Computers and Chemical Engineering 93 (2016) 64–86

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Semantically enabled process synthesis and optimisation

Antonis Kokossis[b], Claudia Labrador-Darder[a], Franjo Cecelja[a,*]

[a] Centre for Process & Information Systems Engineering, University of Surrey, Guildford GU2 7XH, UK
[b] School of Chemical Engineering, National Technical University of Athens, GR-15780 Athens, Greece

A R T I C L E I N F O

Article history:
Received 17 October 2015
Received in revised form 18 April 2016
Accepted 28 May 2016
Available online 9 June 2016

Keywords:
Process synthesis
Ontologies
Tabu search

A B S T R A C T

This paper introduces a new framework to support synthesis of complex engineering problems using a paradigm that combines optimisation with ontological knowledge modelling. The framework registers and analyzes new solutions by introducing a mechanism of digital certificates to translate structural information and solution features through semantics of an ontology. The solutions are respectively clustered by design features. Tested against complex synthesis of reactor networks, the framework offers a potential to visualize optimization in the course of its development and demonstrates noticeable advantages over conventional methods of a similar basis in convergence and performance.

1. Introduction

Most of industrial processes are complex by nature; this is particularly the case with processes involving reaction networks described by highly nonlinear kinetics. Numerous techniques have been developed for design and synthesis of reactor network, i.e. graphical techniques including attainable region technique, simplified approximations in the form of superstructures, and highly analytical representations (Ashley and Linke, 2004; Soltani and Shafiei, 2015; Zhao and Marquardt, 2016). In either case the selection of options from among large number of alternatives is normally supported by optimisation with numerous optimisation approaches reported. Initially, these were deterministic techniques including non-linear programming (NLP) (Achenie and Biegler, 1988) and mixed-integer non-linear programming (MINLP) (Kokossis and Floudas, 1990; Raman and Grossmann, 1991; Kokossis and Floudas, 1994; Jin et al., 2012), among others. More recent approaches focus on stochastic search based optimisation with perhaps Simulated Annealing (Marcoulaki and Kokossis, 1996, 1999; Mehta and Kokossis, 2000; Linke and Kokossis, 2003a), Tabu Search (Wang et al., 1999; Linke and Kokossis, 2003b; Cavin et al., 2004) and Ant Colony (Dorigo et al., 1999; Jayaraman et al., 2000; Dorigo and Blum, 2005) being the most widely applied. Attempts were also made to use the combination of linear programming and stochastic optimisation to find the best synthesis solutions (Jin et al., 2012). The latest advances in stochastic search based on cascading of population and inflection of solutions is particularly attractive as it provides readily access to optimisation solutions at every stage of the process, the search known as the Cascade Algorithm (Labrador-Darder et al., 2009; Kokossis et al., 2011; Cecelja et al., 2014).

Inherent problems with all optimisation techniques have long been realised, and they include (i) tedious analytical considerations, (ii) slow convergence and long computational time (Kokossis et al., 2011), (iii) interpretation of complex and impractical optimisation results (Ashley and Linke, 2004), and (iv) lack of confidence in selecting the options. As reported, complex analytics was mainly addressed by controlled simplifications, e.g. superstructure representation (Yeomans and Grossman, 1999; Pahor et al., 2000; Linke and Kokossis, 2003a), whereas attempts were made to improve slow convergence of deterministic optimisation by simplifying the conceptual content and hence analytics (Raman and Grossmann, 1991; Bauer and Stichlmair, 1996). Similarly, slow convergence of stochastic searches was addressed by parallelising the execution and hence providing larger number of solutions in shorter time (Talbi et al., 1998; Leite and Topping, 1999; Wang et al., 2005; James et al., 2009; Kokossis et al., 2011; Kim et al., 2012; Cecelja et al., 2014).

Application of engineering knowledge in the process synthesis and especially in the process of optimisation helped to both interpret and simplify results, hence to improve the confidence, but also to speed up convergence. Raman and Grossmann (1991) attempted to apply engineering insights as additional logical constraints in MILP optimisation. Similarly, Shah and Kokossis (2001) attempted to further formulate conceptually rich performance model that makes simultaneous use of engineering insights and MILP opti-

* Corresponding author.
E-mail address: f.cecelja@surrey.ac.uk (F. Cecelja).

http://dx.doi.org/10.1016/j.compchemeng.2016.05.018
0098-1354/

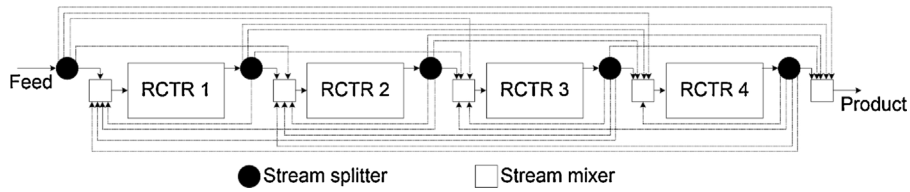

Fig. 1. Single phase superstructure representation.

