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Generating and Analyzing Mathematical Programming Models of Conceptual Process Design by P-graph Software

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Supporting Information

ABSTRACT: The primary aim of process-network synthesis, or PNS in short, is to determine the best process network achieving a desired goal, e.g., producing a set of desired products or satisfy demands. PNS has a long history, and numerous methods for executing it are available. Its acceleratedly increasing importance can be attributed to the need to respond to the rapid emergence of new technologies and fast changes in the economic environment. It is highly desirable that any corporation be able to ascertain if a new technology is viable for its business as well as to assess if its current technology remains sustainable in the changing environment. Herein, a novel method and software for PNS are proposed for generating, optimizing, and analyzing alternative process designs at the conceptual level. The method is illustrated by synthesizing alternative process designs with different network structures for the production of butanol, ethanol, and acetone from grains. Furthermore, the sustainability of the resultant process designs is analyzed. This is executed by varying the payout period and the production rate, i.e., load.

1. INTRODUCTION

Process-network, or process synthesis, problems arise frequently in chemical and allied industries and are of major interest due to their practical relevance. Nevertheless, process synthesis gives rise to a complex combinatorial optimization problem that is generally highly convoluted, and thus, it is extremely difficult to determine its optimal solution. The field of process synthesis has been explored extensively in the past decades,[1−5] and it remains an active research field to this day.[6−10] As such, process synthesis has generated a vast body of literature delineating various methods pertaining to algorithms, approaches, and their applications.

The methods proposed so far for process synthesis can be roughly grouped into two classes. One class deploys heuristic rules based on previous experiences to determine the optimal solution. By nature, however, human experiences are almost always localized: They are gained from only a finite and probably a limited number of observations of specific instances. A heuristic method is relatively easy to implement, but is inherently effective only at the local level. The other class consists of algorithmic, or mathematical programming, methods. These methods tend to be effective for processes of relatively small or modest size; they can be rigorous only when the necessary mathematical-programming models can be explicitly constructed. Nevertheless, these mathematical models are constructed manually. The objective function and the set of constraints need to be externally defined; they are not algorithmically generated.

In the early 1990s, Friedler and Fan and their collaborators[11,12] introduced a mathematically rigorous method based on the P-graph framework that algorithmically yields the mathematical programming model of process synthesis problems. The method resorts to the well-established mathematics of graph theory and is heavily based on a unique class of graphs in representing unambiguously the structures of process networks. Consequently, a set of axioms can be formulated to express the necessary and sufficient combinatorial properties to which a feasible process structure should conform.[11] In turn, these axioms lead to a set of algorithms implementable effectively on computers.[12]

The present work proposes P-graph-based software for solving PNS problems. Besides model generation, other important advantages of the P-graph solvers are that they can algorithmically generate design alternatives and compute optimal configurations of process networks. The only drawback of applying P-graph software for PNS was that incorporating special constraints would need modification of the algorithms and software. The latest version, however, provides model export to popular general purpose optimization engines where model extension and solution can be performed.

The effectiveness of the proposed method is illustrated by applying it to a case study. It introduces the steps of the solution, the underlying mathematical model, and the definition of the globally optimal and suboptimal alternative designs. Furthermore, the detailed analysis executed by software is presented for the case study.

2. CASE STUDY

The process for this case study is from our previous work.[13,14] The best flowsheets are determined for producing butanol, ethanol, and acetone for grains by fermentation and separation of the fermentation broth.

The separations are performed in two stages. The first stage removes water by either extraction (by operating units Extract and SolventStrip) or by adsorption (by operating units

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Table 1. List of Material Streams

ID	description	composition (%)				
		acetone	ethanol	water	butanol	ethyl-hexanol
F	fermentation broth (raw material)	0.606	0.220	97.686	1.488	
A	acetone (product)	100.000				
E	ethanol (product)		100.000			
B	butanol (product)				100.000	
X	ethyl-hexanol					100.000
I1	intermediate	14.667	4.000	46.667	34.667	
I2	intermediate	0.352	0.101		1.309	98.239
I3	intermediate	20.000	5.714		74.286	
W1	waste water		0.057	99.885	0.057	
W2	waste water	0.225	0.112	99.607	0.056	
W3	waste water	10.000	2.500	87.500		

GasStrip and Adsorp). The second stage separates butanol, ethanol, and acetone by one of the two different configurations of distillation columns (Distill1 or Distill2). The details of the problem are given in Tables 1, 2, and 3.

