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Designing Sustainable Supply Chains in the Energy-Water-Food Nexus by the P-graph Methodology

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The P-graph or process graph framework is both a representation and a methodology that can be shown to be extremely useful as a modelling tool in various areas. P-graphs are directed bi-partite graphs that give an unambiguous representation of any process that can be expressed as a network. It is based on rigorous axioms and combinatorial analysis. The result is a maximal structure, solution structures, and an optimal structure of the network for the process of interest. All of these are feasible and meet design requirements. There is freely available software which automates much of the application of the methodology. The P-graph framework is most useful in the initial design phase of a process where the requirements, the feedstocks, the outputs, and the necessary process structure or network may not be precisely defined, but there is a need to generate alternatives which are feasible to start the design process. For this reason, we propose the P-graph framework as an effective means of generating alternative networks which can represent the nexus of energy, water, and food for the purpose of looking for the most cost effective and sustainable options.

1. Introduction

The most widely known definition of sustainability, or more accurately sustainable development, is due to the Brundtland Commission which generally states that sustainable development is “development that meets the needs of the present without compromising the ability of future generations to meet their own needs” (World Commission on Environment and Development, 1987). Given the projected growth of the human population (United Nations, 2015), meeting the aforementioned goal is likely to be difficult. This is important in the context of the energy-food-water nexus because every human being requires a certain amount of energy, water, and food to be able to subsist. Particularly in the context of the modern world with integrated commerce and distribution across the globe, the needs for energy, water, and food are likely to be met through distribution networks that are commonly referred to as supply chains. The goal of the present work is then to explore the application of the P-graph methodology together with concepts of sustainability and sustainability metrics to the design of supply chains that are as sustainable as possible while meeting human needs.

2. The P-graph Framework

The P-graph framework aims to solve various synthesis problems, see (Bertok et al., 2013). Flowsheet design problems or process network synthesis (PNS) arise frequently in the chemical industry. A PNS problem tries to answer the following questions: Which is the best way to produce certain products if a number of units or processing steps are available? What raw materials should we use? Which units will be part of the solution structure? How are they connected?
Process synthesis gives rise to a complex combinatorial problem which is very difficult to solve. This research field has been studied extensively in the past decades and there are still several questions to be answered. The process synthesis methods can be grouped into two classes. The first class deploys heuristic rules based on engineering insights and best practice to determine an acceptable solution

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structure. However, human experiences are gained from only a small number of observations. Sometimes a heuristic method can be effective and very quick. On the other hand, a heuristic solution can be very far from the optimum because it is not a systematic approach. The second class of methods uses mathematical programming. These methods are usually applicable for problems of relatively small or moderate size because of the great execution times. The models can be rigorous only when the mathematical-programming is carefully constructed and nothing is missing from the structural model, (Quaglia et al., 2015).

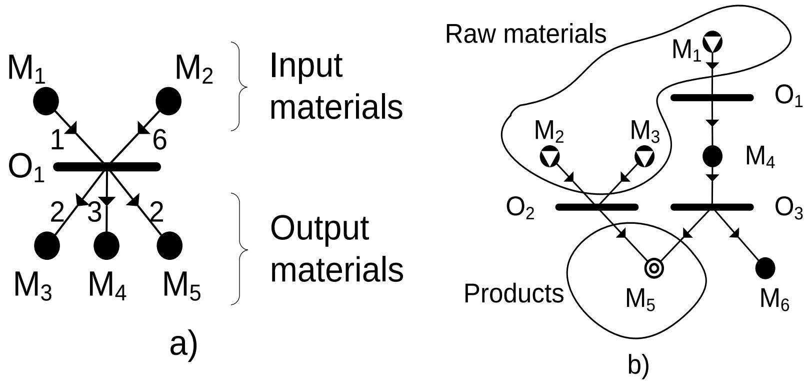


Figure 1: (a) Graphical representation of an operating unit, (b) PNS network involving three operating units and six materials.

