- $\{z\}$: Set of unit operation variables for processes $1, \ldots, N$
- $X(\{z\})$: Equipment scale technology matrix
- $H(\{z\})$: Set of all fundamental models for processes $1, \ldots, N$
- $B(\{z\})$: Equipment scale environmental interventions matrix containing models for $R$ interventions

**Section 6.2.2**

- $X_u$: Value chain upstream cutoff matrix containing product flows from the economy to the value chain ($\$\$)
- $A_{ad}$: Value chain downstream cutoff matrix containing product flows from the value chain to sectors (physical units, normalized by total output of destination sector)
- $X_d$: Value chain downstream cutoff matrix (physical units, not normalized)
- $X_u^E(\{z\})$: Equipment-economy upstream cutoff matrix containing product flows from the economy to processes ($\$\$)
- $X_u^V(\{z\})$: Equipment-value chain upstream cutoff matrix: product flows from the value chain to processes (physical units)
- $A_{ad}^E(\{z\})$: Equipment-economy downstream cutoff matrix: product flows from processes to sectors (physical units, normalized by total output of destination sector)
- $X_{ad}^E(\{z\})$: Equipment-economy downstream cutoff matrix: products flows from processes to sectors, (physical units, not normalized)
Table D.1: Symbol definitions (continued)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$X_d^V({z})$</td>
<td>Equipment-value chain downstream cutoff matrix containing product flows from processes to the value chain (physical units, not normalized)</td>
</tr>
<tr>
<td>$U$</td>
<td>Value chain scale use matrix before disaggregation (physical units)</td>
</tr>
<tr>
<td>$U$</td>
<td>Equipment scale use matrix (physical units)</td>
</tr>
<tr>
<td>$V$</td>
<td>Value chain scale make matrix before disaggregation (physical units)</td>
</tr>
<tr>
<td>$V$</td>
<td>Equipment scale make matrix (physical units)</td>
</tr>
<tr>
<td>$V^*({z})$</td>
<td>Economy scale make matrix after disaggregation ($)</td>
</tr>
<tr>
<td>$U^*({z})$</td>
<td>Economy scale use matrix after disaggregation ($)</td>
</tr>
<tr>
<td>$P_F$</td>
<td>Value chain function permutation matrix relating value chain products to commodities (unitless)</td>
</tr>
<tr>
<td>$P_F$</td>
<td>Value chain activity permutation matrix relating constituent value chain activities to parent sectors (unitless)</td>
</tr>
<tr>
<td>$P_E^F$</td>
<td>Equipment-economy function permutation matrix relating equipment scale products to commodities (unitless)</td>
</tr>
<tr>
<td>$P_E^F$</td>
<td>Equipment-economy process permutation matrix relating constituent processes to parent sectors (unitless)</td>
</tr>
<tr>
<td>$p$</td>
<td>Vector of value chain product prices</td>
</tr>
<tr>
<td>$p$</td>
<td>Vector of equipment scale product prices</td>
</tr>
<tr>
<td>$V^*({z})$</td>
<td>Value chain scale make matrix after disaggregation (physical units)</td>
</tr>
<tr>
<td>$U^*({z})$</td>
<td>Value chain use matrix after disaggregation (physical units)</td>
</tr>
<tr>
<td>$P_F^V$</td>
<td>Equipment-value chain process permutation matrix relating constituent processes to parent value chain activities (unitless)</td>
</tr>
<tr>
<td>$P_F^V$</td>
<td>Equipment-value chain function permutation matrix relating equipment scale products to value chain products (unitless)</td>
</tr>
<tr>
<td>$A^*({z})$</td>
<td>Direct requirements matrix after disaggregation</td>
</tr>
<tr>
<td>$X^*({z})$</td>
<td>Value chain technology matrix after disaggregation (physical units)</td>
</tr>
<tr>
<td>$R$</td>
<td>Economy scale total interventions matrix containing data on $R$ environmental interventions (physical units)</td>
</tr>
<tr>
<td>$B^*({z})$</td>
<td>Economy scale interventions matrix after disaggregation (physical units)</td>
</tr>
</tbody>
</table>

continued
Table D.1: Symbol definitions (continued)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{R}^*({z})$</td>
<td>Economy scale total interventions matrix after disaggregation (physical units)</td>
</tr>
<tr>
<td>$\mathbf{B}^*({z})$</td>
<td>Value chain scale interventions matrix after disaggregation (physical units)</td>
</tr>
</tbody>
</table>

Section 6.2.4

- $\bar{f}$: Final demand from economy scale of P2P system (generally zero, $\$\$)
- $\bar{s}$: Economy scale scaling vector
- $\bar{f}$: Final demand from value chain scale of P2P system (generally zero, physical units)
- $\bar{s}$: Value chain scale scaling vector
- $\bar{f}$: Final demand from equipment scale of P2P system (physical units)
- $\bar{s}$: Equipment scale scaling vector (elements may be non-linear or fixed)
- $\mathbf{X}(\{z\})$: Multi-scale P2P transactions matrix
- $\mathbf{B}(\{z\})$: Multi-scale P2P environmental interventions matrix
- $\bar{s}$: P2P scaling vector
- $\bar{f}$: Final demand from P2P system

D.2 Python code for building and solving a P2P model

D.2.1 Description of data files

The abbreviations for the name of each data file are used as variable names in the model code. Entries marked with an asterisk indicate matrices that may contain variable elements. These matrices can either be read in as “blank” matrices (all zeros) and then re-defined within the code, or they can be defined wholly within the code.

1. EconMake: Economy make table
   - Dimensions: Commodities by Sectors
• Units: Monetary, NOT normalized (millions of USD)

2. EconUse: Economy use table

• Dimensions: Sectors by Commodities
• Units: Monetary, NOT normalized (millions of USD)

3. EconTotalEnvInt: Economy TOTAL interventions matrix

• Dimensions: interventions by Commodities
• Units: Physical, NOT normalized

4. VCMake: Value chain make table

• Dimensions: Activities by value chain products
• Units: Physical

5. VCUse: Value chain use table

• Dimensions: Value chain products by activities
• Units: Physical

6. VCEnvInt: Value chain interventions matrix

• Dimensions: interventions by Value chain products
• Units: Physical

7. *EqMake: Equipment scale make table

Activities and processes must have common product flows in the same units
Must correspond to level of production in make/use tables
• Dimensions: Processes by equipment scale products
• Units: Physical

8. *EqUse: Equipment scale use table

• Dimensions: Equipment scale products by processes
• Units: Physical

9. *EqEnvInt: Equipment scale interventions matrix

• Dimensions: interventions by Products
• Units: Physical

10. VCUpstCut: Value chain upstream cutoff matrix

• Dimensions: Sectors/Commodities by Activities
• Units: Monetary (in USD, not millions of dollars)

11. VCDownCut: Value chain downstream cutoff matrix

• Dimensions: Value chain products by Sectors/Commodities
• Units: Physical per dollar
• Calculations: Normalize by total destination sector output (millions of USD) after disaggregation

12. *EqEconUpstCut: Equipment-Economy upstream cutoff matrix

• Dimensions: Sectors/Commodities by Processes
• Units: Monetary (in USD, not millions of dollars)
13. *EqVCUpstCut: Equipment-Value chain upstream cutoff matrix
   - Dimensions: Value chain products by Processes
   - Units: Physical

14. *EqEconDownCut: Equipment-Economy downstream cutoff matrix
   - Dimensions: Products by Commodities/Sectors
   - Units: Physical per dollar
   - Calculations: Normalize by total destination sector output (millions of USD) after disaggregation

15. *EqVCDownCut: Equipment-Value chain downstream cutoff matrix
   - Dimensions: Products by Activities
   - Units: Physical

