

# Synthesis of Sustainable Energy Supply Chain by the P-graph Framework

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**S** Supporting Information

**ABSTRACT:** The present work proposes a computer-aided methodology for designing sustainable supply chains in terms of sustainability metrics by utilizing the P-graph framework. The methodology is an outcome of the collaboration between the Office of Research and Development (ORD) of the U.S. EPA and the research group led by the creators of the P-graph framework at the University of Pannonia. The integration of supply chain design and sustainability is the main focus of this collaboration. The P-graph framework provides a mathematically rigorous procedure for synthesizing optimal and alternative suboptimal networks subject to multiple objectives and constraints, which include profitability and sustainability in the proposed methodology. Specifically, to evaluate the sustainability of a given process under construction including its supply chain, sustainability metrics are incorporated into the design procedure. The proposed methodology is demonstrated with the optimal design of a supply chain for providing heat and electric power to an agricultural region with relatively limited land area where agricultural wastes can potentially be recovered as renewable resources. The objective functions for optimization comprise the profit and the ecological footprint. The results of the study indicate that, compared to using electricity from the grid and/or natural gas, using renewable energy resources can yield substantial cost reductions of up to 5%, as well as significant ecological footprint reductions of up to 77%. It may, therefore, be possible to design more sustainable supply chains that are both cost-effective and less environmentally damaging.

## 1. INTRODUCTION

**1.1. Sustainability.** At its broadest application, sustainability is thought of in terms of meeting needs—the needs of the present population, as well as the needs of future populations,<sup>1</sup> and at the same time, without causing irreparable damage to the ecological systems that ultimately support these needs. At best, achievement of sustainability while meeting all of these needs is a balancing act. Since sustainability was first defined, numerous questions have risen as to what, exactly, constitutes “needs”, how needs are met, and how progress or achievement of sustainability is measured.

Perhaps the definition is so nebulous because the needs of humanity are many and varied. In satisfying the human condition, themes such as energy, water, food, wastes, safety, economics, and health must be taken into consideration. In attempting to quantify and measure sustainability, many indicators have been developed; the Compendium of Sustainable Development Initiatives database currently contains 894 initiatives.<sup>2</sup> Some of these indicators are more singular in that they are only applicable at a particular level such as an indicator that only measures sustainability of nations or cities. Others can be applied from the global system level to an individual level to a singular process level. However, over time, all of these different sustainability indicators are consistently classified into 3 primary dimensions known as the environmental, economic, and social dimensions. Accounting for all three of these dimensions is known as triple-bottom line accounting.<sup>3</sup>

While it is evident the complexity of sustainability has led to countless indicators to measure sustainability, it remains that

sustainability must be addressed in every decision of human society today. All three dimensions must be addressed to achieve sustainability—what may seem economically sustainable at a certain level may not also be environmentally or socially sustainable. Even now, mass consumerism and societal emphasis on wealth (economic dimension) is overtaxing the ecological system (environmental dimension) beyond what can be supported.<sup>4–7</sup> Therefore, in measuring the sustainability of the energy production processes addressed in this paper, the Ecological Footprint<sup>5</sup> is used in our first attempt in identifying sustainable supply chains. Although the Ecological Footprint does not explicitly address the social dimension in which population health is included, greenhouse gases resulting from the energy production feedstocks are assessed. Because greenhouse gases negatively impact the environment and human health, the social dimension is inherently addressed, and the Ecological Footprint is regarded as a multidimensional indicator.<sup>8</sup>

**1.2. Supply Chain Design.** Businesses use supply chain management<sup>9</sup> to help organize the chain of events associated with a product or service. In the case of a material product, this often includes the flow of raw materials and energy from supply, manufacturing, distribution, usage, and disposal

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processes as well as the flow of the associated necessary information. In the case of a service, there might be more focus on the flow of information, but that information often carries a physical footprint due to the presence of the energy, people, and communication systems needed to initiate and maintain the flow of information. Traditionally, supply chains have been designed and optimized for profit.<sup>10</sup> However, the increasing human population<sup>11</sup> along with increasing prosperity<sup>12</sup> has created a situation where it is not only necessary to organize supply chains for profit but also to assess and address associated environmental concerns. Simply put, many more people who are consuming many more goods and services have created flows of goods, services, and information which present the world with unprecedented environmental challenges in terms of unrestrained resource consumption and/or environmental pollution. Therefore, the design of sustainable supply chains is an effort to meet the consumption needs of the human population within the limits of the Earth.

Supply chains are essentially networks along which material, energy, and information flow for the purpose of meeting some human need whether material or otherwise. Extensive literature currently exists<sup>13</sup> on the design of traditional profit-oriented supply chains, along with a developing body of literature on the design of supply chains for the environment.<sup>14</sup> Here we propose to explore methods for the design of supply chains that are not only profitable but also sustainable. Differences exist between green supply chains that are designed to minimize environmental impact and those that are designed for sustainability, although the two are often related.<sup>15</sup> The main difference is often the time frame under consideration. So both green and sustainable supply chains are designed to minimize environmental impact, but a sustainable supply chain is designed to minimize environmental impacts over the long-term and to ensure that the environment can indefinitely support the material and energetic flow requirements of the supply chain.

Here we propose to design sustainable supply chains using the P-graph framework with the following additional criteria: minimizing supply chain capital and operating cost and maintaining a low ecological footprint of the supply chain feedstock. The P-graph framework is essentially an algorithm for optimal network design, which we are using to design supply chains that are optimal with respect to cost and the ecological footprint of the feedstock. Keeping costs low creates an economic need to conduct operations as profitably as possible. Minimizing the land area needed to support a supply chain's energy feedstock inputs and, for the purposes of this study, achieving a low ecological footprint<sup>5</sup> indicates that operations are being conducted with the smallest possible land use burden on the environment. Together, these two criteria represent a reasonable initial assessment of the sustainability of a proposed or existing supply chain.

