CHEMICAL ENGINEERING TRANSACTIONS

VOL. 70, 2018

A publication of AIDIC

The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Timothy G. Walmsley, Petar S. Varbanov, Rongxin Su, Jiří J. Klemeš

ISBN 978-88-95608-67-9; **ISSN** 2283-9216

DOI: 10.3303/CET1870016

Towards Generalized Process Networks: Prospective New Research Frontiers for the P-graph Framework

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The P-graph framework was originally developed to address Process Network Synthesis (PNS) problems in the preliminary design of chemical plants. P-graph provides a mathematically rigorous and computationally efficient framework for solving PNS problems via the maximal structure generation (MSG), solution structure generation (SSG) and accelerated branch-and-bound (ABB) algorithms. MSG ensures rigorous generation of the maximal structure, while the ad hoc generation of a superstructure as basis for a mathematical programming model can lead to significant modelling errors. In addition, SSG allows the generation of combinatorially feasible network structures that can be utilized for practical decision-making by designers. For very large problems, ABB can reduce the computational effort of reaching globally optimal solutions by multiple orders of magnitude compared to conventional branch-and-bound solvers for Mixed Integer Linear Programming (MILP) models. In addition to conventional PNS problems, P-graph has been applied to the optimization of separation processes, Heat Exchanger Networks (HENs), Combined Heat and Power (CHP) systems, chemical reaction pathways, polygeneration plants, biorefineries, and supply chains. Further non-conventional applications have also been reported, such as the optimisation of office processes, human resource networks, and economic structures at the level of cities or regions. In addition to synthesis and design problems, P-graph has also been applied to operational problems, such as determining the best abnormal operating conditions for process networks. These diverse applications suggest the potential for applying the P-graph framework as a problem-solving strategy for a broad class of generalized process networks, beyond the traditional PNS problems in chemical plant design. This paper surveys recent trends in the P-graph literature and uses bibliometric analysis to identify promising trends and discusses potential directions for novel applications for optimization of generalized process networks, particularly for applications that address critical sustainability issues.

1. Introduction

The P-graph framework was initially developed as a rigorous approach to solving Process Network Synthesis (PNS) problems in plant design applications. This graph-theoretic framework is based on mathematical axioms (Friedler et al., 1992a) that provide a basis for the development of efficient algorithms for PNS (Friedler et al., 1992b). Initial development of the P-graph framework can be traced to the late 1970s (Friedler et al., 1979). Upon its introduction, it presented a viable alternative to Mathematical Programming (MP) models that dominate the Process Systems Engineering (PSE) literature. The P-graph methodology has matured over three decades of development and has been integrated into both basic (Peters et al., 2003), advanced level textbooks (Klemeš et al., 2010), book chapters (Cabezas, 2017) and professional magazines

Please cite this article as: Tan R.R., Aviso K.B., Klemes J.J., Lam H.L., Varbanov P.S., Friedler F., 2018, Towards generalized process networks: prospective new research frontiers for the p-graph framework , Chemical Engineering Transactions, 70, 91-96 DOI:10.3303/CET1870016

(Cabezas et al., 2015). A recent work also documents the pedagogical advantages of P-graph methodology in comparison to equation-based modelling approaches (Lam et al., 2016). The capability to generate both optimal and near-optimal solutions also creates some advantages in the context of Problem-Based Learning (PBL), as it strengthens the interpretation of model solutions into practical engineering decisions (Promentilla et al., 2017).

Three notable previous papers have surveyed developments in P-graph literature. Lam (2013) reviewed developments in PNS as well as extensions applied to the planning of sustainable supply chains for bioenergy systems. A subsequent paper discussed further developments, including trends in the diversification of applications and geographic distribution of research teams working on P-graph (Klemeš and Varbanov, 2015). The most recent article articulated the need for further research in computational and implementation aspects of the P-graph framework, based on an analysis of developments from the original date of inception (Varbanov et al., 2017). In this work, developments in the use of the P-graph framework to address non-conventional problems with PNS-like structure are surveyed; further prospects for future applications in novel problem domains are then considered. Aspects already covered by the three mentioned papers are excluded here. The rest of this paper is organized as follows. Section 2 gives a brief description of the P-graph framework. Section 3 gives a critical appraisal of the P-graph literature trends, focusing on non-conventional applications, while Section 4 describes methodological innovations arising from combining P-graph with other methodologies. Some promising PNS-like problems are then discussed in Section 5. Finally, the conclusions are given in Section 6.