16. VCPrices: Price data for value chain products
   - Dimensions: 1 by Sectors/Commodities
   - Units: Monetary

17. EqPrices: Price data for products
   - Dimensions: 1 by Sectors/Commodities
   - Units: Monetary

5Elements may be zero for products of non-constituent processes and activities
6All prices should be for the same year whenever possible. Must be in units of millions of USD before being used in disaggregation calculations, to match units of economy make and use tables.
18. VCpP: Value chain-Economy process permutation matrix
   - Dimensions: Activities by Commodities/Sectors
   - Units: Dimensionless

19. VCpF: Value chain-Economy product permutation matrix
   - Dimensions: Commodities/Sectors by Value Chain Products
   - Units: Dimensionless

20. EqVCpP: Equipment-Value chain process permutation matrix
   - Dimensions: Processes by Activities
   - Units: Dimensionless

21. EqVCpF: Equipment-Value chain product permutation matrix
   - Dimensions: Value chain Products by Equipment-scale Products
   - Units: Dimensionless

22. EqEconP: Equipment-Economy process permutation matrix
   - Dimensions: Processes by Commodities/Sectors
   - Units: Dimensionless

23. EqEconF: Equipment-Economy product permutation matrix
   - Dimensions: Commodities/Sectors by Equipment-scale Products
   - Units: Dimensionless

D.2.2 Code structure
Figure D.1: Structure of the Python code developed to build and optimize a general P2P model
D.2.3 Model file template

# -*- coding: utf-8 -*-

Created on Wed Dec 3 10:43:08 2014
Updated Thurs Feb 4 2015
Updated Fri Feb 13 2015
Updated Mon Feb 16 2015

This is a model of a toy P2P system and is intended to serve as a basic template for setting up the P2P modeling framework for an arbitrary system. Most of the framework data is read in from .csv files and then passed to the function p2pModel, which calculates the objective function and constraints values.

Chunks of code preceded by a comment that starts with "DNE" ARE NOT TO BE EDITED UNLESS YOU KNOW WHAT YOU ARE DOING. If the preceding comment starts with "Define" or something else, it’s OK to edit.

Within p2pModel:
Inequality constraints are defined as \( f(x) \leq 0 \)
Equality constraints are defined as \( f(x) = 0 \)
The objective function is MINIMIZED. Multiply by \(-1\) to maximize.
@author: rjh

""

from numpy import *

# Define working directory
os.chdir('...')

# Function for reading in data in 2D arrays and storing the data in a variable getnumdata assumes that the data file (.csv) has both row and column names. To change this default functionality, in the definition below change rowNames = 1 to rowNames = 0, and change colNames = 1 to colNames = 0. rowNames and columnNames can also be set each time getnumdata is used - see EqPrices and VCPrices below.

def getnumdata(FileName, rowNames = 1, colNames = 1, missing='nan', fill = 0):
    datafile = open(FileName, 'r')
    356
Var = genfromtxt(datafile, delimiter=',',
               skip_header=colNames,
                missing_values=missing,
                filling_values=fill)

if size(Var.shape) == 1:
    Var = Var[rowNames:]  
elif size(Var.shape) == 2:
    Var = Var[:, rowNames:]  
else:
    Var = 'nan'

return Var

# Function that takes in a vector and diagonalizes it
# to a square matrix.

def hat(Vector):
    Matrix = zeros((Vector.size, Vector.size))
    for i in range(Vector.size):
        Matrix[i,i] = Vector[i]

    return Matrix

# READ IN MULTI-SCALE MODEL DATA ##

# Define number of sectors (equal to number of commodities)
no_sectors = 2
no_commodities = no_sectors

# Define number of activities and value chain products
no_activities = 2
no_vcproducts = 2

# Define number of processes and equipment scale products
no_processes = 2
no_eqproducts = 3

# Equipment scale product prices
EqPrices = hat(getnumdata('EqPrices-toy.csv', rowNames = 1, colNames = 0))

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# Value chain scale product prices
VCPrices = hat(getnumdata('VCPrices-toy.csv', rowNames = 1, colNames = 0))

# Economy make and use matrices
EconMake = getnumdata('EconMake-toy.csv')
EconUse = getnumdata('EconUse-toy.csv')

# Economy TOTAL interventions matrix
EconTotalEnvInt = getnumdata('EconTotalEnvInt-toy.csv')

# Value chain make and use matrices
VCMake = getnumdata('VCMake-toy.csv')
VCUse = getnumdata('VCUse-toy.csv')

# Value chain upstream and downstream cutoff matrices
VCUpstCut = getnumdata('VCUpstCut-toy.csv')
VCDownCut = getnumdata('VCDownCut-toy.csv')

# Value chain interventions matrix
VCEnvInt = getnumdata('VCEnvInt-toy.csv')

# Value chain permutation matrices
VCpF = getnumdata('VCpF-toy.csv')
VCpP = getnumdata('VCpP-toy.csv')

# Equipment scale permutation matrices
EqEconpF = getnumdata('EqEconpF-toy.csv')
EqEconpP = getnumdata('EqEconpP-toy.csv')
EqVCpF = getnumdata('EqVCpF-toy.csv')
EqVCpP = getnumdata('EqVCpP-toy.csv')

#################################################
## SANITY CHECK ON MODEL DATA ##
#################################################

# DNE
dataList = list((EconMake, EconUse, EconTotalEnvInt, VCUse, VCMake, VCUpstCut, VCDownCut, VCPF, VCP, EqEconpF, EqEconpP, EqVCpF, EqVCpP, VCEnvInt))

# DNE
dataFailed = list(ones(14))
dataFailed[0] = EconMake.shape == array([no_commodities, 
no_sectors])
dataFailed[1] = EconUse.shape == array([no_sectors, 
no_commodities])
dataFailed[2] = VCUse.shape == array([no_vcproducts, 
no_activities])
dataFailed[3] = VCMake.shape == array([no_activities, 
no_vcproducts])
dataFailed[4] = VCUpstCut.shape == array([no_sectors, 
no_activities])
dataFailed[5] = VCDownCut.shape == array([no_vcproducts, 
no_sectors])
dataFailed[6] = VCpF.shape == array([no_commodities, 
no_vcproducts])
dataFailed[7] = VCpP.shape == array([no_activities, 
no_sectors])
dataFailed[8] = EqEconpF.shape == array([no_commodities, 
no_eqproducts])
dataFailed[9] = EqEconpP.shape == array([no_processes, 
no_sectors])
dataFailed[10] = EqVCpF.shape == array([no_vcproducts, 
no_eqproducts])
dataFailed[11] = EqVCpP.shape == array([no_processes, 
no_activities])
dataFailed[12] = EconTotalEnvInt.shape[0] == no_sectors
dataFailed[13] = VCEnvInt.shape[0] == no_activities

# DNE
dataFailStatement = array(["Economy make matrix", 
"Economy use matrix", 
"Value chain use matrix", 
"Value chain make matrix", 
"Value chain upstream cutoff matrix", 
"Value chain downstream cutoff matrix", 
"Value chain product permutation matrix", 
"Value chain process permutation matrix", 
"Equipment-economy product permutation matrix", 
"Equipment-economy process permutation matrix", 
"Equipment-value chain product permutation matrix", 
"Equipment-value chain process permutation matrix", 
"Economy interventions matrix", 
"Value chain interventions matrix"])

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# DNE
for i in range(11):
    if dataFailed[i][0] == 0:
        print "----- Dimensional error in model data: ----- 
        print dataFailStatement[i]
        print "Number of rows is 
        print dataList[i].shape[0]
    if dataFailed[i][1] == 0:
        print "----- Dimensional error in model data: -----" 
        print dataFailStatement[i]
        print "Number of columns is 
        print dataList[i].shape[1]

