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On the systematic extraction of knowledge in process synthesis and chemical process design

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Abstract

The paper presents a systematic approach for the extraction, interpretation and exploitation of design knowledge in process synthesis. Knowledge is developed in the course of superstructure optimisation. Semantic models (ontologies) and analytical tools are combined to simplify the superstructures and interpret solutions. In the course of the search the method translates intermediate solutions and upgrades the superstructure model. The approach supports a faster implementation and a transparent interpretation of the solutions. Results are presented for the synthesis problem of reactor networks, essentially addressing the challenges of a multi-level optimization problem. Although presented with stochastic optimization techniques, the proposed method is applicable to general types of models and optimization methods.

Keywords

Knowledge; superstructure optimization; ontology; clustering; decision-making.

1. Introduction

The proliferation of modelling tools has enabled an intensive application of simulation and optimization technology. Process synthesis and design applications employ tools to address the systematic development of process operations and often rely on generic representations that are used to integrate

the available options in exhaustive layouts. Although design solutions can be approached in a single stage, practice dictates the employment of multiple stages - first with the deployment of simple conceptual models and then with the use of more detailed formulations - as intermediate solutions can be reviewed, analyzed and understood. Even in cases where the development of solutions is rigorous and proven, synthesis and design experiments can prove rather inconclusive and difficult to translate. The systematic interpretation of the solution can yield not only to a better understanding of the solution space but also to a systematic reduction of the representation employed (both in size and complexity) and, thus, to much simpler synthesis experiments. The paper presents a systematic approach for the extraction, interpretation and exploitation of chemical process knowledge. The work is demonstrated with the synthesis of isothermal single phase reactor networks that are optimized with the use of stochastic optimisation. The approach is illustrated with the Van de Vusse reaction.

2. Background

The use of stochastic optimization methods in reactor synthesis has proved robust and reliable as the methods can be applied for arbitrary and complex reaction schemes and kinetics [4,5]. Design solutions are selected on the basis of performance and represent special cases out of generic representations that function as reference models (superstructures). The stochastic nature of the approach concludes to a number of alternative solutions, often of high complexity and quite rich in design information. The solutions represent a large pool of competitive designs that may differ – sometimes dramatically - in their layout and operation. Unable to incorporate any type of knowledge that is accumulated in the course of the search, the synthesis process is required to employ exhaustive versions of reference models, an approach that increases the computational burden especially in the study of large industrial problems. Even in cases where the interpretation of the solutions accounts for a precise set of design recommendations, the algorithmic launch of the method - in its current form - does not allow convergence unless a significant number of stochastic experiments meets the required convergence criteria.

The paper offers an alternative approach with the proposition of a knowledge layer around the synthesis search. In the course of the search the optimization translates intermediate solutions to the model and the latter is continuously upgraded to guide the search and the deployment of the superstructure model. The alternative approach not only supports a faster implementation but, more importantly, it supports a transparent interpretation of the synthesis solutions as it concludes to recommendations immediately useful for industrial design groups. Due to its nature, the knowledge model complements the mathematical functions and can be extended as the experiments and the studies about the

process continue. Finally, the model can be used to automatically discover relationships and associations between physico-chemical and economic parameters, design parameters, reactor features, and performance.

3. Methodology

The approach is based on the gradual accumulation of design knowledge and is deployed in the course of synthesis experiments for chemical reactor networks. The method attains knowledge to reduce the synthesis structure with the use of an ontology employed parallel to the optimization search. The latter takes the form of a gradual process whose initial stage is an exhaustive superstructure. The superstructure is optimized and updated at different stages. The transition from one stage to another represents different layers of abstraction. Each stage is assigned a knowledge model populated by features obtained from the solutions. At the highest (initial) level the method employs the largest superstructure and an inappropriate knowledge model. In the course of optimization, the superstructure becomes leaner whereas the knowledge model becomes richer and is populated with solution features and relationships. The components of the methodology are presented in Figure 1.

Different stages of the figure correspond to different superstructures. Each stage links with the ontology and an apparent challenge remains the communication between the optimization experiments and the knowledge model. The communication is addressed with the development of digital certificates that is explained later. The certificates update the ontology which is, in turn, used to update the synthesis model.

