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Process Network Design and Optimisation Using P-graph: The Success, the Challenges and Potential Roadmap

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The P-graph framework is a combinatorial approach to synthesising and optimising process networks. It is very efficient in handling problems with high combinatorial complexity and has shown great superiority in reducing the related computational burden. Over the years, it has proven its efficiency in solving topologically and combinatorically challenging problems. Many successful applications to scientific and real-life problems have been produced, demonstrating the benefit potential. The application areas range from the initial chemical process synthesis to identifying the mechanisms of chemical and biochemical reactions, supply chains optimisation, regional resource planning, crisis management, evacuation planning and business process modelling. There have been tools of several generations implementing the P-graph framework, with a simple user interface, but featuring serious data input requirement. The P-graph framework also allows sensitivity analysis and produces usually a set of recommended solutions as opposed to the usual single output from straight applications of MP.

The current contribution makes a critical overview of the achievements from applying the P-graph framework and the main issues to be dealt with. Based on that, a set of recommendations is made on the necessary future development of the implementations regarding modelling capability, data and algorithmic interfaces, representation of the modelled networks, as well as complexity management.

1. Introduction

Process Network Synthesis usually involves selection of topology, operating units and their capacities, within the context of completing a certain goal – e.g. chemical synthesis, oil refining, food processing, a supply of products, resource harvesting and use. The complexity of the problem arises from the combination of continuous and combinatorial aspects. This increases exponentially with the number of candidate operating units, posing a serious challenge to the solution methods.

One option for modelling and solving such problems is Mathematical Programming (MP) and specifically Mixed Integer Nonlinear Programming (MINLP), used for reducing pre-constructed network superstructures. For large problems, however, applying MP becomes increasingly difficult (Arora and Barak, 2009), due to the usually heuristic construction of superstructures. Such activities are time demanding and error-prone and may miss advantageous options. The structural infeasibilities in the evaluated combinations are discovered by the solvers only after evaluating the constraints. Consequently, practical problems often become too complex to solve. If the problem is then simplified to be solvable, the resulting formulation is usually no longer representative of the original task. In Computational Complexity Theory (Arora and Barak, 2009) these problems are referred to as “intractable”.

The P-graph framework (Friedler et al., 1992) was developed to address this combinatorial challenge for optimising process networks (Friedler et al., 1998). It presents the fundamental concepts, followed by the main algorithms (Friedler et al., 1993), and extensions (Friedler et al., 1995), including Accelerated Branch and Bound optimisation (Friedler et al., 1996). The framework has been presented in detail by Klemeš et al. (2010).

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Many successful applications (Klemeš and Varbanov, 2015) to scientific and real-life problems testify to the efficiency and superiority of the P-graph framework in solving topologically and combinatorically challenging problems, demonstrating the potential benefit. Some of them are also reviewed next. However, the applications have also revealed certain limitations in treating engineering problems – especially dealing with continuous problems where material states are not predefined. An example is water or steam network optimisation where the stream compositions depend on the operating unit sizes. As a result, the success stories and the limitations have been shaping the directions for future development of P-graph. This paper analyses the P-graph framework suitability for a range of Process Systems Engineering problem classes and recommending appropriate focus for the future efforts in its development and applications.

2. Conception and core features

The P-graph framework (Friedler et al., 1992) provides an unambiguous representation of process networks. Combined with the rigorous mathematical toolset of the axioms and theorems, provides advantages over MP for process network optimisation. The main advantages come from exploiting the combinatorial nature of the problem instead of transforming it to equations. The associated instruments – the axioms ensuring representation unambiguity and the algorithms for generating, reducing and optimising the maximal network structure, have several important properties. The algorithms automatically generate, then optimise and reduce the problem superstructure, following the user inputs. This is made possible by exploiting graph theory and advanced set manipulation. The superstructure optimisation avoids the examination of infeasible combinations of binary variable values by applying the Accelerated Branch-and-Bound algorithm (Friedler et al., 1996). As a result, the P-graph approach to network optimisation drastically reduces the combinatorial search space and is more efficient than pure MP measured by the number of options to evaluate.