# DNE
if dataFailed[12] == 0:
    print "----- Dimensional error in model data: -----" 
    print dataFailStatement[i]
    print "Number of elements is 
    print dataList[i].shape

# DNE
if dataFailed[13] == 0:
    print "----- Dimensional error in model data: -----" 
    print dataFailStatement[i]
    print "Number of elements is 
    print dataList[i].shape

#########################################################################
## P2P MODEL FUNCTION
#########################################################################

def p2pModel(vars, return_type, EqPrices = EqPrices,
VCPrices = VCPrices,
    EconMake = EconMake, EconUse = EconUse,
    VCUpstCut = VCUpstCut,
    VCDownCut = VCDownCut, VCMake = VCMake, VCUse = VCUse,
    EconTotalEnvInt = EconTotalEnvInt, VCEnvInt = VCEnvInt,
    VCpF = VCpF, VCpP = VCpP, EqEconpP = EqEconpF,
    EqEconpP = EqEconpP): 

#########################################################################
## CONSTRAINTS ##
#########################################################################
# Define number of constraints in the process models
no_of_eq_ineq_constraints = 3
no_of_eq_equ_constraints = 1

# Define number of constraints in the p2pmodel
no_of_p2pmodel_ineq_constraints = 1
no_of_p2pmodel_equ_constraints = 5

# DNE - Sets up vectors to store constraints
ineq = zeros(no_of_eq_ineq_constraints +
             no_of_p2pmodel_ineq_constraints)
equ = zeros(no_of_eq_equ_constraints +
             no_of_p2pmodel_equ_constraints)

########################################################################
## PARAMETERS AND VARIABLES ##
########################################################################

# Define the number of variables in the process models
no_of_unit_op_vars = 4

# Define process parameters (fixed values used
# throughout model)

# Define individual unit op variables using
# elements in vars, for clarity
# Not required but convenient for defining process model.
z_11 = vars[0]
z_12 = vars[1]
z_21 = vars[2]
z_22 = vars[3]

# DNE - Sets up the scaling vector
p2p_s = concatenate((vars[no_of_unit_op_vars:], array([1, 1])))

########################################################################
## FUNDAMENTAL PROCESS MODELS ##
########################################################################

# Define process models and constraints
equ[0] = z_12 - 0.129*z_21 # = 0
ineq[0] = (z_11*z_12/7)*(1 - z_12/7) - 0.12 # <= 0
ineq[1] = -(z_11*z_12/7)*(1 - z_12/7) # <= 0
ineq[2] = 4.2*z_21*(z_22 - 104) - 3000.0 # <= 0

#########################################################################
## EQUIPMENT SCALE MAKE AND USE MATRICES ##
#########################################################################

# Define equipment scale make matrix using unit operation variables and information from the fundamental process models
# Dimensions = Processes by equipment scale products
EqMake = array([[0, z_12*(z_11 - z_11*z_12/7)*(1 - z_12/7),
                 z_12*(z_11*z_12/7)*(1 - z_12/7)],
                [0.129*z_21, 0, 0]])

# Define equipment scale use matrix similarly
# Dimensions: Equipment scale products by processes
EqUse = array([[z_12, 0],
               [0, 0],
               [0, 0]])

# Define equipment scale environmental interventions matrix
# Dimensions: Number of interventions by processes
EqEnvInt = array([1.78*z_12*(z_11*z_12/7)*(1 - z_12/7),
                   1.4*z_12 + 2.0*z_22])

#########################################################################
## EQUIPMENT SCALE CUTOFF MATRICES ##
#########################################################################

# Variable cutoff flows are inserted into the existing matrices elementwise
# Specify POSITIVE matrix values as the cutoff matrices are multiplied by
# negative 1 when inserted into the multi-scale transactions matrix

# Define process inputs that are produced by the economy
# Dimensions = Commodities (Sectors) by Processes
EqEconUpstCut = array([[0.45*z_12, 0.074*z_21*(z_22 - 104)],
                       [0, 0]])

# Define process outputs that are consumed by the economy
# Dimensions = Equipment scale products by sectors

EqEconDownCut = zeros((EqUse.shape[0], EconUse.shape[1]))

# Define process inputs that are produced by the value chain
# Dimensions = Value chain products by processes

EqVCUpstCut = array([[0.79*z_12, 0],
                    [0, 0.129*z_21]])

# Define process outputs that are consumed by the value chain
# Dimensions: Equipment scale products by activities

EqVCDownCut = zeros((EqUse.shape[0], VCUse.shape[1]))

###############################
## FAILURE CHECK ##
###############################

# Define sanity check on process models
# If values going into p2pModel are nan, that will make all
# of the equality constraints nan as well and will delay the
# optimization process
# Depending on the model, some nan values can be replaced
# with real values using this code
# The variable "failed" is passed back to the optimizer to
# tell it if something went wrong in the calculation of the
# objective function.

failed = 0
if any(any(isnan(EqMake))):
    failed = 1
elif any(any(isnan(EqUse))):
    failed = 1
elif any(any(isnan(EqEnvInt))):
    failed = 1
elif any(any(isnan(EqEconUpstCut))):
    failed = 1
elif any(any(isnan(EqEconDownCut))):
    failed = 1
elif any(any(isnan(EqVCUpstCut))):
    failed = 1
elif any(any(isnan(EqVCDownCut))):
    failed = 1
# DNE - Disaggregate economy make matrix
One = ones((2,1))
EconMakeStar = EconMake - dot(VCPrices, (dot(transpose(VCpP),
    dot(VCMake, transpose(VCpF)))) - dot(EqPrices,
    dot(transpose(EqEconpP), dot(EqMake,
    transpose(EqEconpF)))))
SectorOutputStar = dot(transpose(EconMakeStar), One)

# DNE - Normalize value chain and equipment-economy
# downstream cutoff matrices according to the disaggregated
# total sectoral outputs
for i in range(SectorOutputStar.size):
    for j in range(VCDownCut.shape[1]):
        VCDownCut[i,j] = VCDownCut[i,j]/SectorOutputStar[i]
    for j in range(EqEconDownCut.shape[1]):
        EqEconDownCut[i,j] = EqEconDownCut[i,j]/SectorOutputStar[i]

# DNE - Disaggregated economy use matrix
EconUseStar = EconUse - (dot(VCPrices, dot(VCpF, dot(VCUse, VCpP))) +
    dot(VCPrices, dot(VCpF, VCDownCut)) +
    dot(VCUpstCut, VCpP)) - (dot(EqPrices,
    dot(EqEconpF, dot(EqUse, EqEconpP))) +
    dot(EqPrices, dot(EqEconpF, EqEconDownCut)) +
    dot(EqEconUpstCut, EqEconpP))

# DNE - Disaggregated economy environmental interactions matrix
# Commented lines calculate economy-scale emissions factors
# before disaggregation - they are NOT used to build the p2p model
# but can be un-commented to find out how much of an effect the
# disaggregation calculations have on the economy emissions factors
TotalEconEnvIntStar = zeros(2)
EconEnvIntStar = zeros(2)
for i in range(EconTotalEnvInt.shape[0]):
    TotalEconEnvIntStar[i] = EconTotalEnvInt[i] -
        dot(VCEnvInt, VCpP)[i] -
        dot(EqEnvInt, EqEconpP)[i]
    EconEnvIntStar[i] = TotalEconEnvIntStar[i]/SectorOutputStar[i]
\#EconEnvInt\_original[i] = EconTotalEnvInt[0,i]/SectorOutput[i,0]

\# DNE - Disaggregated direct requirements matrix
Astar = dot(EconUseStar, inv(transpose(EconMakeStar)))

\# DNE - Identity matrix
Imat = eye(Astar.shape[0])

