

N-best Design Options with Strategical Differences in Process Network Synthesis

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The main goal of Process Network Synthesis is usually to find the lowest-cost process for a given problem. Since the model is not able to account for every parameter of an industrial realisation, the decision makers prefer to have alternatives, which can be provided when generating the n-best solutions. This, however, comes with another issue, specifically that several of the near-optimal solutions are almost identical to the optimal one, and only differ in one or two operating units. Thus, the next step to improve the generation of feasible and performant alternatives is to provide process designs with meaningful differences from the optimum. Meaningful differences between designs have to be defined by the decision makers. These are differences that the decision makers consider as major strategic questions, while other changes in the process constitute fine details where simply selecting the lowest cost option is enough. The current work describes a branch-and-bound algorithm that is able to generate the n-best strategically different process designs. The difference between considering and ignoring strategic differences when generating n-best solutions is illustrated via a case study.

1. Introduction

Process network synthesis (PNS) is the procedure of building and configuring a network from a set of available operating units to perform a desired job. Various strategies have been developed for solving PNS problems, such as mathematical programming (Ng et al., 2014), cascade analysis (Foo, 2008), involving metaheuristic optimisation algorithms (Silva et al., 2010), Pinch Analysis (Klemeš and Kravanja, 2013), or the graph-theory-based P-graph framework (Friedler et al., 2022).

The P-graph framework represents the PNS problem as a directed bipartite graph where different types of nodes represent operating units and materials, while the edges define the material flows. This unambiguous representation of the process permits enhanced optimisation performance by exploiting the structure of the process network. Besides the systematic combinatorial tools for synthesis, P-graph also provides an illustrative visual representation for better understanding the internals of the process (Lam et al., 2016).

The wide range of applications proves that the methodology is a powerful tool not only for problems from the chemical industry, but also for any problems whose core is a structure-based process. These applications include azeotropic distillation systems (Feng et al., 2000), biomass networks (How et al., 2016), production scheduling (Frits and Bertok, 2020), heat exchanger network optimisation (Orosz and Friedler, 2020), circular economy implementation (Fan et al., 2020), machine-learning applications (Teng et al., 2022), and wastewater networks (Pimentel et al., 2022).

While the optimal solution of most problems can be generated via different methodologies, a key advantage of the P-graph framework is the inherent capability of generating the n-best design alternatives. As a result, decision makers are not limited to accepting or rejecting a proposal given by the cost-optimal solution; instead, they can review a list of n-best design options and make a decision based on factors not included in the model. This is significantly more important for complex problems, as the mathematical model cannot represent all aspects of real life.

However, similarity between the design options is a common phenomenon when generating the n-best networks based on the objective function alone. Often, the second or third options only differ from the optimal one by some small change, which can be an insignificant detail in the scope of the whole process. For example, if one step of the process can be realised by two different, but similar, operating units, the difference between the best and second-best solution could be to choose the other possible operating unit, while the rest of the process is exactly the same. This is only a local decision that does not affect the structure of the whole process; therefore, the decision maker will simply choose the best one according to the objective function.

To provide a design alternative with meaningful, strategic differences to the decision maker, the standard notion of n-best solutions needs to be revised. The current work presents the extension of the P-graph methodology to the generation of strategically n-best process networks.

2. Motivating example

Figure 1 depicts an example of a P-graph, with some of the operating units (O9, O10, and O11) colored in red. These operating units are termed as *strategically critical* operating units, i.e., these represent the decisions of the process design which the designer deems the most important. While the other operating units also contribute to the final quality of the process, they are less important for the decision maker. Thus, their design is completely left to the optimisation algorithms. Considering the strategically critical operating units, however, the decision maker wants to evaluate the n-best alternatives, as a decision on these operating units significantly influences the final process.

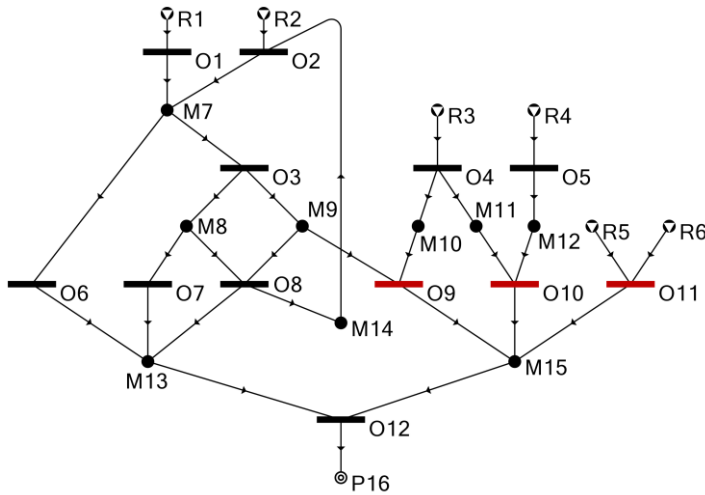


Figure 1: P-graph of motivating example, the strategically critical operating units are marked in red