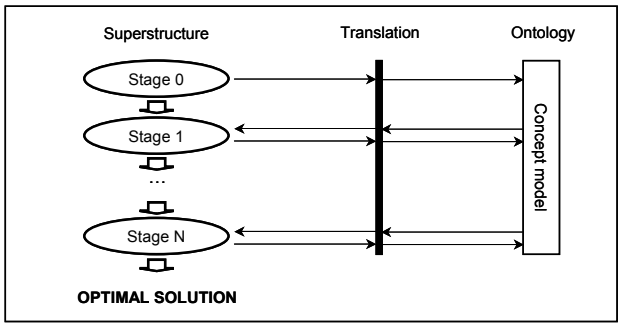


Figure 1 Methodology

3.1. Knowledge representation

The knowledge representation takes the form of a design ontology that is populated by solution features and is composed by synthesis concepts (Figure 2). The ontology consists of two classes of concepts. Input concepts relate directly to the structural and operational components of the superstructure (reactor types and sizes, interconnections, reactor volumes, mixing patterns, recycles, bypasses, temperature profiles). The input concepts represent direct links with the optimization stage and are populated by the solutions of a

particular stage. Output concepts are populated by meta-data retrieved from input concepts. They are used to upgrade the synthesis model or support general analysis. This paper addresses output concepts of the former class which

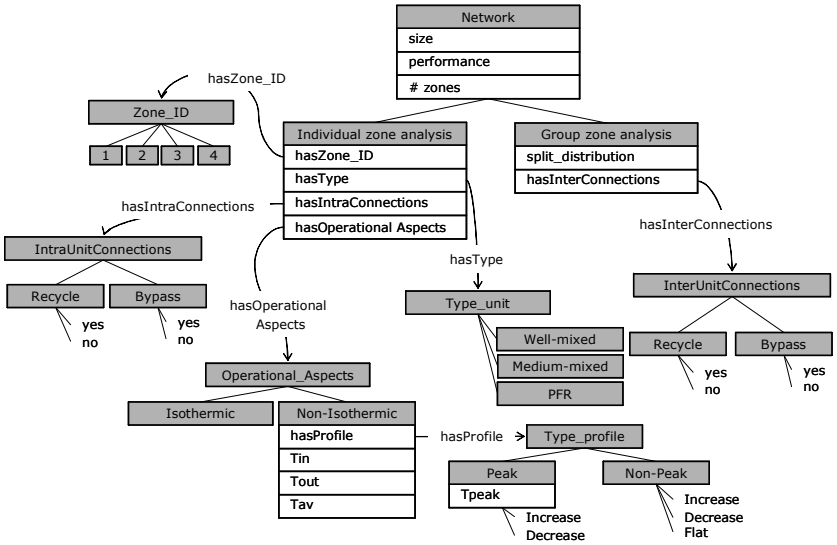
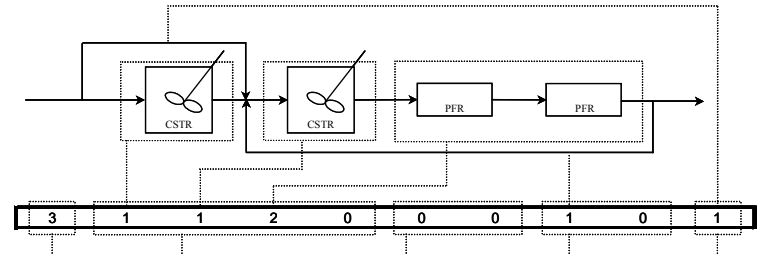


Figure 2 Ontology for the reactors network domain

account for temperature and concentration profiles (increasing, decreasing, mixed), favorable interconnections and hardware, trends in the solution search or previews of selected design features (e.g. splitting feed streams along a PFR).

3.2. Analysis

The approach requires an automated identification of design trends. This is achieved with the use of digital certificates that are issued for different solutions. A more refined stage would assign such a translation to agents. For the purpose of this study the certificates are encoded with a digital vector.



no_zones	mixing per zone		intraconnections				interconnections				feeding (split distribution)	
			recycles		bypasses		recycles		bypasses			
1 … N	1	well-mixed	1	exist	1	exist	1	exist	1	exist	1	exist
	4	mid-mixed	0	do not exist	0	do not exist	0	do not exist	0	do not exist	0	do not exist
	2	PFR										

Figure 3 Synthesis representation and code for a solution

Reactor units are combined into reactive zones depending on the mixing pattern favoured. Each mixing zone is represented by an integer. Recycles and bypasses are classified as intra- and interconnections. Feeding distribution and connections are also binaries. The link between the synthesis representation and the digital certificate is shown in Figure 3. Information is collected as selected data become organised around certificates. The information that is captured by the certificates enables comparisons, analysis of trends and the population of output concepts. For the purposes of the application, the certificates represent the number of reactive zones, the mixing pattern, the feed distribution and the reactor connections.