\# DNE - Disaggregated Leontief matrix
Lstar = Imat - Astar

\# DNE - Disaggregate value chain make matrix
VCMakeStar = VCMake - dot(EqPrices, dot(transpose(EqVCpP), dot(EqMake, transpose(EqVCpF))))

\# DNE - Disaggregate value chain use matrix
VCUseStar = VCUse - dot(EqPrices, dot(EqVCpF, dot(EqUse, EqVCpP))) - dot(EqPrices, dot(EqVCpF, EqVCDownCut)) - dot(EqVCUpstCut, EqVCpP)

\# DNE - Disaggregated value chain technology matrix
VCYStar = transpose(VCMakeStar) - VCUseStar

\# DNE - Equipment scale technology matrix
EqY = transpose(EqMake) - EqUse

\# DNE - Multi-scale transactions matrix
p2p\_X = concatenate((concatenate((Lstar, -VCUpstCut, -EqEconUpstCut), axis = 1),
                        concatenate((-VCDownCut, VCYStar, -EqVCUpstCut), axis = 1),
                        concatenate((-EqEconDownCut, -EqVCDownCut, EqY), axis = 1)),
                        axis = 0)

\# DNE - Multi-scale environmental interactions matrix
p2p\_B = concatenate(((EconEnvIntStar, VCEnvInt, EqEnvInt),
                          axis = 1)

\# Define final demand vector - Very few elements should be non-zero
p2p\_f = zeros(p2p\_X.shape[0] - 2)

\# DNE - Balance equations on system form equality constraints
\# If the model is set up correctly this equation will work
productBalance = dot(p2p_X, p2p_s)

# One last constraint on production of the primary product
ineq[no_of_eq_ineq_constraints] = 10 - productBalance[-2] #<= 0

# Define objective function
# At least the hybrid scaling vector should appear here
# Unit op vars may also appear here
co2_objective = dot(p2p_B, p2p_s)

###################################################
## DEFINE RETURN VALUES ##
###################################################

# Define more elif statements if you have multiple objectives
if return_type == "CO2 Objective":
    return co2_objective
elif return_type == "Inequalities":
    return ineq
elif return_type == "Equalities":
    return equ
elif return_type == "Failure":
    return failed

###################################################

D.2.4 Optimization file template

# -*- coding: utf-8 -*-

Created on Wed Dec 3 12:33:00 2014
Updated Thurs Feb 4 2015
Updated Fri Feb 13 2015
Updated Mon Feb 16 2015

This is a toy P2P model and is intended to serve as a basic template for building other P2P models.

Chunks of code preceded by a comment that starts with "DNE"
ARE NOT TO BE EDITED UNLESS YOU KNOW WHAT YOU ARE DOING.
@author: rjh

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from numpy import *
from pyOpt import Optimization
from pyOpt import ALGENCAN
# ALGENCAN is a reliable and reasonably powerful solver
# but it cannot handle integer variables

# Define working directory
os.chdir('...')

# Run the model file to define the P2P model function
runfile(r'.../p2pModel.py')

###############################################
def getnumdata(FileName, rowNames = 1, colNames = 1, missing='nan', fill = 0):
    datafile = open(FileName, 'r')
    Var = genfromtxt(datafile, delimiter=',',
                     skip_header=colNames,
                     missing_values=missing,
                     filling_values=fill)
    if size(Var.shape) == 1:
        Var = Var[rowNames:]
    elif size(Var.shape) == 2:
        Var = Var[:, rowNames:]
    elif size(Var.shape) > 2:
        Var = 'nan'

    return Var

###############################################

# Change file names if necessary
no_sectors = getnumdata('EconMake-toy.csv').shape[0]
no_activities = getnumdata('VCMake-toy.csv').shape[0]
no_vcpproducts = getnumdata('VCMake-toy.csv').shape[1]
no_processes = 2
no_eqproducts = 3

# Define some data duplicated p2pModel.py here, for
# convenience and to set up

367
# the optimization problem
no_of_eq_ineq_constraints = 3
no_of_eq_equ_constraints = 1
no_of_p2pModel_ineq_constraints = 0
no_of_p2pModel_equ_constraints = no_sectors + no_vcproducts +
no_eqproducts - 2
no_of_unit_op_vars = 4

# DNE - this function calls p2pModel.py to calculate the objective function,
# constraints and the failed flag
def objfunc(vars):
    f = p2pModel(vars, "CO2 Objective")
    g = concatenate((p2pModel(vars, "Equalities"),
                     p2pModel(vars, "Inequalities")), axis = 0)
    fail = p2pModel(vars, "Failure")
    return f,g,fail

# Define lower and upper limits and initial values for ALL variables
# Change both limits and initial values as necessary
UnitOpDown = array([0.3, 0.0, 14.0, 120.0])
UnitOpUp = array([0.8, 1000.0, 50.0, 140.0])
UnitOpInit = 0.5*(UnitOpDown + UnitOpUp)

EconSDown = zeros(no_sectors)
EconSUp = 1000000.0 + EconSDown
EconSInit = 0.5*(EconSDown + EconSUp)

VCSDown = zeros(no_activities)
VCSUp = 1000.0 + VCSDown
VCSInit = 0.5*(VCSDown + VCSUp)

# EqSDown = zeros(no_processes)
# EqSUp = 1000.0 + EqSDown
# EqSInit = 0.5*(EqSDown + EqSUp)

# DNE - Sets up all components in the optimization problem
opt_prob = Optimization('Minimize Objective Function of p2pModel', objfunc)

# DNE - Specifies variables in optimization problem
opt_prob.addVarGroup('UnitOpDesignVars', no_of_unit_op_vars, type='c',
value = UnitOpInit,
lower = UnitOpDown,
upper = UnitOpUp)
opt_prob.addVarGroup('EconScalingVector', no_sectors, type='c',
value = EconSInit,
lower = EconSDown,
upper = EconSUp)

opt_prob.addVarGroup('VCScalingVector', no_activities, type='c',
value = VCSInit,
lower = VCSDown,
upper = VCSUp)

#opt_prob.addVarGroup('EqScalingVector', no_processes, type='c',
#value = EqSInit,
#lower = EqSDown,
#upper = EqSInit)

# DNE - Specifies objective function
opt_prob.addObj('f')

# DNE - Specifies constraints.
# Equality constraints must be specified first.
opt_prob.addConGroup('gE',
no_of_eq_equ_constraints +
no_of_p2pModel_equ_constraints,
'e') # = 0

opt_prob.addConGroup('gI',
no_of_eq_ineq_constraints +
no_of_p2pModel_ineq_constraints,
'i') # <= 0

# DNE - Prints out problem statement
# This can be commented out without
# affecting how the problem solves
print opt_prob

# DNE - Calls optimizer
algencan = ALGENCAN()

# DNE - Solves optimization problem by MINIMIZING
# the objective function and
# prints solution when found.
# WARNING - JUST BECAUSE SOMETHING PRINTS OUT,
# THAT DOES NOT MEAN A FEASIBLE
# SOLUTION WAS FOUND. LOOK AT THE SOLUTION
# FILE CREATED BELOW TO CHECK
# FEASIBILITY
algencan(opt_prob)
print opt_prob.solution(0)

# Change file name as necessary - Saves solution in a
# .txt file located in
# /your/working/directory/goes/here
opt_prob.write2file(outfile="p2pModelOptResults", disp_sols=1)
Appendix E: Model data and other information for P2P case studies

E.1 Model data for the polymer supply chain design demonstration

The process model matrix is given in Equation (E.1).