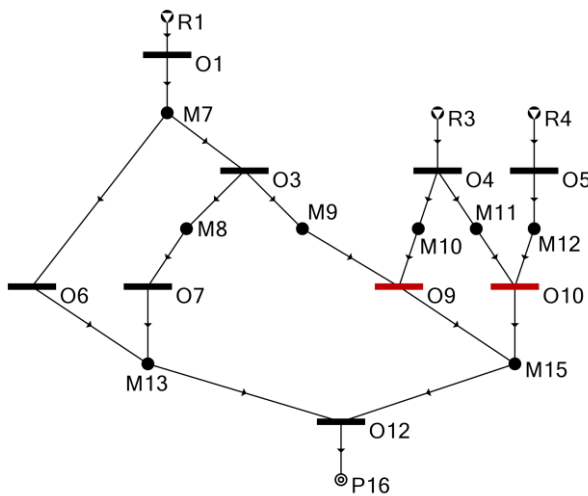


Figure 2: Lowest-cost design option for the motivating example

The goal of the current changes is to provide the decision maker with the lowest-cost process design, as well as the n -best alternatives where all generated alternatives differ from all others in regard to the strategically critical operating units. The cost-optimal design, shown in Figure 2, includes strategically critical operating units O9 and O10. Besides this process design, the decision maker does not wish to see alternative designs that only differ in the non-critical operating units. However, it is important to display alternatives that are strategically different to the cost-optimal solution.

Naturally, since the problem definition has three strategically critical operating units, this limits the number of generated, strategically different processes to eight. However, as usual in PNS problems, some of the networks might not be feasible, or might contain redundant elements that only increase the cost without providing benefit. These networks will be implicitly excluded during the search by the algorithms of the P-graph framework. As a result, the final number of generated, strategically different solutions for the motivating example can be eight or lower.

3. Methodology

Two important observations can be made: (i) for any given potential design network, the set of included critical operating units is unambiguous, and (ii) two network design options are strategically equivalent if they contain exactly the same set of critical operating units. Consequently, the feasible process designs for a PNS problem can be separated into equivalence classes based on which critical operating units their networks contain. For a PNS problem with n critical operating units, 2^n equivalence classes can be defined. For each subset \hat{o} of the critical operating units, there is an equivalence class consisting of the feasible networks where the set of included critical operating units is exactly \hat{o} . Since the networks within an equivalence class are strategically equivalent, and the designer only wishes to receive design options with strategic differences, the set of strategically different solutions consists of the lowest-cost network from each strategic equivalence class. This can be accomplished with the utilisation of the combinatorial algorithms of the P-graph framework.

The P-graph framework provides combinatorial algorithms for PNS, such as algorithm MSG for generating a rigorous superstructure, algorithm SSG for generating combinatorially feasible solutions, and algorithm ABB for generating the best, n -best, or all feasible networks. Since algorithm ABB is capable of generating all feasible solutions as an ordered list, a potential algorithm for determining the structurally different solutions is to generate all feasible solutions (via algorithm ABB) and then select the lowest cost network from each strategic equivalence class. This procedure is shown in Figure 3, where SDSI is the strategically different solution identification algorithm.

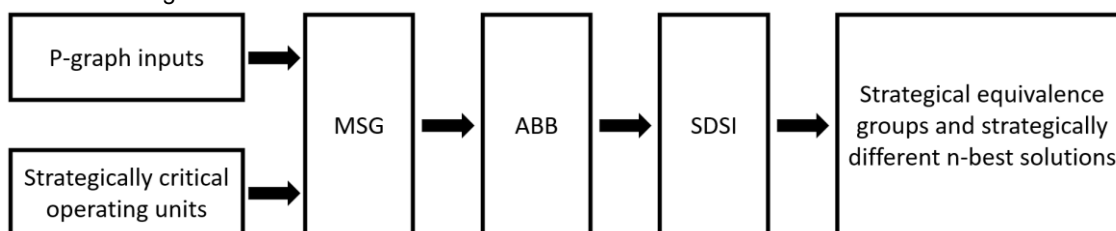


Figure 3: Flow diagram of proposed methodology to identify the n -best strategically different process designs