Friedler et al. (1992) introduced the P-graph (process graph) framework for process network synthesis (PNS) problems in the early 1990s. This framework has three components: the P-graph representation of processing networks; axioms which must be true for the combinatorially feasible solution structures; and algorithms capable to determine the maximal structure, the solution structures, and the optimal structure. Thus, on P-graph we mean two things: the graph representation and the framework itself. Though originally, the P-graph problem was developed for chemical industry problems, it is now used at several area from energy supply chains (Lam et al., 2010) until operational adjustment in plants (Tan et al., 2014).
A PNS problem is given by three factors: what to produce, from what to produce, with what to produce. In other words, the products, the raw materials, and the available operating units must be known. Of course, numerical parameters should be also available. For example, the maximum amount of the raw materials, the minimum amount of the products, the properties of the operating units, and so on. After the inputs are given, the structural model and the mathematical model are generated and solved. The maximal structure (i.e., superstructure), the solution structures, and the optimal structure are displayed.
A P-graph has nodes for materials (circles) and nodes for operating units (horizontal bars). The arcs express if a material is an input or an output of a given operating unit. The numbers on the arcs signify consumption or production rates. Figure 1(a) illustrates that operating unit O_1 converts one units of M_1 and six units of M_2 into two units of M_3, three unit of M_4, and two units of M_5. Figure 1b represents a P-graph with the following operating units O_1, O_2, and O_3, and the following materials M_1, M_2, and M_6. The triangle within the circle indicates that M_1, M_2, and M_3 are raw materials, the double circle indicates that M_5 is the product; and there is no extra sign for a byproduct, M_6, or for an intermediate M_4.

2.1 Axioms and Algorithms

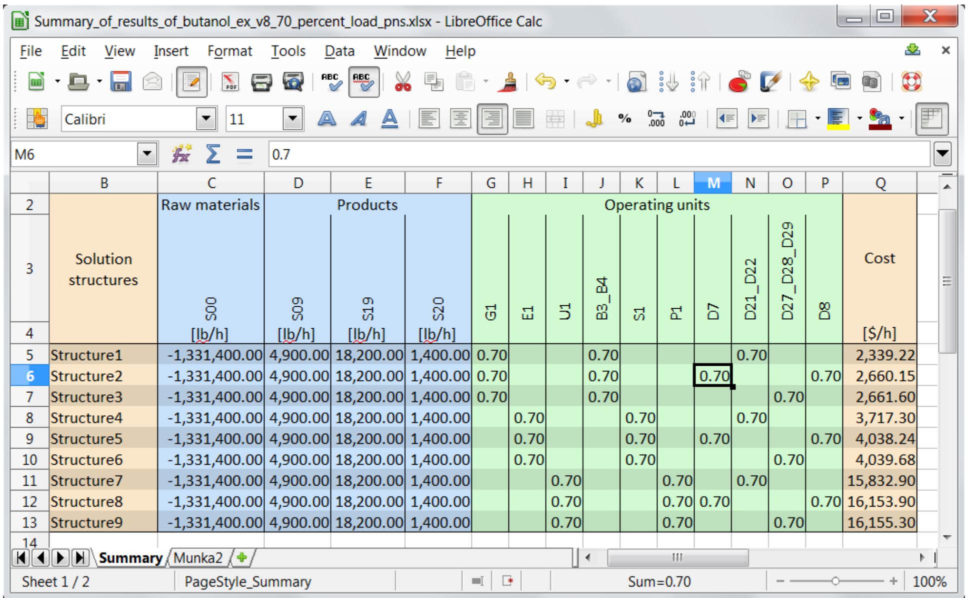
A combinatorially feasible network has to satisfy five properties or axioms. These are the following: (a) every demand is represented in the structure; (b) a material represented in the structure is a resource if and only if it is not an output from any operating unit represented in the structure; (c) every operating unit represented in the structure is defined in the synthesis problem; (d) any operating unit represented in the structure has at least one directed path leading to a product; and (e) if a material belongs to the structure, it must be an input to or output from at least one operating unit represented in the structure.
Based on these axioms effective algorithms have been developed. The maximum structure generator, MSG, determines the structural model, the solution structure generator, SSG, generates each of the solution structures, and the optimal structure generator, ABB, which is based on an accelerated branch-and-bound algorithm, results in the optimal structure, (Friedler et al., 1992).
The MILP model of a process synthesis problem is difficult to solve with a general solver. In contrast, algorithm ABB is able to exploit the structural properties of the problem at hand, thus, it can reach the optimal structure much more effectively.