\[ Y_R(X, C) = \]

\[
\begin{array}{cccccccc}
\text{Elec.} & \text{CE} & \text{NGE} & \text{MAP} & \text{MBP} & \text{CAP} & \text{CBP} & \text{ETPP} \\
1 & 1 & -26.4 & -27.1 & -19.2 & -21.8 & -(4.823(1 - X^2)C^{-0.3} + 3.2) \\
Monom. & 0 & 0 & 1 & 1 & 0 & 0 & -(4.2X^{1.5}C^{-0.5} + 9.2) \\
Catal. & 0 & 0 & 0 & 0 & 1 & 1 & -C \\
Exp.Pol. & 0 & 0 & 0 & 0 & 0 & 0 & 14.7(1 - X^3)C^{0.25} \\
Thm.Pol. & 0 & 0 & 0 & 0 & 0 & 0 & 14.7X^3C^{0.25} \\
\end{array}
\] (E.1)

The columns of \( Y_R(X, C) \) refer to coal electricity (CE), natural gas electricity (NGE), monomer A production (MAP), monomer B production (MBP), catalyst A production (CAP), catalyst B production (CBP) and ETPP. Rows refer to the value chain products: electricity, monomer, catalyst, expanded polymer and thermoformed polymer. Both production cost data and environmental interaction data is required for these processes. The production costs for the supply chain processes, defined as the cost of producing one unit of product, is as follows.

\[ m(X, C) = \begin{bmatrix} 1.3 & 2.1 & 9.8 & 9.8 & 3.2 & 2.1 & 21.25C(1 - X)^{1.5} + 9.8 \end{bmatrix} \] (E.2)
Environmental interactions data consists of CO₂ emissions in kg/unit output for each process in the supply chain. The interactions are constant for all processes save ETPP, which has interactions as functions of \( X \) and \( C \). Equation (E.3) gives the process scale interactions vector \( \mathbf{B}_R(X, C) \).

\[
\mathbf{B}_R(X, C) = \begin{bmatrix} 38 & 30 & 50 & 42 & 20 & 12 & 1.9C^{-0.2}(72X - 64X^4) \end{bmatrix}
\]  

(E.3)

The economy-scale make and use matrices, from which the adjusted direct requirements matrix \( \mathbf{A}^*(X, C) \) is derived, are given in Equations (E.4) and (E.5).

\[
\mathbf{U} =
\begin{bmatrix}
WS & CM & OE & NGE & PGS & OCM & SCM & PM \\
WS & 236 & 349 & 356 & 233 & 345 & 385 & 194 & 262 \\
CM & 394 & 276 & 301 & 315 & 325 & 211 & 226 & 348 \\
OE & 324 & 201 & 259 & 375 & 272 & 363 & 256 & 235 \\
NGE & 140 & 410 & 282 & 397 & 80 & 248 & 85 & 306 \\
PGS & 201 & 373 & 358 & 405 & 94 & 313 & 255 & 176 \\
OCM & 330 & 152 & 411 & 418 & 382 & 177 & 145 & 87 \\
SCM & 331 & 366 & 248 & 89 & 347 & 421 & 163 & 123 \\
PM & 373 & 219 & 98 & 172 & 227 & 232 & 326 & 361 \\
\end{bmatrix}
\]  

(E.4)

\[
\mathbf{V} =
\begin{bmatrix}
WS & CM & OE & NGE & PGS & OCM & SCM & PM \\
WS & 2654 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
CM & 0 & 2693 & 0 & 0 & 0 & 0 & 0 & 0 \\
OE & 0 & 0 & 2636 & 0 & 0 & 0 & 0 & 0 \\
NGE & 0 & 0 & 0 & 2662 & 0 & 0 & 0 & 0 \\
PGS & 0 & 0 & 0 & 0 & 2312 & 0 & 0 & 0 \\
OCM & 0 & 0 & 0 & 0 & 0 & 2685 & 0 & 0 \\
SCM & 0 & 0 & 0 & 0 & 0 & 0 & 2221 & 0 \\
PM & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2413 \\
\end{bmatrix}
\]  

(E.5)
The economy-scale total environmental interactions vector, used to derive the adjusted economy-scale interactions vector \( \overline{B}^*(X, C) \), is given in Equation (E.6).

\[
\mathbf{R} = \begin{bmatrix}
34444 & 12439 & 17471 & 23338 & 22542 & 26931 & 19229 & 30838
\end{bmatrix}
\]  

(E.6)

The upstream cutoff matrix \( Y_u(X, C) \) and the downstream cutoff matrix \( Y_d(X, C) \) are as follows:

\[
Y_u(X, C) = 
\begin{cases}
\text{CE} & 4.10 & 5.03 & 6.12 & 4.35 & 0.8 & 1.2 & (0.4713 + 3.1525X - 4.0225X^2)1.3C^{-0.5} + 3.5 \\
\text{CM} & 0.13 & 0 & 0 & 0 & 0.02 & 0 & 0 \\
\text{OE} & 0 & 0 & 6.72 & 3.88 & 0.13 & 0 & 0 \\
\text{NGE} & 0 & 0.37 & 0 & 0.31 & 0.21 & 0 & 12.8(X - X^4) + 4.78C^{0.5} \\
\text{PGS} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{OCM} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{SCM} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{PM} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00
\end{cases}
\]

(E.7)

\[
Y_d(X, C) = 
\begin{cases}
\text{Elec.} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{Monom.} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{Catal.} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
\text{Exp.Pol.} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & (14.7X^3C^{0.25})/x_{PM} \\
\text{Thm.Pol.} & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00
\end{cases}
\]

(E.8)

The matrix \( \mathbf{I} - \overline{A}^*(X, C) \) is given in individual columns in Equations (E.9) - (E.16).

\[
\begin{bmatrix}
0.91 \\
-0.15 \\
-0.12 \\
-0.05 \\
-0.08 \\
-0.12 \\
-0.12 \\
-0.14
\end{bmatrix}
\]  

(E.9)
\[
\begin{align*}
[I - \mathbf{A}^*(X, C)]_{\text{CM}} &= \begin{bmatrix} -0.13 \\ 0.90 \\ -0.07 \\ -0.15 \\ -0.14 \\ -0.06 \\ -0.14 \\ -0.08 \end{bmatrix} \\
[I - \mathbf{A}^*(X, C)]_{\text{OE}} &= \begin{bmatrix} -0.13 \\ -0.11 \\ 0.90 \\ -0.11 \\ -0.14 \\ -0.16 \\ -0.03 \\ -0.06 \end{bmatrix} \\
[I - \mathbf{A}^*(X, C)]_{\text{NGE}} &= \begin{bmatrix} -0.09 \\ -0.12 \\ -0.14 \\ 0.85 \\ -0.15 \\ -0.16 \\ -0.03 \\ -0.06 \end{bmatrix}
\end{align*}
\]
\[
\begin{bmatrix}
I - \overline{A}^*(X, C)\end{bmatrix}_{\text{PGS}} = \begin{bmatrix}
-0.15 \times 10^{12} C^{0.5} - 3.41 \times 10^{10} X - 1.79 \times 10^{16} C^{0.25} + 4.36 \times 10^{10} X^2 + (5.11 \times 10^9 + 8.80 \times 10^{14} C^{0.5}) X^3 + 3.41 \times 10^{16} X^4 - 4.36 \times 10^{10} X^5 - 5.11 \times 10^9 \\
1.19 \times 10^{16} C^{0.25} X^2 - 2.41 \times 10^9 \\
5.80 \times 10^{16} C^{0.25} X^3 - 3.46 \times 10^9 \\
1.22 \times 10^{16} C^{0.25} X^4 - 2.47 \times 10^9 \\
3.92 \times 10^{16} C^{0.25} X^5 - 2.89 \times 10^9 \\
2.13 \times 10^{18} C^{0.25} X^6 - 5.10 \times 10^9 C^{0.25} + 7.97 \times 10^7 C^{0.75} - 4.13 \times 10^4 C^{0.25} X^2 - 4.27 \times 10^8 C^{0.25} X^3 - 7.97 \times 10^6 C^{0.75} X^2 + 2.13 \times 10^6 C^{0.25} X^7 + 8.47 \times 10^{12} \\
1.00 - 0.93 \times 10^{12} C^{0.25} + 4.88 \times 10^{14} C^{0.25} X^3 - 8.48 \times 10^{16} C^{0.25} X^4 + 8.48 \times 10^{16} C^{0.25} X^5 - 8.48 \times 10^{16} C^{2.25} X^6 + 8.48 \times 10^{16} C^{0.25} X^7 - 8.48 \times 10^{16} C^{2.25} X^8 - 9.94 \times 10^{15} \\
1.22 \times 10^{16} C^{0.25} X^3 - 2.47 \times 10^9 \\
1.45 \times 10^{16} C^{0.25} - 4.25 \times 10^9 C^{0.75} + 2.01 \times 10^{14} C^{0.25} X^2 - 4.25 \times 10^9 C^{0.75} X^3 + 4.25 \times 10^9 C^{0.75} X^4 - 4.25 \times 10^9 C^{0.75} X^5 - 4.07 \times 10^{13} \\
2.63 \times 10^{11} C^{0.25} X^3 - 2.47 \times 10^9 \\
1.45 \times 10^{16} C^{0.25} - 4.25 \times 10^9 C^{0.75} + 2.01 \times 10^{14} C^{0.25} X^2 - 4.25 \times 10^9 C^{0.75} X^3 + 4.25 \times 10^9 C^{0.75} X^4 - 4.25 \times 10^9 C^{0.75} X^5 - 4.07 \times 10^{13} \\
6.02 \times 10^9 C^{0.25} + 1.18 \times 10^{12} C^{0.25} X^3 - 2.41 \times 10^{13} \\
1.22 \times 10^{14} C^{0.25} X^3 - 2.47 \times 10^9 \\
\end{bmatrix}
\]