There are two more points here that merit further discussion. First, why use an integrated indicator such as the ecological footprint and not other simple indicators such as ozone emissions or water quality? Primarily because many variables characterize a supply chain, and integrated indicators offer protection against shifting risks from one environmental criterion to another, i.e. resolving an air pollution problem by creating a water pollution problem. Further, the theory underlying an integrated metric provides a basis for managing many disparate variables that characterize the supply chain, which is something that cannot be done by individually

assessing large numbers of distinct variables with simple indicators.

**1.3. Process Network Synthesis.** A process system or network endeavors to create certain products (or services) from raw materials using a number of processing steps. Process synthesis determines the structure of a process system. Examples of said networks are innumerable and range from food processing plants to chemical production to energy production networks to basically any product utilized in today's society. A good review of the development of process synthesis in the past two and a half decades was completed by Sargent in 2004.<sup>16</sup>

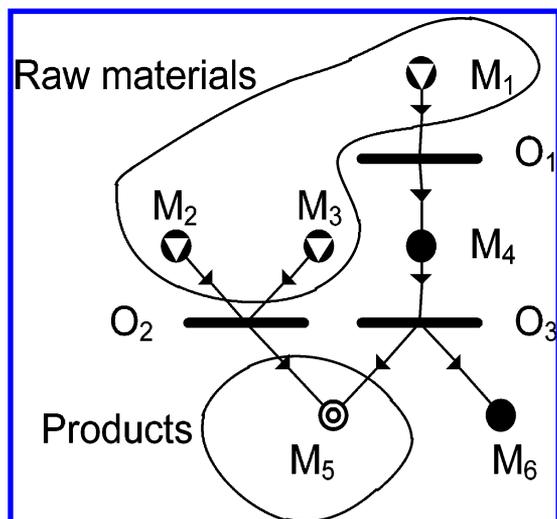
Because of the combinatorial nature of the problem, a multitude of alternative feasible structures comprised of multiple operating units is usually capable of producing the desired products. Process synthesis seeks the optimal network in terms of some objective function, e.g., profit, revenue, sustainability, etc. The determination of the optimal network structure is most frequently referred to as flowsheet design or process-network synthesis (PNS).

PNS is an essential component of process system engineering. Its significance is highlighted by numerous publications in the scientific literature. A computer-aided flowsheet design method has been available,<sup>17</sup> which includes the group contribution approach to predict molecular properties of material species participating in the process to be designed. This method has been further developed for mineral processing flowsheet design.<sup>18</sup> The structural properties, especially the redundancy, of the superstructures of the processes of interest have been explored.<sup>19</sup> A novel representation, the state-task network, has been introduced originally for scheduling problems.<sup>20</sup> This representation includes explicitly both the states (feedstocks, intermediates, and final products) and the tasks (operations) as network nodes. The state-task network and state-equipment network has been applied to aid process synthesis.<sup>21</sup> The mathematical modeling of either of the two representations is performed with generalized disjunctive programming. A similar disjunctive optimization model has been deployed for simultaneous flowsheet optimization and heat integration,<sup>22</sup> systems involving both nonisothermal and isothermal streams have been considered. It has been shown that the latter system gives rise to mixed integer linear programs. The synthesis of separation networks with nonsharp separation has been explored,<sup>23</sup> where the robust optimization capability of the evolutionary algorithms has been deployed in conjunction with the rigorous modeling capability of Aspen Plus.

The P-graph methodology is a graph-theoretical approach utilized for solving PNS problems. In a PNS problem, the maximum available raw materials may be constrained, and the rate of manufacturing of each product must be specified. The P-graphs (process graphs) are bipartite graphs, each comprising nodes for a set of materials, a set of operating units, and arcs linking them. The materials can be the raw materials, intermediates, and products. The operating units are defined in terms of input and output materials, their ratios, and their cost functions.

Figure 1 represents a process network featuring operating units  $O_1$ ,  $O_2$ , and  $O_3$  and materials  $M_1$ - $M_6$ , where  $M_1$ ,  $M_2$ , and  $M_3$  are raw materials;  $M_4$  is an intermediate;  $M_5$  is a product; and  $M_6$  is a byproduct.

P-graph frameworks have been utilized in many areas such as emission reduction,<sup>24</sup> optimal retrofit design for a steam-supply



**Figure 1.** PNS network involving three operating units and six materials.

system,<sup>25</sup> and downstream processes for biochemical production.<sup>26</sup>

**1.4. Ecological Footprint.** The Ecological Footprint is a sustainability metric which calculates the amount of land required to support and assimilate a given human population's consumption and wastes.<sup>5</sup> The metric essentially measures whether a population or economy is living within the means of the population's natural system boundaries. The metric was initially applied at the global level where it was determined approximately as of 1977 that the human population's consumption and wastes required more than 1 planet to maintain those levels of consumption and wastes.<sup>27</sup> Since that time, the metric has gone through several revisions and has been applied from national to individual levels.<sup>27</sup>