The present work proposes the P-graph framework for designing energy supply chains while taking into account sustainability criteria. The proposed method will be illustrated by a case study involving energy production from conventional and renewable sources. The P-graph framework makes it possible to generate design alternatives which will be also demonstrated.

2.2 PNS Studio & PNS Draw

Small examples can be solved manually with the P-graph framework but effective and reliable software tools are needed for medium and large scale problems. These tools have to be user friendly to ease the use of the P-graph framework for the average user. Two software tools have been developed to address these issues. The PNS Studio assists the building of new PNS problems or the modifying of existing ones, and solves these problems. It consists four sections. In the first two, the materials and the operating units can be defined. In the second two their properties can be given, like the name, price, maximum available amount, measurement units, relative flowrates, cost, etc.

One can avoid a lot of syntactic and semantic errors using the PNS Studio. For example, the input and output materials of an operating unit are given with drag-and-drop technique, thus, the misspelling of the name of a material cannot happen. An example of a semantical error is the following: a material is to be deleted from the problem definition, but it is still used by some operating units. In this case the PNS Studio does not allow to finalize the delete operation. These automated checks free the time of the user, thus, he or she can focus on high level modelling issues. It is important to analyse the results of PNS Studio, so the solution structures can be exported into Excel files where parameters are displayed, Figure 2.



Solution structures	Raw materials	Products			Operating units										Cost
	S00	S09	S19	S20	G1	E1	U1	B3_B4	S1	P1	D7	D21_D22	D27_D28_D29	D8	
	[lb/h]	[lb/h]	[lb/h]	[lb/h]											[$/h]
Structure1	-1,331,400.00	4,900.00	18,200.00	1,400.00	0.70			0.70				0.70			2,339.22
Structure2	-1,331,400.00	4,900.00	18,200.00	1,400.00	0.70			0.70			0.70			0.70	2,660.15
Structure3	-1,331,400.00	4,900.00	18,200.00	1,400.00	0.70			0.70					0.70		2,661.60
Structure4	-1,331,400.00	4,900.00	18,200.00	1,400.00		0.70			0.70			0.70			3,717.30
Structure5	-1,331,400.00	4,900.00	18,200.00	1,400.00		0.70			0.70		0.70			0.70	4,038.24
Structure6	-1,331,400.00	4,900.00	18,200.00	1,400.00		0.70			0.70				0.70		4,039.68
Structure7	-1,331,400.00	4,900.00	18,200.00	1,400.00			0.70			0.70		0.70			15,832.90
Structure8	-1,331,400.00	4,900.00	18,200.00	1,400.00			0.70			0.70	0.70			0.70	16,153.90
Structure9	-1,331,400.00	4,900.00	18,200.00	1,400.00			0.70			0.70			0.70		16,155.30

Figure 2: Overview of the optimal and alternative suboptimal process networks in a spreadsheet generated by PNS Studio.

Human beings work better with images, and a graphical problem definition tool, termed as PNS Draw, was also developed. Here you can define problems by drawing materials, operating units, and their connections. Beside structural information, one can provide numerical input as well, e.g., the maximum amount of a raw material. The model defined in PNS Draw can be imported into PNS Studio and the solution structures can be loaded back into PNS Draw. These programs can be downloaded free of charge (P-graph, 2015). In the future a layout engine will be also available which help to draw large P-graphs.