(E.13)

\[
\begin{bmatrix}
I - \overline{A}^*(X, C)\end{bmatrix}_{\text{OCM}} = \begin{bmatrix}
-0.14 \\
-0.08 \\
-0.13 \\
-0.08 \\
-0.12 \\
0.93 \\
-0.16 \\
-0.09 \\
\end{bmatrix}
\]

(E.14)
\[ \hat{\mathbf{B}}(X, C) = \begin{bmatrix} 12.98 & 4.52 & 6.63 & 8.77 & 9.75 & 10.03 & 1.92 \times 10^4 & 1.00 - 3.26 \times 10^{-3} C \frac{1}{2.21 \times 10^3 - 7.25 C} \\ 12.78 \end{bmatrix} \]
Table E.1: Equipment-economy upstream cutoff matrix for the original P2P model.

<table>
<thead>
<tr>
<th></th>
<th>Ethanol plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water ($\text{,}$)</td>
<td>5.28E-04</td>
</tr>
<tr>
<td>Corn grits ($\text{,}$)</td>
<td>7.48E-02</td>
</tr>
</tbody>
</table>

**E.2 Model data for the corn ethanol case study**

The equipment scale model of the corn ethanol plant, the economy scale make and use tables, and the economy scale interventions vector, are all available from the author on request. Electronic copies of all data sets in this section are also available on request.

**E.2.1 Equipment scale matrices**

Tables E.1 - E.4 contain the equipment scale matrices. Entries in *italics* indicate variable element that are scaled by a quantity calculated within the ethanol plant model.

The equipment-economy and equipment-value chain downstream cutoff matrices consisted of all zeros for both the original and the alternative P2P model.

**E.2.2 Value chain models**

Matrices containing the value chain models are given in Tables E.5 - E.11. Value chain models for both the original P2P model and the alternative P2P model are given.
Table E.2: Equipment-value chain upstream cutoff matrix for the original P2P model.

<table>
<thead>
<tr>
<th>Ethanol plant</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen fertilizer (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>P2O5 fertilizer (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>K2O fertilizer (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>CaCO3 fertilizer (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>Herbicide (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>Insecticide (g)</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at field (kg)</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at plant (kg)</td>
<td>-18.00</td>
</tr>
<tr>
<td>Natural gas (kJ)</td>
<td>-0.83</td>
</tr>
<tr>
<td>Coal (kJ)</td>
<td>-0.09</td>
</tr>
<tr>
<td>Electricity (kJ)</td>
<td>-0.07</td>
</tr>
<tr>
<td>Alpha-amylase (kg)</td>
<td>-1.00</td>
</tr>
<tr>
<td>Gluco-amylase (kg)</td>
<td>-1.00</td>
</tr>
<tr>
<td>Yeast (kg)</td>
<td>-1.00</td>
</tr>
<tr>
<td>Urea (kg)</td>
<td>-1.00</td>
</tr>
</tbody>
</table>

Table E.3: Equipment-economy upstream cutoff matrix for the alternative P2P model.

<table>
<thead>
<tr>
<th>Ethanol plant</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Water ($)</td>
<td>5.28E-04</td>
</tr>
<tr>
<td>Corn seeds ($)</td>
<td>0.00</td>
</tr>
<tr>
<td>Natural gas ($)</td>
<td>3.88E-06</td>
</tr>
<tr>
<td>Coal ($)</td>
<td>1.11E-06</td>
</tr>
<tr>
<td>Electricity ($)</td>
<td>1.33E-05</td>
</tr>
<tr>
<td>Alpha-amylase ($)</td>
<td>2.75</td>
</tr>
<tr>
<td>Gluco-amylase ($)</td>
<td>2.75</td>
</tr>
<tr>
<td>Yeast ($)</td>
<td>5.50</td>
</tr>
<tr>
<td>Urea ($)</td>
<td>0.11</td>
</tr>
<tr>
<td>Corn grits ($)</td>
<td>7.48E-02</td>
</tr>
</tbody>
</table>
Table E.4: Equipment-value chain upstream cutoff matrix for the alternative P2P model.

<table>
<thead>
<tr>
<th>Corn at plant (kg)</th>
<th>Ethanol plant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-18.00</td>
</tr>
</tbody>
</table>

E.2.3 Information for permutation matrices

Rather than print out all of the permutation matrices, which consist largely of zeros, the parent sector for each value chain activity and for the ethanol plant is listed in Table E.12. Elements corresponding to these sector-activity and sector-process pairings in the permutation matrices are 1; all other elements are zero. Electronic files containing the permutation matrices are available from the author on request.
Table E.5: Value chain technology matrix for the original P2P model, with the more detailed value chain model (part 1 of 2).

<table>
<thead>
<tr>
<th></th>
<th>Nitrogen fertilizer production</th>
<th>P2O5 fertilizer production</th>
<th>K2O fertilizer production</th>
<th>CaCO3 fertilizer production</th>
<th>Herbicide production</th>
<th>Insecticide production</th>
<th>Corn farming</th>
<th>Corn transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen fertilizer (g)</td>
<td>415.33</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-415.33</td>
<td>0.00</td>
</tr>
<tr>
<td>P2O5 fertilizer (g)</td>
<td>0.00</td>
<td>147.77</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-147.77</td>
<td>0.00</td>
</tr>
<tr>
<td>K2O fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>172.11</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-172.11</td>
<td>0.00</td>
</tr>
<tr>
<td>CaCO3 fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1149.87</td>
<td>0.00</td>
<td>0.00</td>
<td>-1149.87</td>
<td>0.00</td>
</tr>
<tr>
<td>Herbicide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>4.75</td>
<td>0.00</td>
<td>-4.75</td>
<td>0.00</td>
</tr>
<tr>
<td>Insecticide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.40</td>
<td>0.00</td>
<td>-0.40</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at field (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>25.40</td>
<td>-907.19</td>
</tr>
<tr>
<td>Corn at plant (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>907.19</td>
<td>0.00</td>
</tr>
<tr>
<td>Natural gas (kJ)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Coal (kJ)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Electricity (kJ)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Alpha-amylase (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Gluco-amylase (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Yeast (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Urea (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table E.6: Value chain technology matrix for the original P2P model (part 2 of 2).