**1.5. Problem Definition.** Our aim is to present a computer-aided methodology for designing sustainable supply chains in terms of sustainability metrics by utilizing the P-graph framework. For this study, a PNS problem is addressed where the goal is to produce specific amounts of heat and electricity using renewable resources such as grass silage, corn silage, wood, and fossil resources, such as natural gas and electricity from the existing grid. Biogas plants, gas furnaces, and pelletizers are some of the potential operating units. Due to the array of feedstock choices and multifunctionality of generation processes, the modeling of the operating units in this problem is challenging. For example, a biogas plant can process corn silage or grass silage. In the P-graph framework, an operating unit requires well-defined input, and, if an operating unit has two inputs, we must discern whether both inputs are required at the same time, or if one input or the other will suffice. This decision is made automatically by the PNS through application of a modeling technique, and the user is not required to make the choice. Another challenge is the integration of the sustainability metrics into the model itself. Explicitly defined constraints for these metrics are required for this study; however, we want to emphasize that the analysis shown here is meant for illustrating the methodology for a supply chain design. For example, we might look for solutions where the ecological footprint is not larger than a predefined value. The techniques to handle these challenges will be introduced in the following sections, as well as in an accompanying case study. Although logistics is also an

important consideration in supply chain analysis, for the context of this paper, we have focused on the synthesis of the energy supply chains and, in particular, the determination of which raw materials and energy conversion technologies should be used based upon the connections between these elements. The involvement of logistics will be a beneficial extension in subsequent analyses.

## 2. METHODOLOGY

The theoretical results of the P-graph framework have been highlighted by Friedler.<sup>28,29</sup> Yet, theory and practice are two different things, and any framework needs effective implementation and best-practices to be truly useful. If there is no implementation or the framework is too complicated for general use, then the solution to the problem requires considerably more time. Consequently, the framework will not be widely used in research or practice. In this section, different tools are introduced to address P-graph problems. These tools are used to formulate a model to facilitate the synthesis of sustainable energy supply chains.

The P-graph methodology defines how to address a PNS problem by defining how to construct a maximal structure, generate a mathematical programming model, and obtain a solution effectively. Three tools were created to automate the aforementioned procedure: PNS Solver, PNS Studio, and PNS Draw.

**2.1. PNS Tools.** PNS Solver was the first tool developed for the P-graph methodology. Originally, it was intended only for scientific use, with both the input and output files formatted in plain text. For example, the definition of operating unit wood\_chips\_prod is

$$\begin{aligned} \text{fix\_cost} &= 30820, \text{proportional\_cost} = 2.64 \\ \text{wood} + 0.001728 \text{ heat} + 0.000108 \text{ electricity} \\ &+ \text{wood\_chips\_prod\_fix\_cost} + 2.64 \text{ cost} \\ &\geq \text{wood\_chips} \end{aligned}$$

Both the structure and the parameters are given in the input file, but a special format is required. Thus, it is easy to make mistakes. PNS Solver generates both the maximal and the optimal structure and saves it into a text file, which contains the list of the operating units of the optimal structure and their relative sizes. Users are no longer required to construct the maximal structure manually by using the MSG (maximum structure generator) algorithm. Therefore, it is not necessary to create the mathematical model by hand for the structural model, which subsequently can be solved with a solver such as CPLEX. The PNS Solver performs these tasks automatically.

Although the PNS Solver is an excellent tool for determining the optimal structure of a problem, defining the problem and evaluating the result is not adequately supported. Some of these shortcomings are eliminated by PNS Studio. PNS Studio includes PNS Solver and an easy-to-use graphical interface.

PNS Studio consists of four major columnar sections. Materials can be created in the first column. If one selects a material, the property window of that material appears in the third column, where the name, price, maximum available amount, measurement units, and so on, can be specified.

Operating units can be created in the second column. After a new unit is created, the input and output materials can be set with the drag and drop technique. The numerical parameters,

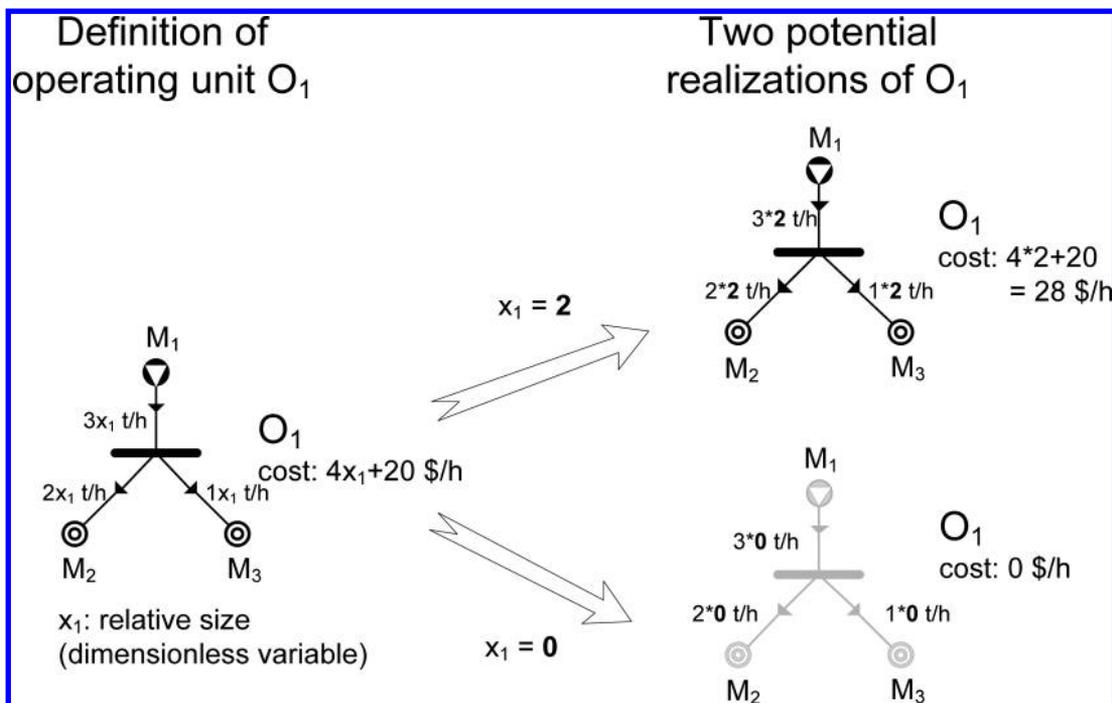


Figure 2. The flows and costs of operating units.

like relative flow rates, cost, etc., can be set in the fourth column.