The formulation and solution of network problems for varying conditions have been also supported (Heckl et al., 2015). This is achieved by special extension of the P-graph model formulation using one operating unit to represent the equipment or facility and further units representing the operation during each of the periods in the considered horizon. More recently this has been extended further to handle partial load limits (Tan and Aviso, 2016).

3. Software tools implementing the P-graph framework

Three generations of tools have implemented the P-graph framework over the years (Klemeš and Varbanov, 2015). The first implementation was command-line software, implementing the core algorithms for superstructure construction and optimisation. The tool required an input of the Process Network Synthesis (PNS) problem in an input text file with a pre-defined syntax. That was later replaced by a Graphical User Interface shell named “PNS Editor”, employing the essentially same code base, but providing more convenient features for editing, saving and problem execution.

The tool offered by the P-graph community (P-graph, 2017) is named “P-Graph Studio”. The tool is freely available for download from the website (P-graph, 2017). It integrates all activities necessary for representing a process network problem as a P-graph and solving the optimisation problem. The features include

- Drawing visually P-graph instances and superstructures. It allows producing well-organised diagrams of P-graphs, containing materials, operating units and connectors
- Editing the properties of the objects and formatting of the complete P-graph diagram
- Export of the resulting diagram to several image formats
- Solving the constructed superstructures to optimality, employing several algorithms: Maximal Structure Generation (MSG) – for building the network superstructures, Solution Structure Generation (SSG) – for enumeration of feasible solutions belonging to the superstructure, Accelerated Branch and Bound (ABB) optimisation – for obtaining the optimal networks
- Modelling for multiperiod optimisation
- Visualisation of the networks, report exporting – including Excel.
- Linear functions are allowed for operating and investment costs of an operating unit.

4. Application Areas

There has been a variety of thematic groups of investigations applying P-graph. These include: Process Synthesis of Chemical and Energy Conversion Systems; Supply Chains, Waste and Resource Management; Modelling Chemical Reactions; Discrete-Event Decision-Making; Combining P-graph algorithms with Mathematical Programming Tools.

4.1 Process Synthesis of Chemical and Energy Conversion Systems

The founding papers finishing with (Friedler et al., 1996) have used illustration examples based on classical Chemical Process Synthesis for generation of chemical conversion flowsheets. This line has been further developed. Lee and Park (1996) combined the use of the P-graph algorithms MSG and SSG for generation of candidate networks in Mass Exchange Networks, then optimised each of them using standard Non-Linear Programming.

An interesting application of P-graph has been published, exploring the biochemical production of butanol from grain feedstock (Liu et al., 2004). The proposed method aims at minimising the overall cost of the resulting downstream processing flowsheet. The procedure starts with the selection of possible processing units and the equipment options for them, followed by algorithmic superstructure generation and generating a set of optimal and near-optimal flowsheets for further selection by engineers. The approach has been extended in a follow-up work on a retrofit problem for the butanol production process (Liu et al., 2006).

Efficient energy conversion networks using fuel cells (Varbanov and Friedler, 2008) and Heat Exchanger Network Synthesis (Nagy et al., 2001) are examples of applying P-graph to energy conversion and recovery systems. Building on that, polygeneration plant optimisation has been investigated by Tan et al. (2014). Optimally synthesising separator networks has also been modelled by Heckl et al. (2010) – including consideration of different separator types – e.g. adding extraction alongside distillation units. A very interesting recent work is the one on optimal design of energy conversion flowsheets (Szlama et al., 2016), where the inputs and outputs for an operating unit are considered as variables. Additional linear constraints are formulated, to model the performance of the operating units.

4.2 Supply Chains, Waste and Resource Management

Regional biorefinery synthesis has been performed by Halasz et al. (2 005). This is an interesting work bridging Process Synthesis and regional resource optimisation. The optimisation of regional energy supply chains with renewables (Lam et al., 2010) has been a very successful area where P-graph based process network optimisation has been applied. This work applies a two-level procedure for the design of regional biomass utilisation networks, minimising the environmental impact. The proposed procedure successfully manages the complexity of the network problem, by simplifying the infrastructure links and their design and tasks.