<table>
<thead>
<tr>
<th></th>
<th>Natural gas production, distribution</th>
<th>Coal production, distribution</th>
<th>Electricity production, distribution</th>
<th>Alpha-amylase production, distribution</th>
<th>Gluco-amylase production, distribution</th>
<th>Yeast production, distribution</th>
<th>Urea production, distribution</th>
<th>Ethanol transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>P2O5 fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>K2O fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>CaCO3 fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Herbicide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Insecticide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at field (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at plant (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Natural gas (kJ)</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Coal (kJ)</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Electricity (kJ)</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Alpha-amylase (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Gluco-amylase (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Yeast (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Urea (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table E.7: Value chain upstream cutoffs for the original P2P model.

<table>
<thead>
<tr>
<th></th>
<th>Nitrogen fertilizer production</th>
<th>P2O5 fertilizer production</th>
<th>K2O fertilizer production</th>
<th>CaCO3 fertilizer production</th>
<th>Herbicide production, distribution</th>
<th>Insecticide production, distribution</th>
<th>Corn farming</th>
<th>Corn transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water use ($)</td>
<td>4.59E-03</td>
<td>3.16E-03</td>
<td>5.84E-04</td>
<td>5.04E-02</td>
<td>3.04E-06</td>
<td>2.55E-07</td>
<td>2.92E-01</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn seed ($)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>4.62E-01</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Natural gas production, distribution</th>
<th>Coal production, distribution</th>
<th>Electricity production, distribution</th>
<th>Alpha-amylase production, distribution</th>
<th>Gluco-amylase production, distribution</th>
<th>Yeast production, distribution</th>
<th>Urea production, distribution</th>
<th>Ethanol transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water use ($)</td>
<td>3.43E-09</td>
<td>8.80E-09</td>
<td>1.01E-06</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.74E-03</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn seed ($)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table E.8: Value chain scale environmental interventions vector for the original P2P model.

<table>
<thead>
<tr>
<th></th>
<th>Nitrogen fertilizer production</th>
<th>P2O5 fertilizer production</th>
<th>K2O fertilizer production</th>
<th>CaCO3 fertilizer production</th>
<th>Herbicide production, distribution</th>
<th>Insecticide production, distribution</th>
<th>Corn farming</th>
<th>Corn transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>kg CO2 emissions</td>
<td>1690.44</td>
<td>248.49</td>
<td>617.43</td>
<td>15.67</td>
<td>95.24</td>
<td>9.34</td>
<td>892.45</td>
<td>50297.16</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Natural gas production, distribution</th>
<th>Coal production, distribution</th>
<th>Electricity production, distribution</th>
<th>Alpha-amylase production, distribution</th>
<th>Gluco-amylase production, distribution</th>
<th>Yeast production, distribution</th>
<th>Urea production, distribution</th>
<th>Ethanol transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>kg CO2 emissions</td>
<td>0.01</td>
<td>0.00</td>
<td>0.16</td>
<td>1468.65</td>
<td>6550.30</td>
<td>2520.88</td>
<td>1116.20</td>
<td>134.57</td>
</tr>
</tbody>
</table>
Table E.9: Value chain technology matrix for the alternative P2P model, with the less detailed value chain model.

<table>
<thead>
<tr>
<th></th>
<th>Nitrogen fertilizer production</th>
<th>P&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;5&lt;/sub&gt; fertilizer production</th>
<th>K&lt;sub&gt;2&lt;/sub&gt;O fertilizer production</th>
<th>CaCO&lt;sub&gt;3&lt;/sub&gt; fertilizer production</th>
<th>Herbicide production</th>
<th>Insecticide production</th>
<th>Corn farming</th>
<th>Corn transp.</th>
<th>Ethanol transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen fertilizer (g)</td>
<td>415.33</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-415.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>P&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;5&lt;/sub&gt; fertilizer (g)</td>
<td>0.00</td>
<td>147.77</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-147.77</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>K&lt;sub&gt;2&lt;/sub&gt;O fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>172.11</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-172.11</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>CaCO&lt;sub&gt;3&lt;/sub&gt; fertilizer (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1149.87</td>
<td>0.00</td>
<td>0.00</td>
<td>-1149.87</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Herbicide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>4.75</td>
<td>0.00</td>
<td>-4.75</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Insecticide (g)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.40</td>
<td>-0.40</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at field (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>25.40</td>
<td>-907.19</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn at plant (kg)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>907.19</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table E.10: Value chain upstream cutoff matrix for the alternative P2P model.

<table>
<thead>
<tr>
<th></th>
<th>Nitrogen fertilizer production</th>
<th>P2O5 fertilizer production</th>
<th>K2O fertilizer production</th>
<th>CaCO3 fertilizer production</th>
<th>Herbicide production, distribution</th>
<th>Insecticide production, distribution</th>
<th>Corn farming</th>
<th>Corn transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water use ($)</td>
<td>4.59E-03</td>
<td>3.16E-03</td>
<td>5.84E-04</td>
<td>5.04E-02</td>
<td>3.04E-06</td>
<td>2.55E-07</td>
<td>2.92E-01</td>
<td>0.00</td>
</tr>
<tr>
<td>Corn seed ($)</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>4.62E-01</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table E.11: Value chain scale environmental interventions vector for the alternative P2P model.

<table>
<thead>
<tr>
<th>Nitrogen fertilizer production</th>
<th>P_{2}O_{5} fertilizer production</th>
<th>K_{2}O fertilizer production</th>
<th>CaCO_{3} fertilizer production</th>
<th>Herbicide production</th>
<th>Insecticide production</th>
<th>Corn farming</th>
<th>Corn transp.</th>
<th>Ethanol transp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>kg CO_{2} emissions</td>
<td>1690.44</td>
<td>248.49</td>
<td>617.43</td>
<td>15.67</td>
<td>95.24</td>
<td>9.34</td>
<td>892.45</td>
<td>50297.16</td>
</tr>
<tr>
<td>Parent</td>
<td>Activity</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------------------------------------</td>
<td>-----------------------------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td>Nitrogen fertilizer production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td>P2O5 fertilizer production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td>K2O fertilizer production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer manufacturing</td>
<td>CaCO3 fertilizer production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pesticide and other agricultural chemical manufacturing</td>
<td>Herbicide production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pesticide and other agricultural chemical manufacturing</td>
<td>Insecticide production</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grain farming</td>
<td>Corn farming</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rail transportation</td>
<td>Corn transportation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Truck transportation</td>
<td>Ethanol transportation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parent</td>
<td>Process</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other basic organic chemical manufacturing</td>
<td>Ethanol plant</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
E.3 Code for implementing pseudo-equilibrium procedure

Data used in implementing this code and for the case study of Section 8.3 can be obtained from the author on request.

```python
# -*- coding: utf-8 -*-

##
Created on Mon Mar 30 11:10:53 2015
Revised June 7-12 2015

Code to apply pseudo-equilibrium method developed by Jun-Ki Choi (Energy Policy, 2010) to an economic input-output model. Original MATLAB code supplied by Prof. Choi has been adapted to Python and altered to model the effects of a CO2 emissions tax rather than the original carbon tax.

Commented-out block of code at the end writes the new economy model and some diagnostic data to file. Uncomment to generate a model under a new emissions tax value and to check calculations.
@author: Jun-Ki Choi, Rebecca Hanes

##

from numpy import *

os.chdir('/home/rjhanes/Dropbox/Research/ActiveResearch/SustainableDesign/Equilibrium/Pseudo/OptimizationFiles')

def getmatrix(FileName, rowNames = 1, colNames = 1, missing='nan', fill=0):
    datafile = open(FileName, 'r')
    Var = genfromtxt(datafile, delimiter=',',
                     skip_header=colNames,
                     missing_values=missing,
                     filling_values=fill)
    if size(Var.shape) == 1:
        Var = Var[rowNames:]
    elif size(Var.shape) == 2:
        Var = Var[:, rowNames:]
    elif size(Var.shape) > 2:
        Var = 'nan'
```

