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Conceptual design and optimization of chemical processes under uncertainty by two-stage programming

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ABSTRACT

This contribution presents a method and a tool for modelling and optimizing process superstructures in the early phase of process design where the models of the processing units and other data are inaccurate. To adequately deal with this uncertainty, we employ a two-stage formulation where the operational parameters can be adapted to the realization of the uncertainty while the design parameters are the first-stage decisions. The uncertainty is represented by a set of discrete scenarios and the optimization problem is solved by stage decomposition. The approach is implemented in the computer tool FSOpt (Flow sheet Superstructure Optimization) FSOpt provides a flexible environment for the modelling of the unit operations and the generation of superstructures and algorithms for the translation of the superstructure into non-linear programming models.

The approach is applied to two case studies, the hydroformylation of dodec-1-ene and the separation of an azeotropic mixture of water and formic acid.

1. Introduction

In this contribution, process synthesis is understood as the choice of the best options from a set of promising design candidates during the early stage of process development. This decision has to be made under incomplete information, as not all alternatives have been explored in experimental work on the laboratory and pilot plant level and the models of some operations are inaccurate, also information on cost and prices is usually tentative. The need for explicitly including uncertainty into the decision making process for process synthesis has already been discussed by Grossmann and Sargent (1978) and Acevedo and Pistikopoulos (1996).

The amount of information that is available during the early process synthesis phase is usually rather limited and the process models are of different levels of quality. For some process steps only semi-quantitative information may be available. The aim of our work is to find the best structures in the presence of these uncertainties using mathematical programming techniques.

During the development of a new process, one of the main challenges is to stop the laboratory or pilot plant experiments as soon as sufficient information has been gathered. The quantification of the point in time when the information is sufficient is usually difficult. In this work, it is assumed that no further experiments have to be scheduled when the uncertainty in the parameters (obtained from the available experimental data) has no influence on the ranking of the design alternatives any more so that options that are not promising do not have to be pursued further and the effort can be focused on one or few design alternatives. In design optimization, both design parameters and operational parameters must be specified to evaluate a design. However, while the design parameters cannot be changed any more after the plant has been built and the true behaviour of the different units is observed.

The operating parameters can be adapted to the realization of the uncertainties. Obviously, this potential for recourse should be taken into account in the selection process which is why we employ a two-stage optimization approach where the design parameters e.g. the number of trays of a column or the size of a reactor are the first stage variables while the operating parameters, e.g. the reaction temperature or the reflux ratio of a column are the recourse parameters that are adapted to the uncertainties. The uncertainty is represented in the optimization by a finite set of discrete scenarios.

The approach is implemented in the computer tool FSOpt (Flowsheet Superstructure Optimization) using a stage decomposition approach to solve the resulting optimization problems. The first stage variables (design decisions and design parameters) are optimized by an evolutionary algorithm. The design candidates are

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evaluated after optimizing the operational parameters using a NLP solver. This is similar to the solution technique for mixed-integer two-stage stochastic programmes proposed in Till et al. (2007) and Tometzki and Engell (2010).

The models and the superstructures are described using the language Modelica, and executable code for optimization is automatically generated from the object-oriented models within the tool FSOpt. This provides the user with an abstract way to formulate the models without having to deal with the details of the implementation in the actual solver. The availability of high-level constructs like objects, inheritance and connections increases the chance for model reuse and easier maintenance due to better readability and separation of concerns.

The modelling concept of FSOpt and the model transformations by symbolic algorithms are described and we demonstrate the capabilities of the tool FSOpt in its present extended form for two challenging case studies.

The first case study features the design of a process for the hydroformylation of dodec-1-ene, which has already been discussed in previous work (Steimel et al., 2013, 2014). In this contribution the model formulation has been improved and new uncertainties are considered.

The second case study deals with the separation of a mixture of formic acid, water, methyl-formate and methanol which is part of the Kemira–Leonard process for the production of formic acid. In this case study the presence of an azeotrope between water and formic acid necessitates the use of non-ideal thermodynamics which are implemented using the Wilson equation. The complex thermodynamic equilibrium calculations pose challenges for the modelling and the optimization as discussed below.