Hence, some error is completely eliminated using PNS Studio. Previously, in PNS Solver, inattention or typos could cause an invalid operating unit. For example, specifying that operating unit 4 produces material 12 could be made, even if material 12 was not defined at all. Now dragging a material which is not defined to an operating unit is not possible. On the other hand, deleting a material which is already used by an operating unit causes a warning dialogue box to pop up. PNS Studio shifts the workload of the users so they do not have to concentrate on the syntax of the problem; the syntax is done automatically, so instead of dealing with various modeling issues, more attention can be focused on the semantics. The results of PNS Studio can be exported into easy-to-use Excel files, where not only are the relative sizes of the operating units displayed but also the consumption or production of each material, along with the associated costs.

PNS Draw goes one step further in that it facilitates the graphical representation of a P-graph. It is human nature that pictures are more easily comprehended than textual descriptions. Thus, a new tool was developed which is capable of drawing P-graphs. By placing and connecting materials and operating units on the canvas, the problem is defined. The result can then be exported into PNS Studio, and the solution can be displayed again in PNS Draw. All of these tools can be downloaded from <http://www.p-graph.com>.

It is worth noting that drawing large P-graphs cleanly can be a challenge, so, we are working on a layout engine specifically designed for P-graphs which can alleviate some of this burden.

**2.2. Ecological Footprint Calculation.** The ecological footprint ( $EF$ ) is typically computed using 6 types of land area required for consumption/assimilation: cropland, grazing land, forest land for timber and wood products, fishing grounds, built-up land and forest land for carbon uptake.<sup>27</sup> The Ecological Footprint of a process ( $EF_p$ ) is calculated for each land type by dividing the amount of product harvested ( $P$ ) by

the national yield factor of that product ( $Y_N$ ) and then multiplying the result by the corresponding land type yield factor ( $YF$ ) and land type equivalence factor ( $EQF$ ) as shown in eq 1.

$$EF_p = \frac{P}{Y_N} \cdot YF \cdot EQF \quad (1)$$

(See ref 27.)

The land type yield factor ( $YF$ ) is calculated by dividing the national product yield ( $Y_N$ ) by world product yield ( $Y_W$ ).

$$YF = \frac{Y_N}{Y_W} \quad (2)$$

(See ref 27.)

The equivalence factor is calculated for each land type by dividing that land type's maximum productivity by the average productivity of all productive land types.

$$EQF = \frac{\text{maximum productivity (land type)}}{\text{Av productivity (all productive land types)}} \quad (3)$$

(See ref 27.)

The multiplication by the  $YF$  and  $EQF$  normalizes all products consumed or all generated wastes into equitable units of global hectares. Global hectares are then aggregated by land type into the total number of global hectares required to support a given population's natural resource demands or in our case a supply chain.

To address waste assimilation, a carbon footprint is calculated in terms of global hectares of forest land for carbon uptake. Calculation of the carbon footprint ( $EF_C$ ) involves reducing the amount of  $CO_2$  emitted ( $P_C$ ) by the amount of  $CO_2$  sequestered by the oceans ( $S_{Ocean}$ ) and then standardizing this amount by the amount of the average rate of carbon to  $CO_2$  sequestered by forestland (ha) at world average yield ( $YC$ ).<sup>27</sup> This amount is then converted to global hectares by a final multiplication of the equivalence factor ( $EQF$ ).<sup>27</sup>

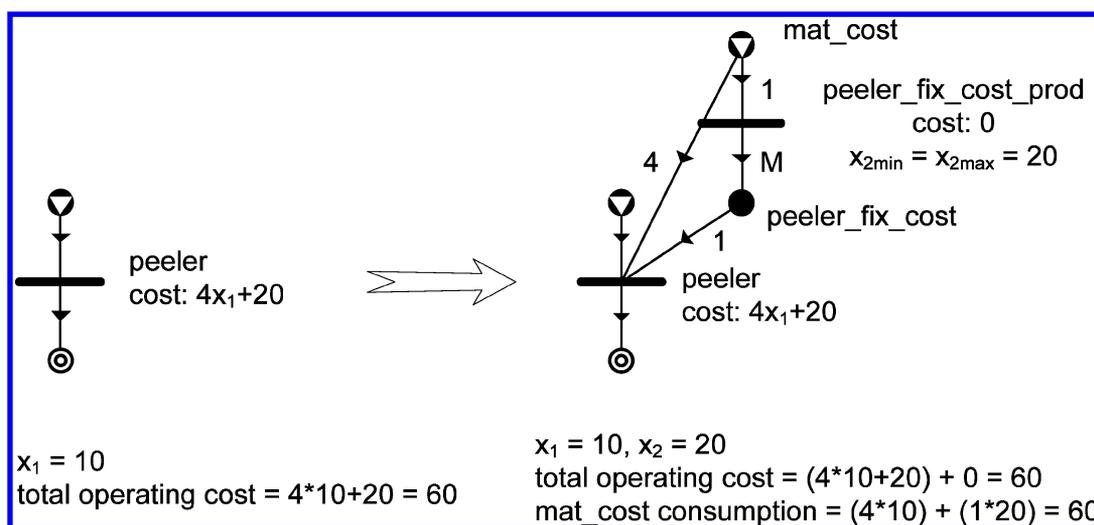


Figure 3. Transforming an operating unit to handle material *mat\_cost*.

$$EF_C = \frac{P_C \cdot (1 - S_{Ocean})}{Y_C} \cdot EQF \quad (4)$$

(See ref 27.)

