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Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets

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ABSTRACT

Designing chemical processes is a multi-criteria optimization problem with conflicting objectives. It can efficiently be solved using Pareto sets. These sets contain all solutions for which an improvement in any objective can only be achieved by accepting a decline in at least one other objective. This work integrates a novel algorithm to determine Pareto sets in a state-of-the-art steady-state flow sheet simulator. An approximation of predefined accuracy of the Pareto set, which can be convex or non-convex, is calculated. The decision maker can then navigate interactively on the Pareto set and explore the different optimal solutions. His decision is, hence, embedded in the knowledge of the entire Pareto set. The application of the method is illustrated by an example in which a distillation process for the separation of an azeotropic mixture (acetone + chloroform) is designed. Two process variants are compared: a pressure-swing and an entrainer distillation.

1. Introduction

Optimization in chemical process design is usually not focusing on just one economic objective. Rather, two levels of objective criteria are often considered: design criteria and final decision criteria. The first group contains, for example, product purities, column duties and reboil ratios. The second group consists of hard economic objectives like investment and operating costs, often more softer environmental issues as sustainability key figures and objectives regarding health and safety. Thus, almost every design decision in process engineering is a compromise between multiple conflicting objectives.

In practical process design, the engineer often tries to find an optimal solution in the multi-dimensional objective space by an empirical iterative change of the process parameters in the design space. Usually, this procedure is continued until either a solution is found which fulfills certain requirements, or some deadline is reached where a solution has to be delivered. This procedure may lead to good results, however, no guarantee on optimality can be given. Furthermore, the empirical optimization only covers restricted areas in both the design and objective space, so that only limited information on the trade-offs between the different objectives is available and the decision cannot be based on an overview of the full solution space. This limitation may lead to overlooking interesting solutions.

It is by far not necessary to calculate all feasible solutions. In principle, only best compromises need to be studied. These are solutions where an improvement in any objective can only be achieved by accepting a worsening in at least one other objective. The respective solutions are called Pareto-optimal (Geoffrion, 1968) and the set comprising all these solutions is the Pareto set, often also called the Pareto frontier because the Pareto set lies on the border between feasible and infeasible solutions.

A common strategy to find single Pareto-optimal solutions is to weight the objectives and subsequently optimize the weighted sum. A drawback of this approach is that the weights have to be chosen beforehand. As the choice of the weights is ambiguous, many solutions will not be accepted without exploring alternative choices. Hence, this approach is, in practice, also empirical and iterative. Furthermore, it is difficult to extend this approach to "soft" objectives, describing safety, environmental, sustainable, or social issues. These are difficult to weight and compare directly to technical or economic objectives. Moreover, not every Pareto-optimal solution can be found by the weighted sum approach: namely if the Pareto set is not convex (Chankong & Haimes, 1983; Haimes, 1977).

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The chemical engineering literature describes many algorithms to determine Pareto-optimal solutions more systematically and efficiently than the weighting approach. They can be classified in deterministic and stochastic algorithms. Deterministic algorithms on the one hand, like for example derivative-based methods, are time-efficient and yield accurate results for the optima, however, they usually only find the local optimum related to the starting point. Examples of deterministic algorithms in process design are goal programming techniques (Chakraborty & Linninger, 2002), including the ε-constraint method (Hugo, Ciumei, Buxton, & Pistikopoulos, 2004), or weighting approaches with methodical variation of the weights (Lim, Floquet, Joulia, & Kim, 1999). On the other hand, stochastic algorithms try to find the global optimum by sampling large areas of the objective space, which also leads to time-consuming and less accurate procedures. For examples of stochastic algorithms in process design see Gutirrez-Antonio and Briones-Ramirez (2009), Leyland (2002), or Micovic, Beierling, Lutze, Sadowski, and Górak (2013). Evolutionary approaches in particular are intensively used for stochastic algorithms as they can be applied straightforward to any process simulation, are robust and somewhat insensitive to local optima. For general reviews and classifications of algorithms to find Pareto-optimal solutions the reader is referred to Andersson (2000), Bhaskar, Gupta, and Ray (2000), or Rangaiah (2008).

There have also been efforts to create multi-purpose numerical tools which apply multi-criteria optimization techniques to arbitrary models in a black box. An example is the commercial tool modeFRONTIER[1] that has been successfully coupled to chemical process simulators (Altendorfner, 2008). To ensure robustness the software uses an evolutionary algorithm. Using this type of algorithm the user has to accept, however, a computationally expensive calculation, and gets only an approximation of the Pareto set. Additionally, the accuracy of this approximation is not known.