An interesting contribution on waste minimisation has been that of Halim and Srinivasan (2002a). This is the first of a series of three3 publications and the most highly cited from the series. The paper has formulated a hierarchical decision-making procedure embedding P-graph and its application in the overall workflow. Using a cause-and-effect based analysis, the work provides the complete algorithm and an illustrative case study. That work was later followed by extensions developing an intelligent decision support system (Halim and Srinivasan, 2002b) and adaptation to batch processes (Halim and Srinivasan, 2006).

A case of crisis management via re-routing resources and production tasks on an industrial site has been investigated (Tan et al., 2016). This work provides problem formulation and a procedure using P-graph for optimising the response to failures in plant operation.

4.3 Modelling Chemical Reactions

Another successful application area has been the modelling of biochemical reactions. Seo et al. (2001) applied P-graph to the pathway identification in biochemical reactions, followed by (Fan et al., 2002) which dealt with identifying reaction mechanisms in catalytic reactions. The latter paper presents a mathematically exact method based on P-graph by synthesising networks of pathways and evaluating them. The authors applied specially developed software tools and the results have indicated higher efficiency than other combinatorial approaches. Those works have been extended by Lee et al. (2005) to analysing metabolic pathways. A further application has been the Fischer-Tropsch synthesis of hydrocarbons from syngas (Lin et al., 2009).

4.4 Discrete-Event Decision-Making

There have been works dedicated to discrete-event decision-making. A typical example is workflow modelling (Tick, 2007), which has extended the P-graph mathematical toolset to model and synthesise workflows as networks. Another particularly practical and potentially very important work has been the determination of the event-dependent dynamically-optimal evacuation routes (Garcia-Ojeda et al., 2012) for large buildings and industrial sites.

4.5 Combining P-graph algorithms with Mathematical Programming Tools

Bertók et al. (2012) have provided a method for generating and analysing Mathematical Programming models for Process Synthesis problems. This work illustrates the power of the P-graph framework and the potential flexibility that is possible if this is combined with other tools supporting Mathematical Programming. The latter can be GAMS, LINDO, Excel or ILOG CPLEX. The highest value of this development lies in the opportunity for seamlessly integrating the P-graph framework into the overall process optimisation workflow, keeping its crucial advantage – the mathematically rigorous superstructure generation.

5. Analysis and the way forward

The reviewed high-quality works illustrate clearly the power and appeal of the P-graph framework, as well as its efficiency in tackling combinatorial challenges within a diverse set of application areas. The popularity of the published works shows a trend of growing impact and the need for further development.

The main achievements of the framework and its application have been in the unrivalled reduction of combinatorial burden on solvers compared with straight application of Mathematical Programming. There have been serious strengths. One of them is the simplicity and the user friendliness of the offered P-graph tool (P-graph, 2017). The users do not need very advanced training to apply it. The interface and the required data input are simple, as is the interpretation of the results. Required is, of course, sufficient knowledge of the modelled subject area and sound engineering or modelling judgement. The P-graph framework allows sensitivity analysis and produces usually a set of several recommended solutions.

The P-graph applications have been useful in modelling problems with clearly identifiable discrete alternatives and their combinations. This can be witnessed by the reviewed works on supply chain optimisation, chemical process synthesis, chemical reaction modelling, workflow optimisation, evacuation route planning.

The framework, however, has also certain limitations. They seem rooted mainly in the current implementation philosophy of the tools. One is the complicated user interaction for larger problems in terms of both data entry and preparation. The P-graph extension for modelling multiperiod problems offers this modelling flexibility at the cost of amplifying the data requirement.

A second key issue is the inability of the framework implementations to tackle efficiently network optimisation problems where the process performance and the stream properties vary with the process unit capacity or cases where component-wise mass balance or enthalpy balances are necessary. Such are, for instance, Heat Exchanger Networks (HEN), Water Integration and CHP system synthesis. The problem here is the difficulty of identifying specific states of the materials or streams involved in the considered problems. A typical example is a HEN problem, where the temperature of a stream after a heat exchanger would vary with the duty. In this context, it is unclear what value to assign to a "material" that models such a stream. This is an open issue, which is necessary to consider in an open discussion – whether and how to handle it, or keep the current limitations in place.