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return matrix(Var)

def getarray(FileName, rowNames = 1, colNames = 1,
            missing='nan', fill=0):
    datafile = open(FileName, 'r')
    Var = genfromtxt(datafile, delimiter=',',
                     skip_header=colNames,
                     missing_values=missing,
                     filling_values=fill)
    if size(Var.shape) == 1:
        Var = Var[rowNames:]
    elif size(Var.shape) == 2:
        Var = Var[:, rowNames:]
    elif size(Var.shape) > 2:
        Var = 'nan'
    return Var

def hat(Matrix):
    if Matrix.shape[0] == 1:
        return diag(array(Matrix)[0,:])
    elif Matrix.shape[1] == 1:
        return diag(array(Matrix)[:,0])
    else:
        return nan

###
C = 0.055  # Dollars per kg CO2  ($10 per U.S. ton CO2 is  
            # current emissions tax in BC, Canada)
###
##  Read in data
# Industry-by-commodity make matrix
EconMake = getmatrix('EconMake2007.csv') #MM$
# Commodity-by-industry use matrix
EconUse = getmatrix('EconUse2007.csv') #MM$
# Total commodity output vector
CommOutput = getmatrix('TotalCommodityOutput2007.csv') #MM$
# Total industry output vector
IndOutput = getmatrix('TotalIndustryOutput2007.csv') #MM$
# Monetary final demand vector
FinalDemand_pretax = getmatrix('FinalDemand2007.csv') #MM$

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# Elasticity values
Elasticity = getmatrix('Elasticities.csv',
    rowNames = 0, colNames = 0)

# Total CO2 emissions for each sector
EconTotalCO2 = getmatrix('EconTotalEnvInt2007.csv',
    rowNames = 0, colNames = 0)  # kg CO2
# CO2 emissions factors for each sector
EconCO2_pretax = divide(transpose(EconTotalCO2),
    IndOutput)  # kg CO2 per million dollars

# Total value added for each sector
# Value added for grain farming is
# -156 million due to subsidies
V_pretax = getmatrix('EconTotalValueAdded2007.csv')  # MM$
# Value added per dollar industry output
V_pretax_norm = divide(transpose(V_pretax),
    IndOutput)

I = eye(EconUse.shape[0])

# Industry-by-industry direct requirements matrix, pre-tax
A_pretax = EconMake*inv(hat(CommOutput))*EconUse*inv(hat(IndOutput))
# Industry-by-industry transactions matrix, pre-tax
Z_pretax = A_pretax*hat(IndOutput)  # MM$

# Calculate amount of emissions tax for each sector
tax = (1/1000000.0)*C*EconTotalCO2  # MM$

## Cost Push Model ##
# Calculate change in value added due to emissions tax
V_posttax = V_pretax + transpose(tax)  # MM$

# Fraction change in value added
del_V = divide((V_posttax - V_pretax), V_pretax)

# Percentage change in value added in normalized form
del_K = transpose(multiply(transpose(V_pretax_norm), del_V))

# Total percentage price change calculated via cost push
del_P = linalg.inv(I - transpose(A_pretax))*transpose(del_K)

# Post-tax transactions matrix
\[ Z_{\text{posttax}} = \text{transpose}(\text{transpose}(Z_{\text{pretax}})*(I + \hat{\text{del}}_P)) \] #MM$

\[ \text{EconUse}_{\text{posttax}} = \text{transpose}(\text{transpose}(\text{EconUse})*(I + \hat{\text{del}}_P)) \] #MM$

\[ \text{EconMake}_{\text{posttax}} = \text{EconMake}*(I + \hat{\text{del}}_P) \] #MM$

# Industry output post-price change, pre-demand change
# These values are all much greater than the pretax industry outputs
\[ X_{\text{interm}} = (I + \hat{\text{del}}_P)\text{transpose}(\text{IndOutput}) \] #MM$

# Monetary final demand post-price change, pre-demand change
\[ \text{FinalDemand}_{\text{interm}} = (I + \hat{\text{del}}_P)\text{FinalDemand}_{\text{pretax}} \] #MM$

# Post-tax industry-industry direct requirements matrix
\[ A_{\text{posttax}} = Z_{\text{posttax}}\text{linalg.inv}(\hat{X}_{\text{interm}}) \]

## Demand Pull Model ##
# Change in final demand
\[ \text{del}_\text{FinalDemand} = \text{multiply}(\text{transpose}(\text{Elasticity}), \text{del}_P) \]

# Post-tax (post-price change and post-demand change)
# final demand
\[ \text{FinalDemand}_{\text{posttax}} = (I + \hat{\text{del}}_{\text{FinalDemand}})\text{FinalDemand}_{\text{interm}} \] #MM$

# Post tax industry output
\[ \text{IndOutput}_{\text{posttax}} = \text{linalg.inv}(I - A_{\text{posttax}})\text{FinalDemand}_{\text{posttax}} \] #MM$

# Post tax CO2 emissions factors for each sector
\[ \text{EconCO2}_{\text{posttax}} = \text{EconCO2}_{\text{pretax}}\text{linalg.inv}(I + \hat{\text{del}}_P) \] #kg CO2 per dollar output

# Post tax total CO2 emissions for each sector
\[ \text{EconTotalCO2}_{\text{posttax}} = \text{multiply}(\text{transpose}(\text{EconCO2}_{\text{posttax}}), \text{IndOutput}_{\text{posttax}}) \] #kg CO2

\[ \text{TotalCO2}_\text{pct\_change} = 100*\text{divide}((\text{EconTotalCO2}_{\text{posttax}} - \text{EconTotalCO2}_\text{pretax}) , \text{EconTotalCO2}) \]

\[ \text{EmissionsFactor}_\text{pct\_change} = 100*\text{divide}((\text{EconCO2}_{\text{posttax}} - \text{EconCO2}_\text{pretax}) , \text{EconCO2}_\text{pretax}) \]

\[ \text{FinalDemand}_\text{pct\_change} = 100*\text{divide}((\text{FinalDemand}_{\text{posttax}} - \text{FinalDemand}_\text{pretax}) , \text{FinalDemand}_\text{pretax}) \]

\[ \text{IndOutput}_\text{pct\_change} = 100*\text{divide}((\text{IndOutput}_{\text{posttax}} - \text{IndOutput}_\text{pretax}) , \text{IndOutput}_\text{pretax}) \]
transpose(IndOutput)), transpose(IndOutput))

savetxt('EconUse-50.csv', EconUse_posttax, delimiter=','
savetxt('EconMake-50.csv', EconMake_posttax, delimiter=','
savetxt('EconTotalEnvInt-50.csv', EconTotalCO2_posttax
    delimiter=','
savetxt('PctPriceChange-50.csv', del_P, delimiter=','
savetxt('TotalCO2-pct-change-50.csv', TotalCO2_pct_change,
    delimiter=','
savetxt('EmissionsFactor-pct-change-50.csv',
    EmissionsFactor_pct_change, delimiter=','
savetxt('FinalDemand-pct-change-50.csv',
    FinalDemand_pct_change, delimiter=','
savetxt('IndustryOutput-pct-change-50.csv',
    IndOutput_pct_change, delimiter=',')
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