The previously introduced motivating example includes three strategically critical operating units: O9, O10, and O11. Therefore, the feasible solutions can be partitioned into 8 equivalence classes. However, some of these equivalence classes might not have any feasible solutions. For example, at least one of the critical operating units is necessary for the process, so there are no feasible solutions without any of the critical operating units. Furthermore, adding zero-sized, i.e., unused, operating units to a feasible network does not lead to infeasibility, only impracticality or cost inefficiency. Consequently, algorithm ABB only generates feasible networks with redundancy-free configurations, i.e., networks where the optimal configuration utilises every included operating unit. As a result of this behaviour, some equivalence classes, i.e., {O9,O11}, {O10,O11}, and {O9,O10,O11}, do not have any redundancy-free feasible solutions.

The 26 feasible networks generated for the motivating examples are partitioned into 4 strategical equivalence classes, where the identifying critical operating units are {O9}, {O10}, {O11}, and {O9,O11}. Table 1 lists all equivalence classes, and where applicable, the number of feasible networks and the cost-optimal feasible network in each equivalence class. The ranking of the equivalence class is the cost-based ranking of their *lowest-cost* networks. As a result of the generation procedure, the set of strategically different solutions is created from the cost-optimal networks for each equivalence class. Therefore, it will contain 4 feasible solutions.

Table 1: Strategic equivalence classes and their lowest-cost network of the motivating example

Ranking	Strategically critical operating units	Number of feasible networks in equivalence class	Optimal network in equivalence class
-	-	-	-
#4	O9	7	O1,O3,O4,O6,O7,O9,O12
#3	O10	6	O1,O6,O4,O5,O10,O12
#2	O11	7	O1,O6,O11,O12
#1	O9,O10	6	O1,O3,O4,O5,O6,O7,O9,O10,O12
-	O9,O11	-	-
-	O10,O11	-	-
-	O9,O10,O11	-	-

4. Case study

A larger case study is introduced to show the difference between standard n-best and strategic n-best solutions. This case study is a problem of industrial symbiosis, where three companies (A, B and C) are producing different products. Company A produces biodiesel from *Chorella sp. microalgae*. It is a large factory with multiple facilities to grow the microalgae, and these can be combined with one or more of 9 upgrading technologies to convert the lipids to biodiesel (Lim et al., 2022). Company B is a smaller enterprise which also uses *Chorella sp. microalgae* to create biochar (Zhang et al., 2022). This biochar then serves as an absorbent for wastewater treatment to remove ammonia pollutants, which is especially important in the case of agricultural wastewater. Finally, Company C utilises anaerobic digestion of manure and corn silage to produce power and heat (Vondra et al., 2019). The three companies have multiple options for cooperation through contracts to increase their economic efficiency. Naturally, these contracts are dependent on the individual operations of the companies. However, if the possibility is already considered in the design phase, it can lead to more beneficial process designs for all companies.

While the internal designs of the processes have to be determined, in terms of the whole system, the most important decisions are the contracts, i.e., these will be the strategically critical decisions. There are 6 potential contracts, which are represented as inter-company material- or energy transfers:

- Company A can take clean water directly from Company B,
- Company A can take some of the CO₂ that is produced in Company C as a byproduct,
- Company A also needs energy, which Company C can supply,
- Company C can take some of the biodiesel from Company A to convert into energy,
- Company B needs grown microalgae, which Company A can supply, and
- Company B can take wastewater from Company C and treat it.

Integrating these potential material- and energy transfers between the companies can greatly impact their internal process designs. The main decisions in Company A are the technologies to utilize to produce biodiesel. Company B does not have many options structurally, but it can define the operating capacities as a result of the availability and price of its input materials. Finally, Company C can choose between different ratios of corn silage and manure. The P-graph maximal structure of the whole network is shown in Figure 4, where the 6 strategically critical operating units, representing the potential contracts, are shown in red.

The case study has 19 strategically different feasible networks. These are all the *lowest-cost* networks from their respective equivalence classes. Table 2 lists which critical operating units exist in each network, i.e., which inter-company connections are *utilised*. The number of feasible networks of each equivalence class can also be seen in the last column. Note that the problem has 3,080 feasible networks in total, so the reduction in the number of generated networks is significant. If the goal was to generate the best 10 design options, the conventional network generation would only generate networks from the same *strategic* equivalence class. In fact, the first 72 networks belong to the same equivalence class. Therefore, the *second-best* strategically different solution is only in 73rd place among the whole set of networks. However, with the current method, all 10 would be significantly different from each other, while still satisfying the philosophy of n-best solutions.