The mathematical rigour of the P-graph framework allows future developments. Several directions are possible and a serious debate should be held on prioritising them, carefully weighing the relevance and potential benefits against costs in terms of development efforts and need for funding. Solutions to each of the outlined challenges are analysed.

The complexity of data entry is mainly implementation issue, but it can also be linked to the potential development of the P-graph framework in terms of improved concepts. In this direction, tools enabling data conversion between flowsheeting environments and P-graph can be a large part of the solution. In terms of framework development, hierarchical graphs can be also useful, allowing to have nodes, containing sub-graphs. This may bring about a serious scalability advantage concerning both the model storage and its visualisation.

With respect to the multiperiod modelling, there are several assumptions made in the tool implementations, which are not explicitly stated. For instance, rigorous material balances are applied around operating units, while around "material" nodes the balances are open – as long as material consumption does not exceed its influx, the system is considered feasible. These assumptions should be thoroughly analysed and their implications documented in the knowledge base of P-graph.

The current difficulty in handling more sophisticated mass and energy balances using the P-graph tools can be tackled by further developing the symbiosis of the P-graph tools with Mathematical Programming tools. The reviewed article (Bertók et al., 2012) has the potential to perform such a link more efficiently. Another potential development avenue can come from the hybrid applications of P-graph with other methods, such as Monte Carlo Simulation (Tan et al., 2017).

6. Conclusions and potential development directions

From the overview and analysis, it has become apparent that the P-graph framework has offered a mathematically rigorous paradigm for Process Network Optimisation and Synthesis. It provides a set of axioms and algorithms for superstructure generation and reduction in an efficient way, very much superior to most other methods. It has proven very successful in many areas such as supply chains, regional development, reaction

pathways identification, energy conversion. In solving all such problems, it has demonstrated a great strength in reducing the combinatorial complexity, generating a set of alternative solution recommendations – preserving the valuable interaction with the tool users instead of isolating them from the decision-making process.
Another very useful feature is the framework's flexibility in combining it with other procedures and network optimisation principles. The successful application to regional renewable resources utilisation by Lam et al. (2010) has clearly illustrated this where the P-graph application stage is preceded by resource targeting, regional clustering and formulation of a series of network synthesis problems to pass to the P-graph algorithm.
The discussed limitations also form drivers for potential further research and development aiming for improvements. One prospective direction of future work will obviously concern bridging the gap between the formulations of the real network optimisation problems and the requirements of the P-graph framework implementations for clear-cut input of fixed states/materials and fixed performance of operating units. A potential way of addressing this are to provide application-specific wrapper algorithms, which would translate the domain-specific problems into the required mathematical representations.
Another potential innovation stemming from this issue is to develop ways of allowing more complex and realistic internal models for the operating units. In fact, the P-graph mathematical fundamentals do not require exactly proportional models with fixed performance. While this development may not constitute a significant chemical or process engineering innovation, in terms of information technology, modelling semantics, modelling paradigm evolution and enabling further widespread application of the P-graph concept and framework, this has the potential to become a major step forward.
Another potential avenue for future innovation may be the combination of P-graph with Mathematical Programming. Such a suggestion has also been made in (Lam, 2013). This would require the interaction of experts on P-graph with those on Mathematical Programming. A possible way for future development is the generator of Mathematical Programming models based on P-graph (Bertók et al., 2012). P-graph tools can be applied for generating good initial points for problems with Non-Linear Programming or Mixed-Integer Non-Linear Programming models. A step toward such modelling flexibility has also been (Szlama et al., 2016).
In terms of improving the user experience in the tool implementations, users have been very happy with the export capability to Excel. This points to another potentially very useful development – providing data import from Excel, within a pre-defined syntax. This can be a productive avenue for discussions between the users and the tool developers, ultimately providing a feature that can save a lot of modelling time.

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