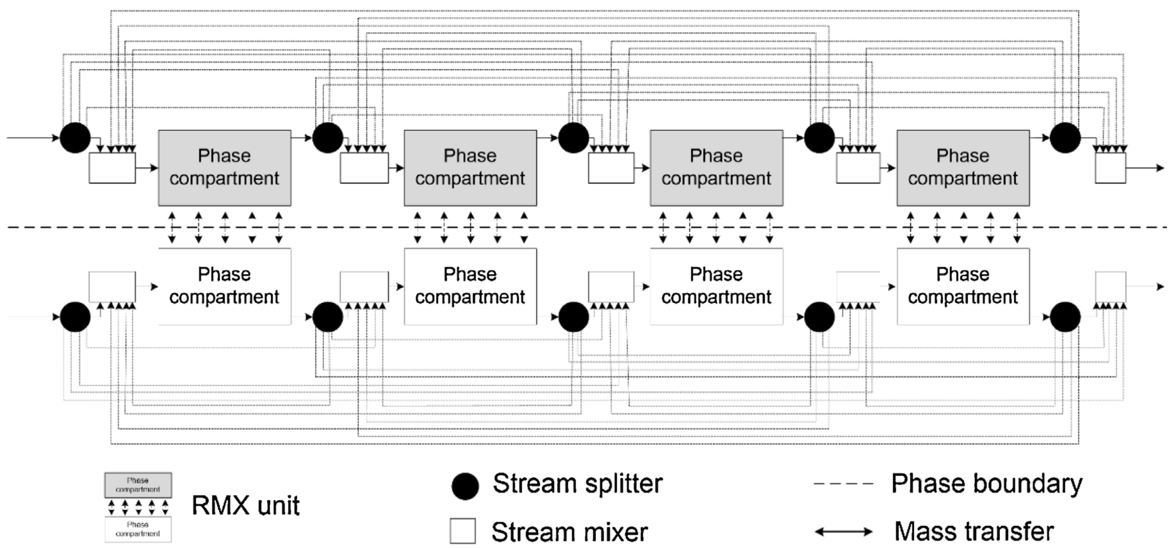

Fig. 2. Superstructure representation of a two-phase system.

misation and later to systematically formulate overall framework (Shah and Kokossis 2002). To our knowledge, the first attempt to create a knowledge model of a complex process, a reactor network, was reported by Jacobs et al. (1996) who formalised it using production rules. The initial intention was to use knowledge model alone to support selection of reactors in the process of reactor network design, and then to automate derivation of reactor strategy (Jacobs and Jansweijer, 2000). Production rules were also used by Ashley and Linke to model reactor networks and to better understand the system to guide the optimal search using stochastic optimisation in the form of Tabu search (Ashley and Linke, 2004), and consequently to analyse results. Ontological approach to model knowledge was used by Kokossis et al. (2008) to extract and interpret knowledge generated in the process of optimising reactor network using Simulated Annealing, which was further expanded to cascade solutions and to guide search using Cascade Algorithm (Kokossis et al., 2011), as well as to parallel execution (Cecelja et al., 2014). An attempt was made by Cecelja et al. (2011) to use both production rules and ontology for integrated interpretation of solutions and acquisition of optimisation knowledge to guide the search in the process of reactor network synthesis using Cascade Algorithm. The use of production rules and ontology towards using, and in particular integrating of processing technologies, was demonstrated by Raafat et al. (2013), the process which was then fully elaborated for practical use (Cecelja et al., 2015).

Interpretation and assuring the confidence in obtained results, however, still remains a problem. Majority of proposed synthesis solutions were either compared with those obtained using different approaches, or compared with 'similar' solutions already proven in practice. The application of knowledge engineering is overwhelmingly 'static' in the sense that reported knowledge models capture existing analytical or experimental facts and without any attempt to get better insight into the problem, to learn from available experimental or otherwise available options or past experience. We speculate that design compromises are always possible, if the consequences are made obvious.

This paper presents an approach to model, acquire and beneficially employ knowledge in process synthesis to (i) interpret solutions for better understanding of the problem, comparison and increased confidence, (ii) to learn from the progress of optimisation and to guide the search towards the optimum solution within predefined and on-the-fly created constraints, and (iii) simplify solutions dynamically and in line with problem formulation to speed up the search and to adjust to specification vary. The proposed approach is based on the hypothesis that (i) the 'best' solution could always be replaced by 'sufficiently good' solution, and (ii) the optimisation based on explicit knowledge is the best way to generate solutions whereas knowledge based on associations, the tacit knowledge, is the best way of selecting solutions. To this end, a widely used, robust and sufficiently adaptable algorithm of Tabu search is used to generate candidate solutions and to optimise. Tacit knowledge about the application and optimisation postulate is modelled using ontologies supported by production rules. While ontologies are used for expanding knowledge base through capturing evolving solution features, for solution interpretation and to share, production rules were employed to model the dynamics of constraints, to simplify solutions and to guide the search.

The reactor network synthesis with superstructure network has been used to demonstrate the approach because it has been deployed extensively in single phase (Kokossis and Floudas, 1990) multiphase problems (Mehta and Kokossis, 2000) applications. The superstructure integrates Continuous Steering Tank Reactor (CSTR) and Plug Flow Reactor (PFR) reactor units that are interconnected through mixers and splitters (Fig. 1).

The superstructure representation of multiphase reactor networks is built around generic reactor/mass exchanger units (RMX) (Linke and Kokossis, 2003a), which enables a flexible and compact representation of fundamental phenomena exploited in the pro-