Table 2. List of Operating Units

	name	description
o_1	GasStrip	gas stripping unit
o_2	Extract	extracting unit
o_3	SolventStrip	solvent stripping unit
o_4	Adsorp	adsorbing unit
o_5	Distill1	distilling unit
o_6	Distill2	distilling unit

The aim of process synthesis is to determine if the adsorption is economically viable for various payback periods and also if the risk of potentially decreasing demands resulting in partial load operation entails an alternative design. Since the proposed algorithm and software result in the ranked list of the best networks, the robustness of the design alternatives are highlighted as well.

3. METHOD

The P-graph framework involves a series of steps from the formal definition of a process synthesis problem, through the creation of the mathematical model, to the generation of structurally alternative solutions. Each of the steps is algorithmic and computer-aided; see Figure 1.

At the outset, the set of candidate operating units needs to be given by their input and output materials, as well as their capacities, i.e., the flow rates of their inlet and outlet streams. The upper bound on the availability of the raw materials and the lower bound on the required amount of desired products can be defined as well. For each intermediate material or byproduct stream, the gross production must be non-negative, i.e., at least the amount consumed must be produced.

In process synthesis, the best network structures are constructed by interconnecting subsets of the operating units defined in the problem. For the best structures, the optimal load of the operating units is computed as well besides the set of operating units incorporated. Variable x_i is assigned to each candidate operating unit o_i expressing its load. In the solution of the optimization $x_i = 1$ signifies full load, $0 < x_i < 1$ signifies partial load, and $x_i = 0$ signifies exclusion of operating unit o_i from the flowsheet. It is assumed that the flow rates of the inlet and outlet streams increase and decrease proportionally to the load; see Figure 2. All the information can be defined graphically by software PNS Draw or in tabular form by PNS Studio.[15]

The P-graph representation expresses the structural or combinatorial properties of a PNS problem and resultant structures unambiguously. For instance, if an operating unit has multiple inlet streams, each of the streams needs to be provided for the operation of the unit, which is a logical AND constraint. If a material can be produced by two or more operating units,

Table 3. Table of Operating Units

name	inlet streams [kg/h]	outlet streams [kg/h]	investment cost [US$]	operating cost [US$/year]
GasStrip	F (744 150)	W1 (713 400) I1 (30 750)	2 180 000	871 000
Extract	F (744 150) X (800 320)	W2 (729 800) I2 (814 670)	1 189 000	5 231 000
SolventStrip	I2 (814 670)	X (800 320) I3 (14 350)	1 914 000	864 000
Adsorp	I1 (30 750)	I3 (14 350) W3 (16 400)	3 806 000	132 000
Distill1	I3 (14 350)	A (2 870) E (820) B (10 660)	3 124 000	1 246 000
Distill2	I3 (14 350)	A (2 870) E (820) B (10 660)	4 156 000	1 658 000