### 3. MODELING ENERGY SUPPLY CHAINS BY P-GRAPHS

**3.1. Cost Calculation.** While various sustainability metrics are gaining importance, the cost or profit of a solution always remains a major factor of influence. In addressing cost we will first explain how cost is handled within the P-graph methodology and then introduce a modeling technique to implement a constraint for the total cost.

The cost of a network contains the cost of the raw materials plus the cost of the operating units in the network minus the price of the products. If the cost is negative, then the network creates profit. The cost of an operating unit has two constituents: investment cost and operating cost. Both types of costs can have a fixed part and a proportional part. Usually, through a payout period the investment cost is annualized, thus, the overall cost function has a single fixed part and a single proportional part. This cost function is used to calculate the cost of an operating unit based on its relative size. Figure 2 highlights the difference between the definition of operating unit  $O_1$ , where the relative size is denoted with  $x_1$ , and 2 potential realizations of  $O_1$  with relative sizes of 2 and 0, respectively.

This type of cost representation is adequate as long as cost is the only objective of the optimization. If there are other objectives, e.g., higher levels of process sustainability, then we may want to handle the total cost as a constraint.

**3.2. Introduction of Cost as a Material.** A modeling technique is proposed here to handle cost as a single material, thus an upper limit can be imposed on cost. A new material called *mat\_cost* must be introduced for the whole network. The former cost parameters facilitate the optimization, while *mat\_cost* restricts the search for total cost using the P-graph methodology. The total cost of a network and the consumed *mat\_cost* in the same network must coincide. Thus, a new operating unit and a new intermediate material must be introduced for each operating unit in the original network, which is illustrated in Figure 3. In this figure a peeler unit has two additional inlet materials, *mat\_cost* and *peeler\_fix\_cost*

with relative flow rates of 4 and 1, respectively. The first relative flow rate, 4, equals the proportional part of the peeler's cost. Only the new operating unit (*peeler\_fix\_cost\_prod*) is capable of producing *peeler\_fix\_cost*, but then the relative size of this new operating unit must be 20, which is the fixed part of the total cost of the peeler unit.

In this example, the relative size of the peeler unit is 10. Consequently, the cost of the original network (the left side) is 60. The cost of the new layout is also 60 because the cost of the peeler unit remains unchanged and the new operating unit (*peeler\_fix\_cost\_prod*) does not have costs.

In the new layout, 40 units of *mat\_cost* are consumed directly by the peeler unit and 20 units by the new operating unit. The new operating unit always consumes 20 units of *mat\_cost* if the peeler is active independently from the relative size of the peeler unit. The total *mat\_cost* consumption is 60, which matches the cost of the network.

Similarly, if some ordinary raw material has costs, then its consumption has to incur the consumption of an appropriate amount of *mat\_cost*. For example, if electricity is purchased from the grid for 149 €/MWh, then the operating unit representing the purchase should have a connection from *mat\_cost* with a relative flow rate of 149.

**3.3. Modeling Ecological Footprint.** The Ecological Footprint is a common tool used to assess sustainability. There are different types of footprint calculations, e.g., the carbon footprint, the sustainable process index, the ecological footprint, etc. These footprints are additive in that the footprint of a network can be calculated by summarizing the footprints of its components. Our aim is to account for the ecological footprint of each of the different solution networks and create a method within the P-graph methodology to limit the search for those networks whose total ecological footprint is below a given threshold.

The initial structure must be transformed to reach the aforementioned goals. This transformation is illustrated by Figure 4. A new material node termed as ecological footprint is introduced, and the node will be the inlet for such operating units which contribute to the ecological footprint generation. For example, operating unit  $O_1$  consumes 4.97 ha from the ecological footprint if the relative size of  $O_1$  is 1. The exact value of the aforementioned ratio is proportional with the footprint contribution of  $O_1$ . If the footprint belongs to a raw

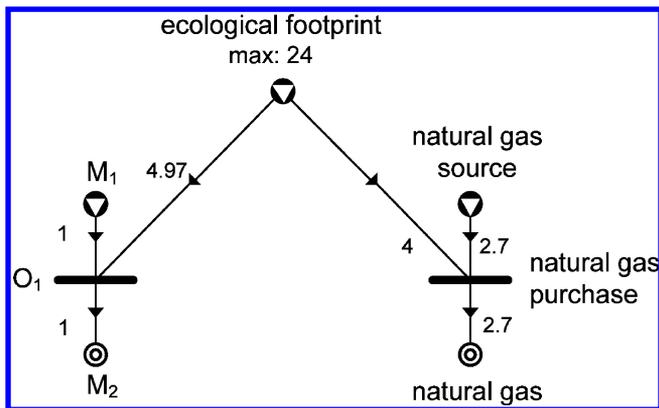


Figure 4. Handling the ecological footprint.

material, then an operating unit has to be introduced to represent the purchase, and the footprint material will be the inlet of this unit.

The ecological footprint of the transformed network is equal to the consumption of the material with the same name. An upper limit can be set for this material, because the P-graph framework allows setting an upper limit for raw materials. This ensures that only those structures are considered in the optimization process whose corresponding ecological footprint is below the set limit.

#### 4. CASE STUDY

The case study chosen to illustrate the methodology being developed here is that of a supply chain designed to produce both heat and electricity used in a geographical district. The maximal structure of the supply chain including all of the possibilities under consideration is illustrated in Figure 5, and

the corresponding data can be found in the Appendix in the Supporting Information.