2. P-graph framework

P-graph is a rigorous framework based on graph theory for solving PNS problems. Five axioms for PNS were proposed by Friedler et al. (1992a) for generic PNS problems in the context of the design of process plants. Computationally efficient algorithms were then developed by taking advantage of the inherent information in PNS problems based on these axioms (Friedler et al., 1992b). Given a predefined set of system component units and streams, it is possible to use the P-graph framework to develop a maximal structure, which represents the union of all combinatorially feasible process networks (Friedler et al., 1993). Unlike ad hoc superstructures used in many PSE applications, maximal structures are generated rigorously via the Maximal Structure Generation (MSG) algorithm, which eliminates the risk of human error that may lead to incorrect problem specification. The Solution Structure Generation (SSG) algorithm allows the rigorous identification of all combinatorially feasible networks that are subsets of the maximal structure. Once flowrate constraints and other boundary conditions are specified, in principle a unique optimum can be determined for each solution structure, if such a solution exists. The Accelerated Branch and Bound (ABB) algorithm allows the efficient determination of the optimal solution to a PNS problem, reducing the solution space dramatically by eliminating the combinatorially infeasible and redundant solutions (Friedler et al., 1996). The natural capability to generate the n-best (i.e., optimal and near-optimal) solutions to a PNS problem is another important advantage, especially for practical engineering decision-making (Promentilla et al., 2017). P-graph software (P-graph Studio), technical support and on-line tutorials are available via a dedicated website (P-graph, 2018), while a more detailed tutorial on the topic can be found in Peters et al. (2003).

3. Current literature on P-graph approach to non-conventional problems

This section discusses the application of P-graph to PNS-like problems. Such extensions are typically developed as a result of analogous problem structures. For example, the equivalence of PNS to set covering problems in Operations Research (OR) was established by Imreh et al. (2000). In other cases, the similarity of novel problems to the classical PNS problem has not necessarily been established with rigorous mathematical proof, but merely demonstrated with examples.

The earliest extensions of P-graph methodology to problems outside of pure process design were applications to the analysis of chemical reaction pathways (Fan et al., 2002). In such problems, each elementary reaction is represented as an operating unit whose input-output ratios are defined by stoichiometry. Specific applications include the catalytic partial oxidation of methanol (Lin et al., 2008), catalytic decomposition of methanol (Lin et al., 2010) and methanation of CO_2 with hydrogen (Díaz-Alvarado et al., 2018). Biochemical reactions have also been modelled in this manner (Seo et al., 2011). A tutorial on this topic is given in the textbook of Peters et al. (2003).

Chong et al. (2014) developed a P-graph approach to the problem of optimal retrofitting of a fleet of fossil fuel-fired power plants for CO_2 capture and storage (CCS). The model considers mass (CO_2) and energy (electricity) balance issues in such systems. Tan et al. (2017) proposed a P-graph method to solve general Carbon Management Network (CMN) problems. The CMN problem is structurally similar to Resource

Conservation Network (RCN) problems in Process Integration (PI), but was further shown to be equivalent to PNS. This method was applied to problems involving carbon-constrained energy planning, and to the allocation of CO_2 in a CCS network with power plant sources and geological storage sinks. The use of Monte Carlo simulation to assess the robustness of the n-best solutions was also demonstrated (Tan et al., 2017).

In addition to these PNS-like problems, the P-graph framework has been applied to a wide range of applications not traditionally covered by PSE. For example, Tick (2007) developed a P-graph approach to the optimisation of business process workflows. Subsequently, fuzzy P-graph (Tick, 2009) and robust P-graph (Tick et al., 2013) extensions were developed to account for imprecision in problem specification in practical cases. Preliminary results on the use of P-graph for the design of multi-agent systems in organizations were reported by Garcia-Ojeda et al. (2015). Aviso et al. (2017) used P-graph to determine the optimal and near-optimal reassignment of personnel in an organisation under abnormal operating conditions. Other notable non-conventional applications include optimisation of emergency evacuation routes (Garcia-Ojeda et al., 2012), vehicle assignment (Barany et al., 2011), vehicle maintenance schedules (Adonyi et al., 2013) and logistics (Tick, 2013).

Aviso et al. (2015) demonstrated that economic input-output (IO) systems can be represented by P-graph. This approach was applied to the problem of reallocating production capacity at the level of cities, regions or countries during crises caused by disruptive events due to climate change. It should be noted that the previously mentioned application to workforce reallocation (Aviso et al., 2017) is also based on the similarity of IO model optimisation to the generic PNS problem. Given the broad applicability of IO models to a wide array of problems, this similarity suggests the potential to also apply P-graph methodology to such cases.

4. Extended and hybrid P-graph approaches

In addition to its use as a stand-alone methodology for static PNS problems, the P-graph framework has been extended to deal with problems of a special structure as demanded by specific applications. It has also been combined with other methods into hybrid problem-solving approaches.

Although originally developed for static or steady-state PNS problems, a multi-period variant was developed by Heckl et al. (2015). This extension is now incorporated in the latest version of P-graph Studio (P-graph, 2018). The multi-period variant was further improved to account for part-load operating limits by Tan and Aviso (2016). In addition to being used as a stand-alone tool, P-graph has also been used in conjunction with MP models. For example, Bertok et al. (2013) used P-graph to rigorously generate MILP models for PNS problems. A similar approach was developed by Voll et al. (2013), who used P-graph to generate an initial superstructure for distributed energy systems. The initial superstructure was then used to develop a full MILP formulation for the design problem. Another interesting development with important engineering applications is the integration of reliability theory in PNS (Holló, 2013). The limitation imposed by linearity assumptions in PNS problems has been relaxed in a recent paper reporting the use of variable IO ratios (Szlama, et al., 2016).