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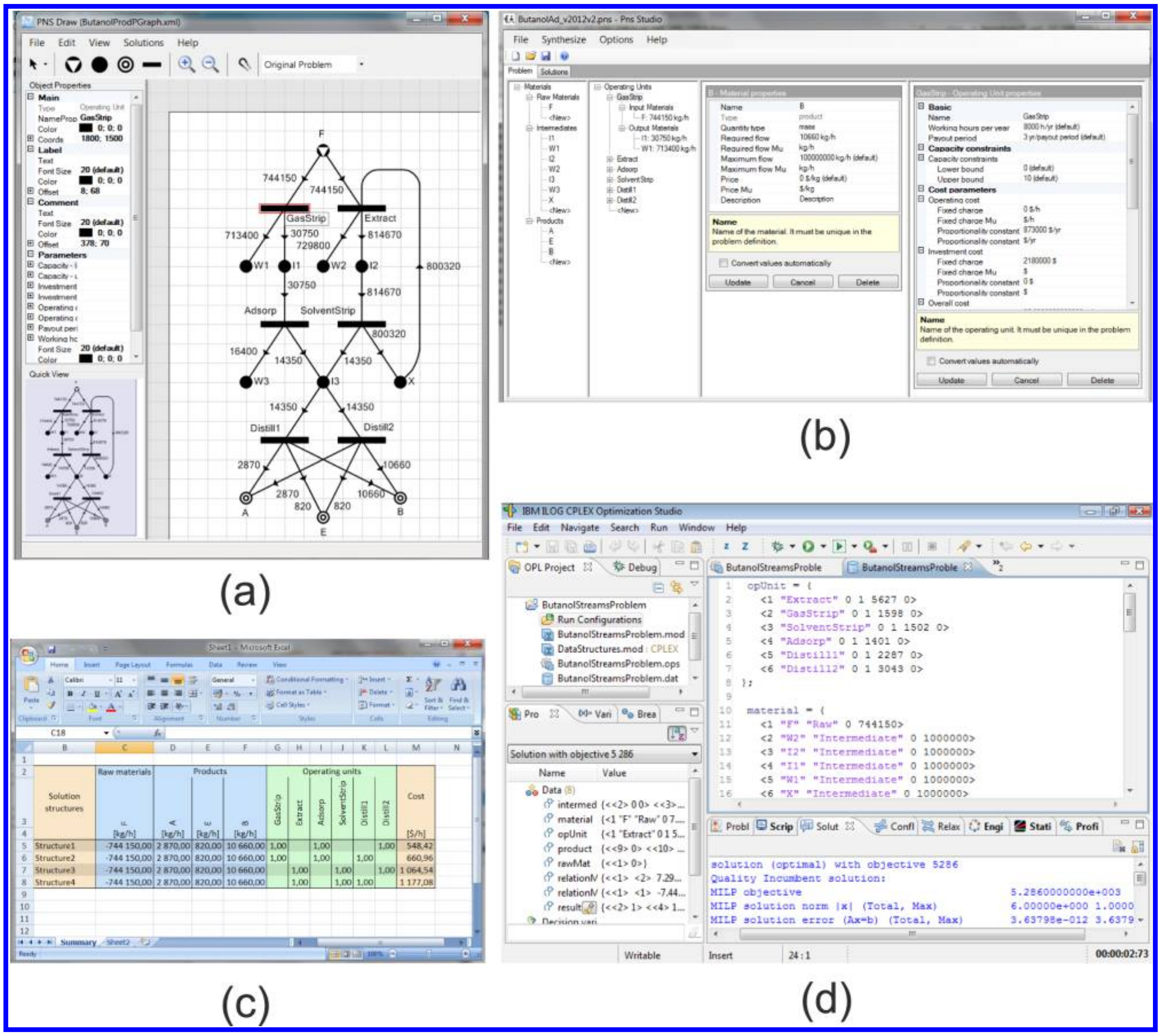

Figure 1. Software for process synthesis: (a) PNS Draw, (b) PNS Studio, (c) Report in MS Excel, and (d) mathematical model in IBM ILOG CPLEX.

then any combination of them can be sufficient for the production of the material, which is a logical OR condition.[11]

The above-mentioned constraints and graphical representation lead formally to the inherent properties of the process structures.[11] Algorithm MSG (Maximal Structure Generator) yields a rigorous superstructure by eliminating exactly those materials and operating units which cannot belong to any combinatorially feasible structure.[16] Algorithm SSG[17] (Solution Structure Generator) generates each combinatorially feasible structure exactly once. The elimination of one or more materials or operating units from the sets defined in the synthesis problem by algorithm MSG in practice implies that the input is incomplete or inconsistent. Executing algorithm MSG in PNS Studio renders it possible to verify whether the input is entered correctly. Note that typically no algorithmic support is available for general purpose mathematical modeling tools to ascertain if part of the model will never be required in the solution. Figure 2 depicts the maximal structure generated by algorithm MSG for the case study; it contains each operating unit defined in the problem.

For determining the best structures and the optimal loads of the operating units, algorithm ABB is executed in PNS Studio.[18] The objective is to minimize the overall annual cost of the process. The overall cost is the sum of the costs of the operating units and the prices of the raw materials. The annual cost of an operating unit is the sum of its operating cost and annualized investment cost. For each operating unit PNS studio considers a linear function with a fixed charge expressing both the expanses arising regardless the volume of the activity and the increase in cost proportional to the growth of mass load; see Figure 3.

The mathematical optimization model[19] can be exported from the PNS Studio to a mathematical modeling environment, e.g., IBM ILOG CPLEX. Editing the optimization model itself enables the incorporation of special constraints undefined in the PNS problem and to obtain the optimal solution by the solver in the modeling environment.