The goal is to meet the heat and electricity requirement of this district, 5000 and 2000 MWh/yr respectively. Naturally, conventional nonrenewable methods are available, such as obtaining electricity from the grid and heat from natural gas combustion. This district also has some renewable energy sources available like corn silage, grass silage, corn cobs, and wood. Additionally, available are several energy conversion technologies such as those used in biogas plants, biogas CHP (combined heat and power) plants, gas burners, pelletizers, and furnaces. Note that, some operating units, e.g., a pelletizer, are available only in certain sizes, the corresponding data are used to construct the cost function. The economic data were obtained from Luttenberger et al.<sup>30</sup>

Some operating units in Figure 5 represent an activity instead of an actual operating unit. For example, the electricity feeder represents the purchase of the electricity from the grid. Consequently, this operating unit has no associated cost, and both its input and output flow rate is 1. The operating unit "wood production" means the cutting of wood. Its input is the area available for this purpose. There is a specific limit on the area for wood production, and it is worth noting that in this particular example, 2 distinct areas for corn production are used. One area is used only for silage production, and the other is used for the production of corn straw pellets.

If an operating unit has two operating modes, such as a gas burner being used to combust either natural gas or biogas, then more than one operating unit is used to represent it. One operating unit represents the physical equipment (gas burner) which produces a hypothetical material (gas burner capacity), one operating unit represents biogas burning, and the another represents natural gas burning.

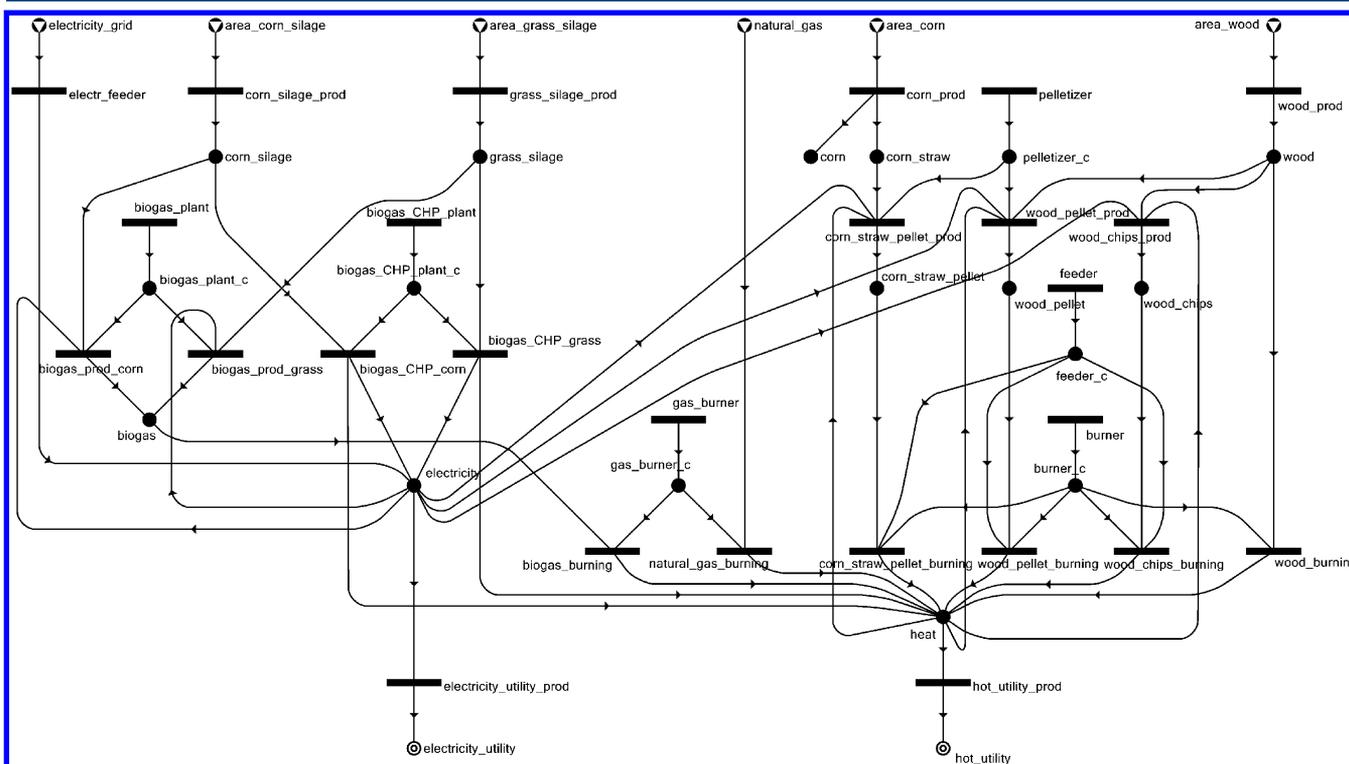


Figure 5. Maximal structure of case study supply chain including all configurations.