Hakanen, Hakala, and Manninen (2006) presented an interactive tool that couples a process simulator and a deterministic multi-criteria optimization algorithm. To avoid an expensive approximation of the complete Pareto set they use an interactive algorithm: individual Pareto optimal points are subsequently calculated until the user terminates the algorithm. Thereby, the user specifies the search direction by updating constraints on the objectives. The major drawback of this interactive method is that the user only explores parts of the Pareto set. Which parts of the Pareto set he explores is somewhat intuitive and dependent on the user's experience.

In this work we present a tool, which couples a commercial process simulator with multi-criteria techniques and overcomes the earlier mentioned drawbacks related to calculation speed, accuracy and Pareto set exploration. The work is inspired by the concepts for determining and visualizing the Pareto set reviewed by Küfer et al. (2009, chap. 5). The basic idea is to first, efficiently determine an approximation of the complete Pareto set of a given chemical process design problem. This allows the decision maker to focus his attention only on relevant solutions, so that the decision process is facilitated. We calculate the approximation of the Pareto set by using a combination of evolutionary and efficient derivative-based algorithms. During a short initial evolutionary phase, a variety of starting points close to the expected Pareto surface is generated. From these starting points, a sequential quadratic-programming algorithm is applied to find the Pareto points. We calculate only a minimum number of Pareto points to approximate the full Pareto set to an accuracy which is set by the user a priori. Unnecessary computationally expensive simulations are thus avoided. The Pareto points are calculated using a method which combines a sandwiching and a hyperboxing algorithm. Therefore, also non-convex Pareto sets can be efficiently approximated.

The decision maker can then interactively explore the Pareto set by navigating with a graphical user interface (GUI). Graphical sliders are used for this purpose, each corresponding to one objective. By moving one slider, the other sliders are updated in real time, i.e., information on the trade-offs between the best compromises is directly visualized. Further, the GUI allows a simultaneous visualization of different Pareto sets which enables comparing different variants of the process based on different flow sheets. The areas that are explored can successively be restricted to those which are identified as the most promising. Thus, we postpone the restriction to a limited area of the decision space until the decision maker has got insight into the complete set of optimal solutions. This interactive multi-criteria optimization (IMCO) maintains full flexibility until the final choice of the design point. This choice is, hence, embedded in the knowledge of alternative designs. All choices are left to the decision maker, who is efficiently supported by the tool in all steps of the design.

The tool can in principle deal with an arbitrary number of objectives in calculation as well as in visualization. As it is integrated into a state-of-the-art process simulator, its applications range from optimization of single apparatuses up to the design of new plants. Rather than treating the simulator as a black box model, the algorithms are directly coupled with the flow sheet solver which leads to high speed and robustness. This could in principle be done with any state-of-the art process simulator, provided that the source code is available. For reasons explained below in more detail, it cannot be expected to achieve a similar performance if the process simulator is only addressed as a black box.

In the following, we first describe the MCO methods used in the present work together with their implementation, and then illustrate their application in a case study in which two processes for separating chloroform from acetone are compared: an entrainer and a pressure-swing distillation.

2. Method for MCO in chemical process design by navigation on Pareto sets

2.1. Overview

The MCO chemical process design problem which is addressed in the present work is of general nature. In principle, any problem, for which a process simulation can be set up, can be addressed. The MCO methods described in the present work were implemented in CHEMASIM, a steady-state flow sheet simulator which was developed and is maintained by BASF SE (Hegner & Schoenmakers, 1985). The methods are generic in the sense that in principle any other flow sheet simulator could have been used. The main reason to choose CHEMASIM was that it is an equation-oriented simulator thus allowing for flexible and unified handling of all model parameters/variables and also providing fast convergence by suitable initial guesses. Furthermore, the source code was available for the present study and CHEMASIM developers were able to join the team. Other advantages of CHEMASIM are its efficiency and robustness[2] which make it a good choice for the endeavor.

Fig. 1 shows a scheme of process optimization based on process simulation and serves for defining the nomenclature used in the following. The process simulation has input variables, some of

[1] Product of ESTECO, Trieste, Italy.

[2] To solve the non-linear model equations, a set of process variables as a start point has to be given to the solver. Empirically we found that the CHEMASIM solver is more robust to perturbations in this start point and converges faster than other process simulators. Both properties are crucial during the optimization process.