The article is structured as follows. The theoretical background and the state of the art concerning the optimization of superstructures and modelling the uncertainties are summarized briefly in Sections 2 and 3. Section 4 provides a short overview of two-stage stochastic programmes and related solution techniques. In Section 5 the main features of the tool FSOpt are discussed. Section 6 describes the first case study and highlights some interesting results. The second case study is presented in Section 7. The article closes with Section 8, which consists of a discussion, some concluding remarks, and an outlook on future research.

2. Superstructure optimization using mathematical programming

An overview of mathematical programming for process synthesis is given in Grossmann et al. (1999). Despite remarkable progress in recent years, there are still many open problems. One of them, related especially to the early design phase, is that algorithm-based short cut models are not suitable for rigorous optimization.

Secondly, the size of the flowsheets and the level of detail of the models are still limited. Examples reported in the literature cover flowsheets exhibiting one or two distillation columns (c.f. Dowling et al., 2014; Dowling and Biegler, 2015), auxiliary separation units (Skiborowski et al., 2014) or reaction steps (Recker et al., 2015). If the level of detail of the model increases, robust convergence of the solution is still difficult to achieve and requires sophisticated semi-automated initialization techniques (Dowling and Biegler, 2015; Skiborowski et al., 2014). If complex networks are synthesized the underlying models are often simplified (Quaglia et al., 2014) and/or only models of a single kind of unit are considered. Examples for this can be found in water treatment network synthesis (Tanvir and Mujtaba, 2008; Khor et al., 2012).

In most of these examples the design problem is modelled as a superstructure, which is a graph containing all combinations of process units and connections that are considered.

Several methods for expressing superstructures as mathematical programming problems exist. Classically, superstructures are modelled as mixed-integer non-linear programmes (MINLP) in which the integer decisions are relaxed using Big-M formulations (Grossmann et al., 2000). A newer approach for modelling superstructures is Generalized Disjunctive Programming which is based on logic propositions and disjunctions (Yeomans and Grossmann, 1999; Lee et al., 2003). This approach allows the grouping of equations into disjunctive sets, for which efficient relaxations can be calculated using a convex-hull approximation. With better relaxations the optimization performs faster, as larger parts of the tree can be pruned during the search. A problem in MINLP-based approaches is the need to solve the relaxed root problem. If this problem is large and difficult to solve, most MINLP algorithms will fail to solve the overall optimization problem as no starting point can be found.

A recent approach for modelling block-oriented superstructures (Friedman et al., 2013), exploits the hierarchical, highly structured topology that is inherent in most superstructures. This approach has been implemented in the Pyomo modelling framework (Hart et al., 2011).

One difficulty of solving mathematical programming problems that arise from superstructure optimization is due to the integrality of some decision variables, leading to huge disjoint search spaces. The approach in Dowling and Biegler (2015) aims at finding better relaxations than those that result from the use of standard MINLP techniques. For distillation columns the relaxation is based on a physically realizable tray bypass.

A second major problem is the existence of (often many) local minima in flowsheet optimization problems (Urselmann et al., 2011). This calls for the use of rigorous global optimization algorithms which however are not yet able to solve problems beyond the optimization of a single apparatus (Ballerstein et al., 2011).

When uncertainties are considered by modelling them as a number of discrete scenarios, the problem size increases proportional to the number of scenarios. This further increases the difficulty of solving the resulting optimization problems. In the context of the two-stage stochastic optimization formulation, we employ a stage decomposition approach so that the scenario sub-problems can be solved by standard NLP solvers. The first stage problems are highly non-convex with disjunct feasibility sets and we use an evolutionary algorithm to generate good, though not provable optimal solutions.

3. Handling uncertainty in design optimization

The seminal article by Grossmann and Sargent (1978) discussed the need to include uncertainty into the decision making process in process optimization. Since then, many approaches have been presented in the literature, four of which will be described in the following section.

The goal of parametric programming (Acevedo and Pistikopoulos, 1996) is to find a description of the solutions of the design problem depending on the uncertainties in a closed form. The idea to map the uncertainty space to the solution space using single function is intriguing, but so far limited to few uncertain parameters, due to the need of repeated optimizations of a parametric master problem and NLP sub-problems. Another approach which does not require explicit sampling of the uncertainty space was presented by Pistikopoulos and Ierapetritou (1995). For uncertainties that are described by continuous probability distribution functions a two-stage stochastic programming problem is formulated which considers economic aspects as well as process feasibility. Another example of process optimization without scenario sampling is given in Rooney et al. (2003), in which