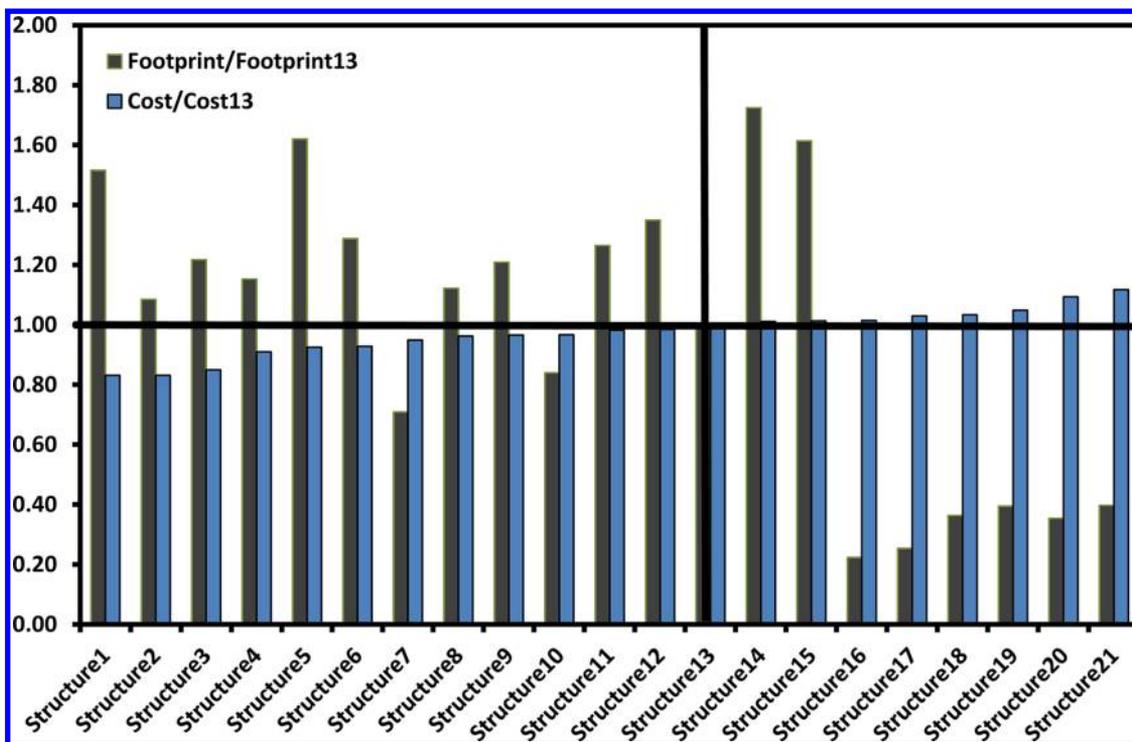


Figure 6. Comparison of 21 different supply chain structures designed to generate 18.0 TJ of heat and 7.2 TJ of electricity per year. The supply chains are compared on the basis of cost and ecological footprint relative to Structure 13, using electricity from the grid and natural gas.

Table 1. Raw Materials, Cost, and Ecological Footprint for the 21 Supply Chain Structures

Solution structures	Electricity_grid	Natural_gas	area_corn	area_corn_silage	area_grass_silage	area_wood	cost	Cost Divided By cost(13)	Cost Change %	footprint	Footprint Divided by footprint(13)	Footprint Change %
	[TJ/yr]	[m <sup>3</sup> /yr]	[ha/yr]	[ha/yr]	[ha/yr]	[ha/yr]	[€/yr]			[global ha]		
Structure 1	7.37					500.00	476,363	0.83	-16.86	1,046.81	1.52	51.58
Structure 2				117.69		367.73	476,433	0.83	-16.85	749.28	1.08	8.50
Structure 3					128.54	367.73	486,852	0.85	-15.03	840.65	1.22	21.73
Structure 4				120.03		393.66	521,283	0.91	-9.02	796.21	1.15	15.29
Structure 5	7.57					539.13	530,210	0.93	-7.46	1,119.21	1.62	62.06
Structure 6					131.10	393.66	531,909	0.93	-7.16	889.40	1.29	28.78
<b>Structure 7</b>		<b>399,272</b>		<b>116.30</b>			<b>543,711</b>	<b>0.95</b>	<b>-5.10</b>	<b>489.71</b>	<b>0.71</b>	<b>-29.09</b>
Structure 8			72.96	126.77			551,507	0.96	-3.74	774.86	1.12	12.20
Structure 9				124.78		380.69	553,388	0.97	-3.42	835.02	1.21	20.91
<b>Structure 10</b>		<b>399,272</b>			<b>127.02</b>		<b>554,007</b>	<b>0.97</b>	<b>-3.31</b>	<b>580.00</b>	<b>0.84</b>	<b>-16.02</b>
Structure 11			72.96		138.46		562,730	0.98	-1.78	873.29	1.26	26.45
Structure 12					136.29	380.69	564,435	0.99	-1.49	931.90	1.35	34.94
<b>Structure 13</b>	<b>7.25</b>	<b>540,588</b>					<b>572,956</b>	<b>1.00</b>	<b>0.00</b>	<b>690.61</b>	<b>1.00</b>	<b>0.00</b>
Structure 14	7.99					529.10	579,343	1.01	1.11	1,190.91	1.72	72.44
Structure 15	8.17		102.04				580,439	1.01	1.31	1,114.72	1.61	61.41
<b>Structure 16</b>				<b>214.45</b>			<b>581,310</b>	<b>1.01</b>	<b>1.46</b>	<b>154.24</b>	<b>0.22</b>	<b>-77.67</b>
<b>Structure 17</b>				<b>125.12</b>	<b>98.01</b>		<b>589,975</b>	<b>1.03</b>	<b>2.97</b>	<b>175.19</b>	<b>0.25</b>	<b>-74.63</b>
<b>Structure 18</b>			<b>90.05</b>	<b>135.88</b>			<b>592,323</b>	<b>1.03</b>	<b>3.38</b>	<b>250.82</b>	<b>0.36</b>	<b>-63.68</b>
<b>Structure 19</b>				<b>234.67</b>			<b>601,052</b>	<b>1.05</b>	<b>4.90</b>	<b>272.33</b>	<b>0.39</b>	<b>-60.57</b>
Structure 20	7.95			125.00			626,618	1.09	9.37	244.35	0.35	-64.62
Structure 21	8.02				136.36		640,169	1.12	11.73	274.22	0.40	-60.29

Figure 5 displays the original model before any of the transformation detailed in the previous section had been carried out. You can see that biogas can be produced in a normal plant

or in a CHP plant. The inlet of both plants can be either corn or grass silage. Pellets can be produced from corn straw or from wood. On the other hand, wood chips also can be created from

wood or wood can be burned directly. Additionally, burning pellets and chips requires a feeder unit which has investment cost, but burning wood requires manual work which has proportional cost.