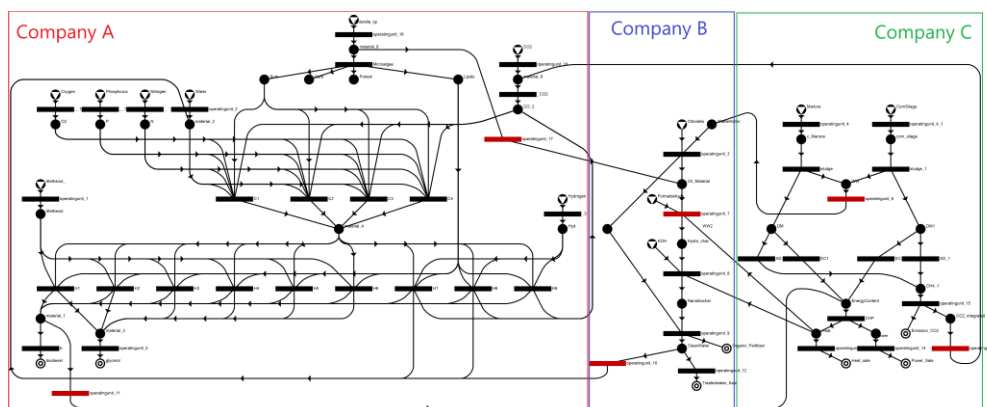


Figure 4: Maximal structure for the 3-company industrial symbiosis case study, the red operating units representing the connections between companies are considered as critical

Table 2: Existence of critical operating units in the strategically different feasible networks for the case study, "Inc" indicates that the connection is included in the network, "Exc" indicates that it is excluded

Profit of best network in the equivalence class (M EUR/y)	A → B Microalgae	B → A Water	A → C Diesel	C → A CO ₂	C → B Wastewater	C → B Heat	Number of different networks in the equivalence class
6.826	Exc	Exc	Inc	Exc	Exc	Exc	144
5.406	Exc	Inc	Inc	Exc	Inc	Inc	72
5.378	Exc	Exc	Inc	Exc	Inc	Inc	72
4.989	Exc	Inc	Inc	Inc	Inc	Inc	328
4.963	Exc	Exc	Inc	Inc	Inc	Inc	328
4.020	Exc	Exc	Exc	Exc	Exc	Exc	147
3.872	Exc	Exc	Inc	Inc	Exc	Exc	132
3.559	Exc	Exc	Exc	Inc	Exc	Exc	128
3.365	Inc	Inc	Inc	Exc	Inc	Inc	106
3.231	Exc	Exc	Exc	Exc	Inc	Inc	74
3.200	Inc	Inc	Exc	Exc	Inc	Inc	108
3.177	Exc	Inc	Exc	Exc	Inc	Inc	72
3.165	Inc	Inc	Inc	Inc	Inc	Inc	424
3.033	Inc	Inc	Exc	Inc	Inc	Inc	324
2.856	Exc	Inc	Exc	Inc	Inc	Inc	188
2.842	Exc	Exc	Exc	Inc	Inc	Inc	188
2.841	Inc	Exc	Inc	Inc	Inc	Inc	172
2.830	Inc	Exc	Exc	Inc	Inc	Inc	72
0.405	Inc	Exc	Exc	Exc	Inc	Inc	1

5. Conclusions

When designing a process, it is beneficial to provide alternative design options to the decision maker. However, when these alternatives are selected based on cost, they are often too similar to the cost-optimal solution. The current work presented a methodology for generating strategically different n-best design options for Process Network Synthesis problems. The decision maker can define the strategically critical operations in the process, which indicate meaningful differences between different designs. Based on the combinatorial algorithms of the P-graph framework, the methodology is able to generate alternative design options where any two solutions are different according to the preferences of the designer. The difference between generating n-best solutions with and without considering strategically critical decisions was demonstrated via a case study. Without defining the critical decisions, the problem had 3,080 feasible solutions. However, as the designer defined 6 operating units to represent the strategically critical decisions, it was discovered that the 72 lowest-cost solutions were strategically identical. Finally, the problem only had 19 strategically different feasible solutions. This shows the capability to provide the decision maker with meaningful choices when presenting alternative designs.

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