Algorithm ABB has a major advantage compared to general purpose solvers. It provides not only the globally optimal, but also the *n*-best suboptimal structures or flowsheets. The

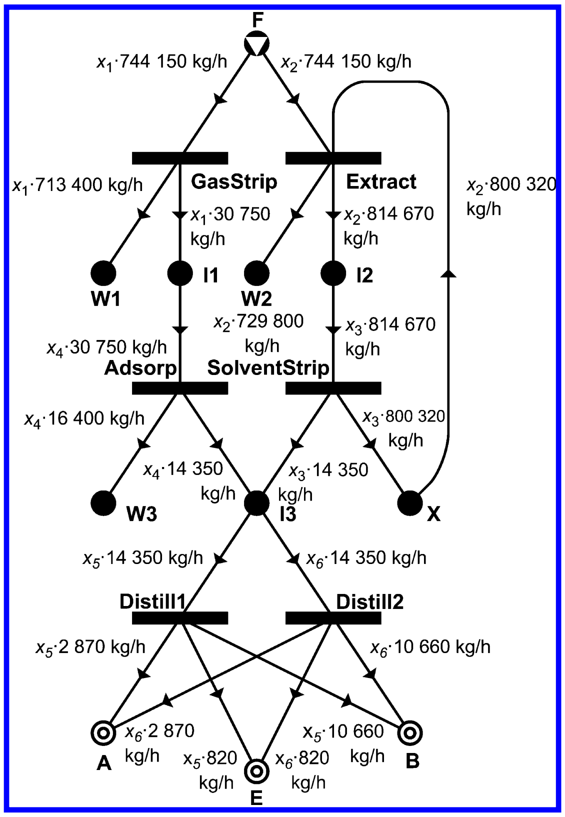

Figure 2. Maximal structure for the case study.

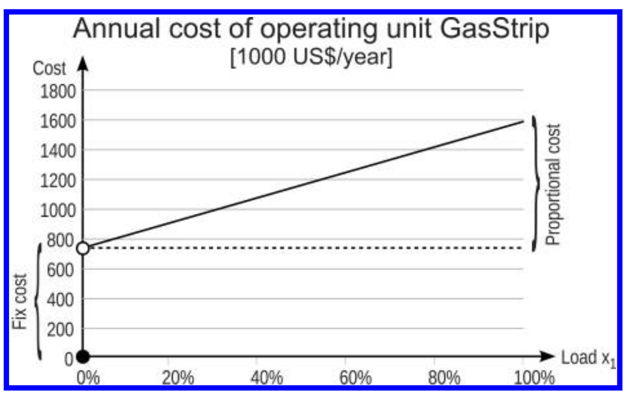

Figure 3. Cost function for an operating unit.

number n is given by the user prior to executing algorithm ABB. A structure is defined to be suboptimal if it does not involve a better substructure. For the structures generated by algorithm ABB in PNS Studio, a detailed report can be exported to Microsoft Excel. Note that for a general mathematical model, it is difficult to define the second best solution.

In rapidly varying economic and technological environments, the robustness of a structure or flowsheet is more important than its optimality under a set of fixed conditions. This implies that generating and analyzing alternative structures are essential for conceptual process design.

For facilitating the implementation of the method, a series of appendices is provided in the Supporting Information: Appendix A: Combinatorial model of PNS, Appendix B: Parametric model of PNS, and Appendix C: The MILP model of PNS.

4. SOFTWARE FRAMEWORK

The software implementations of algorithms MSG, SSG, and ABB are freely available on the Web site www.p-graph.com with additional software tools for solving synthesis problems. This section introduces two software that can be used to define, model, and solve synthesis problems via the P-graph framework.

4.1. PNS Draw. The P-graph framework has the advantage over ordinary MILP models that it is based on an unambiguous graph representation and therefore it is more expressive; it helps to understand the structure of the problem more than an ordinary MILP model. This is exploited by the software PNS Draw.

PNS Draw is a modeling tool used to define synthesis problems graphically. First, the structure of the process has to be drawn and then the appropriate parameters and properties of the operating units (e.g., name, fix cost, proportional cost) and materials (e.g., name, type, required flow) can be given. The flow rates between materials and operating units can be set on the edges; by default, it is set to be 1. PNS Draw automatically ensures that an operating unit can be only connected to a material and vice versa, i.e., it does not allow to connect operating units to operating units or materials to materials. Note, that cost parameters are optional and not required parameters; it is possible to create models where only the structure of the process is of interest.

Models created in PNS Draw can be exported either to .xml format or to .png and .svg image formats. The former can be fed to PNS Studio for further modeling or calculations while the latter can be used for illustration purposes.

4.2. PNS Studio. PNS Studio is a software that implements algorithms MSG, SSG, and ABB, and therefore, it is primarily used as a solver for process synthesis problems. Furthermore, it is also capable of constructing process synthesis models.