The approach makes a repeated use of clustering to classify solutions. Clusters are selected around features of the output concepts. Their objective is to: (i) set up a new optimization stage, and (ii) customize features of the optimization search (mainly the intensification stages of the Tabu search). The acquisition of knowledge is subsequently guiding the search towards high performance regions branching off those superstructure features that are of limited importance.

4. Case study

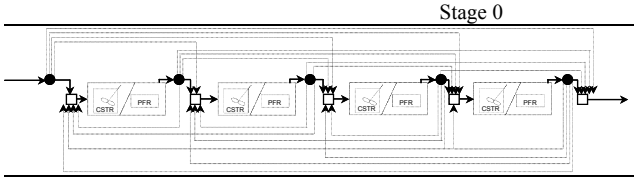
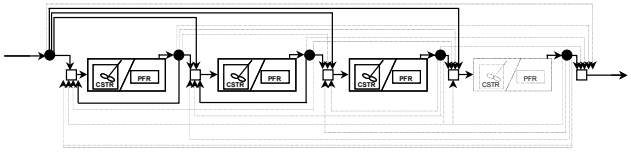
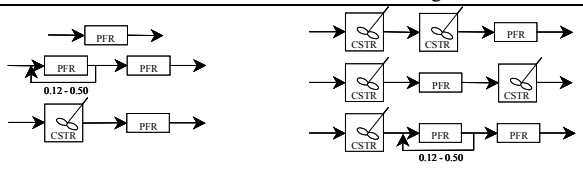
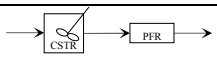
The methodology is illustrated with the Van de Vusse reaction maximised with respect to the outlet concentration of B. Feed conditions and the superstructure representation follow [7]. Computer experiments are performed for a neighbourhood size of 7. The Tabu List contains a single entry. The initial solution is formed by two PFRs in series. The best 50%, 10%, 5% and 1% of the clusters generated are selected in each resulting stage (N=4). Results are summarized in Table 1. The reduction of the superstructure is attained as digital certificates emerge with common features. Clustering identifies promising features whereas irrelevant features are gradually excluded. Stage 1 eliminates connectivities in the final reaction zone, Stage 2 removes feed distribution, whereas the ultimate and penultimate stages break down the synthesis search into a pool of optimal and near-optimal designs.

5. Discussion and Conclusions

The work represents a systematic synthesis methodology that combines knowledge models and optimization. The work is applied to the synthesis problem of reactor networks, essentially addressing the challenges of a multi-level optimization problem (with different levels of abstraction accounting for the different stages of Figure 1). The benefits of the work would become apparent in large-scale and complex networks of chemical reactions. This work is currently in progress. The work is also applicable to other types of models and optimization techniques. For instance, one could disengage stochastic

optimization at selected stages of the search to engage mathematical programming tools in the form of non-linear (NLP) or mixed-integer non-linear programming tools (MINLP). Moreover, the concept itself can be used with techniques entirely residing in mathematical programming.

Table 1. Evolution of the superstructure and results for Van de Vusse.

Superstructure	Code clusters	Max. obj.
Stage 0		
	-	-
Stage 1		
	1 2 0 0 0 0 0 0 0 0	3.56
	1 4 0 0 0 0 0 0 0 0	3.36
	2 1 1 0 0 0 0 0 0 0	3.43
	2 2 2 0 0 0 0 0 0 1	3.52
	2 4 2 0 0 0 0 0 0 0	3.60
	2 2 1 0 0 0 0 0 0 0	3.48
	2 1 2 0 0 0 0 0 0 0	3.64
	2 1 4 0 0 0 0 0 0 0	3.58
	3 1 4 2 0 0 0 0 0 0	3.63
	3 1 1 2 0 0 0 0 0 0	3.51
	3 1 2 1 0 0 0 0 0 0	3.63
	3 1 4 1 0 0 0 0 0 0	3.60
	3 2 4 2 0 0 0 0 0 0	3.52
…		
…		
Stage N-1		
	1 2 0 0 0 0 0 0 0 0	3.62
	2 4 2 0 0 0 0 0 0 0	3.61
	2 1 2 0 0 0 0 0 0 0	3.65
	3 1 1 2 0 0 0 0 0 0	3.62
	3 1 2 1 0 0 0 0 0 0	3.63
	3 1 4 2 0 0 0 0 0 0	3.63
Stage N		
	2 1 2 0 0 0 0 0 0 0	3.66

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