3. Sustainability

For purposes of the current analysis we use two well-known integrated sustainability metrics: Ecological Footprint (EF) and Emergy Analysis (EA). The ecological footprint has been used to analyse sustainability (Čuček et al., 2012). Emergy analysis has been used to evaluate electricity (Ulgiati and Brown, 2002). More recently, they have both been used to analyse the sustainability of energy supply chains (Vance et al., 2013). The Ecological Footprint assesses the amount of productive and assimilative land required to support a population's consumption and remediate the wastes (Wackernagel and Rees, 1996). The EF normalizes different types of productive areas for easier comparison (arable land, forest land, pasture land, sea, energy land, built land), and includes all Earth surfaces. EA calculates the amount of solar energy required to produce products and services, or sustain systems (Odum and Nilsson, 1996). Emergy is roughly the sum total of the thermodynamic work of all forms done by solar, tidal, and geothermal energy in the creation and operation of products or services, or a supply chain. The sustainability concept underlying the analysis is that a supply chain is most sustainable when the ecological footprint and the emergy input are as small as possible.

4. Sustainable Supply Chain Design Concepts

In designing supply chains for sustainability, we assume that: (1) the ecological footprint of the supply chain is dominated by the feed stocks and inputs, and (2) the emergy input of the supply chain is also dominated by the feed stocks and inputs. These simplify the analysis without significantly degrading the validly of the results, because the largest amount mass and energy associated with supply chains is generally in the flow through not the required infrastructure. These assumptions together with the P-graph method and the sustainability metrics were used to develop a supply chain designed to produce electricity and heat. The maximal structure of the supply chain is illustrated in Figure 3.

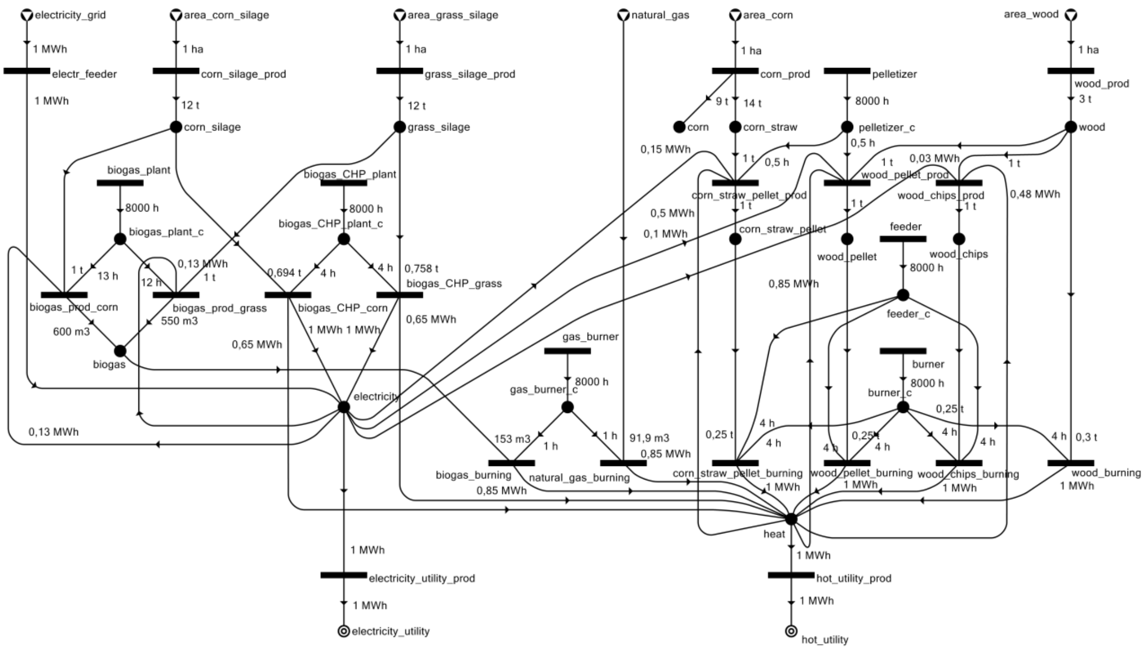


Figure 3: Maximal structure of the illustrative example.