Tick (2007) first proposed the fuzzy P-graph formulation and applied it to business process workflow optimization. This work is based on the concept of fuzzy optimization with “soft” constraints, which may exist in practical situations where data uncertainty prevents precise specification of the optimization problem (Zimmermann, 1978). A variant of fuzzy P-graph has recently been applied to the design of energy systems with uncertain demands (Aviso and Tan, 2017). P-graph was combined with the ε-constraint method to determine Pareto frontiers in vector optimization problems in the context of sustainable supply chain planning (Vance et al., 2015). This approach is valuable due to the inherently multi-dimensional nature of many practical engineering problems. In particular, the trade-off between economic and environmental considerations can be addressed in this manner. In principle, a unique solution for implementation can then be selected from the Pareto frontier; in practice, decision analysis methods, such as the Analytic Hierarchy Process (AHP) (Saaty, 1980), may be further combined with P-graph to make this final step more systematic.

One powerful feature of the P-graph framework is the capability to identify optimal and near-optimal solutions. Tan et al. (2017) proposed a hybrid approach with Monte Carlo simulation being used as a second stage to gauge the quality of the generated n-best solutions. In such cases, near-optimal solutions with objective values that are only marginally worse than the mathematical optimum under nominal design conditions, may prove to be superior over a broader range of non-ideal, perturbed states. Lakner et al. (2017) examined the startability of the reaction networks generated by P-graph algorithms in two ways: by P-graph algorithm and by Petri net algorithm.

5. Potential future P-graph applications

There is considerable potential to apply P-graph methodology to non-conventional PNS-like problems. Some promising directions are discussed here.
The applicability of P-graph to model economic IO systems, which has been demonstrated by Aviso et al., (2015), presents interesting possibilities for further extension. IO methodology is mature and can be used for the analysis of linear networks (Miller and Blair, 2009). The optimisation of IO models via P-graph approach potentially extends beyond economic networks. For example, the use of P-graph to optimise workforce allocation (Aviso et al., 2017) results directly from such problems being represented in an IO framework (Correa and Craft, 1999), while the P-graph allocation of infrastructure inoperability (Tan et al., 2015) makes use of the inoperability input-output model proposed by Haimes and Jiang (2001) which has been used for the analysis of disruptive events (Santos and Haimes, 2004). IO models have been used for the low-resolution analysis of natural ecosystems and food chains (Hannon, 1973). Optimal ecosystem management can potentially be represented as a PNS problem and solved using P-graph. The mathematical framework used in popular decision analysis methods such as AHP (Saaty, 1980) and Decision-Making Trial and Evaluation Laboratory (DEMATEL) (Gabus and Fontela, 1972) are also similar enough to IO calculations to suggest that P-graph can be used to develop improvements or extensions of these tools.
The P-graph framework and its software implementation (P-graph, 2018) offers a particularly simple interface, ease of modelling and high computational efficiency. As long as the modelled problem can be represented as a network of materials/streams/states and operations/transitions, this set of features can be especially useful for spreading to more areas. The usual PI approach is based on setting performance targets before system synthesis or design (Klemeš et al., 2018). Targeting is based on obtaining upper bounds on system performance and lower bounds on its cost, using simplified models. In the case of Heat Integration (Klemeš et al., 2018), thermodynamic calculations have been the basis of a simplified model represented by Composite Curves, roblem Tables and the associated targeting tools for HENs. Ong et al., (2017) successfully applied P-graph to Total Sites. In the case of spatially challenging problems, typical for Supply Chains, targeting can be performed using simplified PNS problem formulations – such as for waste management (Walmsley et al., 2017).
The problem of optimal allocation of resources (e.g., public or private research and development funding) in innovation networks can also be represented in PNS form. Innovation networks consist of sets of interdependent developing technologies which serve as components of larger technological systems (Lange et al., 2013). In such cases, successful commercial deployment is contingent on the technological maturity of the system components. This presents a PNS-like problem for which probability of research and development success can be represented as a component reliability parameter using the approach of Holló (2013).

6. Conclusions

This work has given a comprehensive survey of applications of the P-graph framework to non-conventional problems with the PNS-like structure. Extended and hybrid P-graph approaches have also been reviewed. Opportunities for future applications have also been proposed based on similarities in problem structure domain. A disjunctive search in Scopus using the terms “P-graph” or “Process Network Synthesis” yields 271 documents (cited a combined 2,792 times), including 105 from 2013 to the present. The papers cited here represent only a minority of the total P-graph literature, indicating plenty of opportunity for future expansion.

Acknowledgements

The authors also gratefully acknowledge the EC project fund No. CZ.02.1.01/0.0/0.0/15 003/0000456, provided to Sustainable Process Integration Laboratory - SPIL funded as the Operational Programme Research, Development, and Education of the Czech Ministry of Education, Youth and Sports by EU European Structural and Investment Funds, Operational Programme Research, Development and Education under a collaboration agreement with Pétér Pázmany Catholic University, Budapest.

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