**4.1. Economic Considerations.** The economic considerations included in our analysis are limited to the capital and operating costs and profit normally considered in engineering economics. We do not for example consider the monetary value of environmental damage due to the operation of a supply chain. The reason for this approach is to offer an analysis of sustainable supply chains that is as close as possible to mainstream decision making as commonly practiced. This cannot and should not be interpreted as an implication that other considerations are not important. Rather, the omission simply represents the authors' efforts to present an analysis which is simple and useful under realistic circumstances. Note that obtaining hard cost data in the engineering economics area can prove difficult. For example, the price of a fermentation plant depends on the negotiations between the seller and the buyer. Therefore, for these analyses, the cost parameters come from Luttenberger et al.; we accept these data as self-consistent and valid. If more appropriate values emerge, they can be easily substituted in subsequent analyses. However, we would like to reiterate that the focus in this article is on the methodology, itself.

**4.2. Computational Results.** The principal results from this study include 21 different supply chain structures, which are illustrated in Figure 6 with further details given in Table 1 and the Appendix in the Supporting Information. The illustrative example is relatively small, so for this case study, the number of solutions is 21. Note that supply chain Structure 13 represents the use of electricity from the grid and natural gas - the most common current state of affairs - to produce heat (18.00 TJ per year) and electricity (7.20 TJ per year). We will, therefore, use Structure 13 as our reference point to determine whether the other alternative supply chain structures are more or less sustainable than "business as usual" represented by Structure 13. All of the structures are ranked by relative cost and relative ecological footprint to our reference Structure 13. Details of all of the 21 supply chains considered in this study can be found in Table 1. Note that the thick vertical and horizontal crossed black lines in Figure 6 mark the location and the relative cost and footprint of Structure 13.

Structures which are less costly and environmentally better than reference Structure 13 are those below the horizontal line at 1.0, where the relative cost and footprint are less than one. By simple inspection, two different favorable structures become apparent in Figure 6 moving from left to right: Structures 7 and 10. Structure 7 costs approximately 5% less than Structure 13 with a 29% decrease in ecological footprint, while the cost decrease for Structure 10 is about 3% and the corresponding decrease in ecological footprint 16%. In terms of raw feedstock, both Structures 7 and 10 use natural gas, but Structure 7 supplements that with corn silage while 10 uses grass silage. While both Structures 7 and 10 are environmentally better than 13, structure selection depends partly on the relative availability of grass or corn silage at a given locale and other business circumstances.

If one is willing to consider modest increases in cost to reduce the environmental impact, then Structures 16, 17, 18, and 19 become attractive as well. Structure 16 has approximately a 1.5% increase in cost, but a 78% decrease in ecological footprint using corn silage as the sole feedstock.

Structure 17 has a 3% increase in cost with a 75% decrease in ecological footprint using corn silage and grass silage both as feedstocks. Structure 18 has a 3% increase in cost with a 64% decrease in ecological footprint again using corn silage and grass silage as feedstocks. Lastly, Structure 19 has a 5% increase in cost with a 60% decrease in ecological footprint using only grass silage as feedstock. Superficially, it would seem that Structure 16 is the optimal choice with a relatively small increase in cost and a relatively large decrease in ecological footprint, but exactly which of these is best under a particular set of circumstances could depend on actual local conditions such as the availability of a particular feedstock at a given location as already mentioned.

## 5. CONCLUDING REMARKS

This work presents a synthesis of the P-graph methodology for process design incorporating concepts from the science of sustainability to produce a powerful methodology for the design of sustainable supply chains. The methodology is illustrated by exploring 21 different alternative supply chain structures designed to produce heat (18.00 TJ per year) and electricity (7.20 TJ per year) simultaneously. The use of different feedstocks or inputs singly and in combination is explored, including natural gas and electricity from the grid and various renewable resources (grass silage, corn silage, corn, and wood). A different structure is needed for each class of feedstock such that the branches in Figure 5 which have no flow of mass are deleted. The case study is relatively moderate, thus degeneration, i.e., many solutions at the same objective value, has not emerged here. Admittedly, the costs of the first two solutions are very close (476 363 and 476 433). Ranking these 21 different structures according to cost and ecological footprint demonstrates that feasible supply chains can be found which seem to be cheaper and more sustainable than the usual practice of using electricity from the grid and natural gas. The cost savings and reductions in ecological footprint can range as high as 5% and 77%, respectively, and they are, therefore, significant from an economic and environmental perspective. Note, however, that we recognize that the ecological footprint is not the only sustainability indicator that can or should be used. The size constraint of this paper did not allow for the inclusion of additional sustainability indicators. We are currently preparing a second paper which includes a different sustainability indicator, and it will demonstrate how more than one indicator can be considered and may further contribute to the design of sustainable supply chains.

## ■ ASSOCIATED CONTENT

### 📄 Supporting Information

P-graph framework; parameters of the PNS model of the illustrative example; scope, collecting data; results. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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### Notes

The authors declare no competing financial interest.

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