5. Case study

A case study is presented in this section to demonstrate the synthesis of an energy supply chains with the P-graph framework. The case study of (Vance et al., 2013) is extended here by including emergy analysis. Now three objectives are taken into account: ecological footprint, cost, and emergy. Another important issue to handle is that some units have multi-periodic behaviour. It means that the amount of the demand can differ from period to period, moreover the input and output can change between periods. By definitions the maximal structure includes all the solution structures. The figure contains the modelling step executed for the multi-period operation.

The goal of the structure is to produce 5,000 MWh/y heat and 2,000 MWh/y electricity for a given district. The demands appear at the bottom as electricity_utility and heat_utility. Both non-renewable and renewable energy sources are available. Example for the former is the natural gas and electricity from the grid; and example for the latter is corn silage, grass silage, corn cobs, and wood. Biogas plants, gas burners, biogas CHP (combined heat and power) plants, pelletizers, and regular furnaces are among the available energy conversion technologies. Operating units represent these technologies but not all operating unit is connected to a physical unit, e.g., electric feeder. The numeric parameters were taken from (Luttenberger et al., 2008).

Biogas can be created from corn silage and grass silage or these two materials can be fed into the biogas CHP plant. The area for the wood production is limited. The wood can be burnt directly or it can be transformed into wood chips and wood pellet. If an operating unit is multi-periodic, e.g. the biogas plant, then three operating unit represents this process.

Table 1: Inputs to twenty one energy supply chain structures

Solution structures	electricity grid [TJ/y]	natural gas [m³/y]	area corn [ha/y]	area corn silage [ha/y]	area grass silage [ha/y]	area wood [ha/y]
Structure #01	7.37					500.00
Structure #02				117.69		367.73
Structure #03					128.54	367.73
Structure #04				120.03		393.66
Structure #05	7.57					539.13
Structure #06					131.10	393.66
Structure #07		399,272		116.30		
Structure #08			72.96	126.77		
Structure #09				124.78		380.69
Structure #10		399,272			127.02	
Structure #11			72.96		138.46	
Structure #12					136.29	380.69
Structure #13	7.25	540,588				
Structure #14	7.99					529.10
Structure #15	8.17		102.04			
Structure #16				214.45		
Structure #17				125.12	98.01	
Structure #18				90.05	135.88	
Structure #19					234.67	
Structure #20	7.95			125.00		
Structure #21	8.02				136.36	

Table 2: Cost and sustainability analysis of selected supply chains

Structure	Metric	% Change	Feedstock
Structure #13	Cost	0.0 %	Natural Gas
	Footprint	0.0 %	Grid Electricity
	Emergy	0.0 %	
Structure #8	Cost	-3.7 %	Corn Straw
	Footprint	+12.0 %	Corn Silage
	Emergy	-89.0 %	
Structure #11	Cost	-1.8 %	Corn Straw
	Footprint	+26.0 %	Grass Silage
	Emergy	-77.0 %	
Structure #15	Cost	+1.3 %	Corn Straw
	Footprint	+61.0 %	Grid Electricity
	Emergy	-26.0 %	

6. Conclusions

Starting from the maximal structure (Figure 3), twenty one different supply chains were developed and analysed as shown in Table 1. Of these, the most relevant to the issues of water, energy, and food are Structures 8, 11, and 15 which involve corn – a human and animal food, electricity and heat which are forms of energy, and implicitly the water required to raise the corn. Note that Structure 13 represents the reference or "business as usual" case of using electricity from the grid and heat from burning natural gas. These four supply chains structures are further analysed in Table 2. Compared to the reference Structure 13, Structure 8 is optimal if a reduction in cost and a relatively good sustainability performance are desired. However, if increased production of corn is desired, then Structure 15 is preferable because it produces approximately 40 % more corn. In summary, what is important here is that there is a well-known connection between water, energy, and food such that different supply chain designs lead to different options and sustainability performance. The case study illustrates how the P-graph method along with sustainability and cost considerations can be used to design different supply chains to meet the needs of specific locales, business climates, and environmental conditions. As usual for a complex problem like this one, there is no ultimate answer. But the method demonstrated here synthesizes the choices into a logical frame-work from which rational decisions can be made.

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