As a modeling tool, it uses a "tree-view" that provides a clear overview of the actual problem under consideration and makes it possible to edit the properties of multiple materials and operating units in parallel. The handling of measurement units is aided with automated conversions.

As a solver, PNS Studio can generate the maximal structure, the combinatorial feasible structures, and the globally optimal and suboptimal solutions of the problem. In the latter case the objective can be either cost minimization or profit maximization. PNS Studio provides a double pane view of solutions to compare alternatives.

Models and initial structures created in PNS Drawn can be imported into PNS Studio where they can be further edited. It is also possible to export brief or more detailed reports from PNS Studio to Microsoft Excel.

5. RESULTS AND DISCUSSION

Two explorations have been performed by the method and software proposed in the current contribution to assess the robustness of the optimality of the best structures in a rapidly changing environment. Two sources of risk are taken into account. First, the annual costs and ranks of the best process structures are evaluated under various payout periods. Second, production costs by alternative flowsheets are assessed for different product demands.

The first exploration clarifies how the resultant optimal structures vary under different payout periods. Figure 4 shows the annual cost of the globally optimal and suboptimal

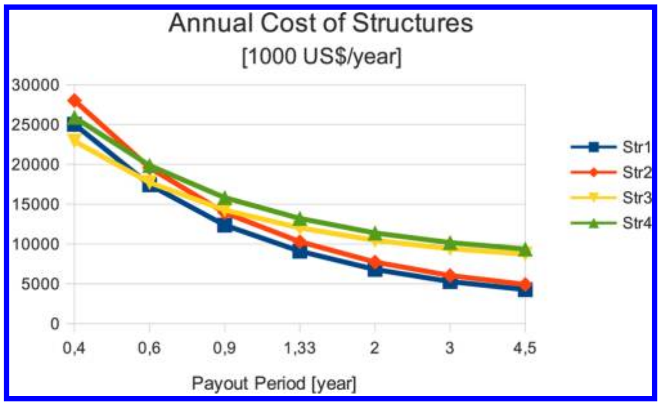

Figure 4. Annual cost of alternative structures as a function of the payout period.

structures as a function of the payout period. This figure is depicted by Microsoft Excel from the report on the globally optimal and three suboptimal structures for the case study computed via PNS Studio. The analysis highlights that the ranking of the structures changes appreciably depending on the payout period. Nevertheless, it remains invariant for a wide range of values.

For the second exploration, it is presumed that the investment costs of the operating units of given capacities are fixed, while their operating costs are proportional to the mass load. Figure 5 illustrates the changes in the production costs of

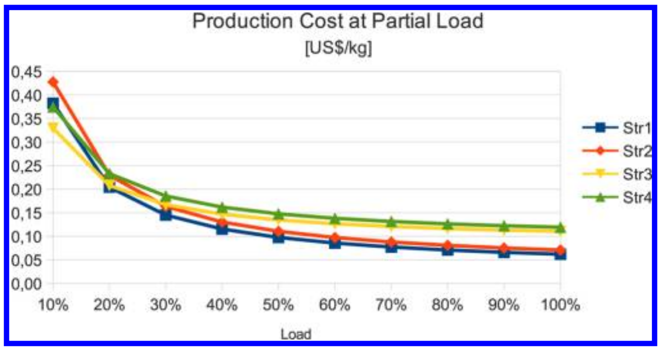

Figure 5. Production cost at partial load by alternative structures.

different flowsheets as a function of the mass load of the process. This figure is also depicted by Microsoft Excel from the report on the globally optimal and three additional suboptimal structures for the case study computed in PNS Studio. As can be seen, not only the per kg production cost but also the order of the best structures may vary substantially depending on the load of the process.

6. CONCLUSION

The P-graph framework, implemented in software PNS Draw and PNS Studio, provides us a mathematically rigorous approach for formulating and solving process synthesis problems, as well as of analyzing the resultant flowsheets with the aid of the built-in optimizer, in MS Excel, or even in IBM ILOG CPLEX. Algorithm MSG (Maximal Structure Generation) can verify if a problem is entered without the loss of essential interconnections among the candidate operating units and related material streams. The best structures computed by algorithm ABB render it possible to select the most appropriate flowsheet under various scenarios representing expected or unexpected situations.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Appendix A: Combinatorial model of PNS; Appendix B: Parametric model of PNS; Appendix C: The MILP model of PNS; Appendix D: Software framework; and Appendix E: Detailed data on the Case Study. 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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