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Decision Support for Process Development in the Chemical Industry

Norbert Asprion,[a] Sergej Blagov,[a] Oliver Ryll,[a] Richard Welke,[b] Anton Winterfeld,[b] Agnes Dittel,[b] Michael Bortz,[b] Karl-Heinz Küfer,[b] Jakob Burger,[c] Andreas Scheithauer,[c] Hans Hasse [c]

[a]BASF SE,
Carl-Bosch-Str. 38, 67056 Ludwigshafen, Germany, norbert.asprion@basf.com

[b]Fraunhofer Institut für Techno- und Wirtschaftsmathematik,
Fraunhofer-Platz 1, 67663 Kaiserslautern, Germany

[c]Lehrstuhl für Thermodynamik, University of Kaiserslautern,
Erwin-Schrödinger-Str. 44, 67663 Kaiserslautern, Germany

Process development in chemical industry is a multiobjective optimization problem. Objectives of this optimization are for example product quality, raw material and investment cost, energy efficiency, reliability or health, safety, and environmental issues. Parameters for this optimization are, e.g., feed stock, utilities, process configuration, equipment, operating parameters, and site.
In process design, the developer usually generates a certain number of process variants by varying process parameters intuitively. The process is usually stopped if a solution is found that is acceptable regarding all or at least most criteria, optimality cannot be guaranteed. The present paper describes a feasible alternative approach, which is a real multiobjective optimization based on the Pareto optimality concept. The Pareto front describes a set of solutions where no improvement in one objective can be reached without at least getting worse in another objective. The Pareto front allows investigating the trade-offs between different objectives, but the final choice of the design is left to the user. In the present work the multiobjective optimization is used together with a decision support system, which allows navigating within the Pareto front and thereby finding the best compromise between the objectives in a rational and efficient way.

1. Introduction

At the time being optimization of a process design is usually an iterative process including subsequent steps of simulation, basic design and economic evaluation. This optimization process will typically end due to limited time resources. As a result an improved but probably sub-optimal process design will be obtained, since many different, partly conflicting objectives have to be met in an acceptable range. This is a typical multiobjective optimization problem which is not yet accounted for in the developer's workflow.

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One step forward to overcome this situation is the concept of the intelligent total cost minimization approach (i-TCM) presented by Wiesel and Polt (2006). In that approach the different objectives are weighted with costs to a total cost function which can be minimized. One drawback of that method is that other, not cost related objectives can not be included. Furthermore, the approach suffers from the typical drawbacks of weight-based multiobjective optimizations (cf. Miettinen, 1999). One example is the strong dependency of results on the chosen (or assumed) weighting factors. An alternative promising approach is studying the different objectives individually and investigating sensitivities. For example it might be interesting to investigate different price scenarios for the raw materials and to see the impact on the different objectives. In the present approach theses studies are carried out not taking the entire solution space of the process design problem as a basis but only on the relevant subset of the Pareto optimal solutions, i.e. on the Pareto front. As the Pareto front has a considerably lower dimensionality than the entire solutions space, this considerably facilitates the search for the most advantageous design, which will, when using the present approach, always be Pareto-optimal. To support the choice of the final design an interactive new decision support system the so-called “Pareto-Navigation System” (Monz, 2006) is used in the present work. The work does not aim at presenting a comprehensive overview of the technique, but rather illustrates the main ideas by a simple example. The tools and methods used for that preliminary study will be continuously improved in order to allow routine applications in the future.

Note that Pareto navigations are very compatible with the process engineer skills and his freedom to choose the final solution according to any complex criteria he may wish to apply. In fact, Pareto navigation has been intuitively used for a long time in process engineering. The best known example for this is probably the N,Q-curve for designing distillation columns, see e.g. Billet (1973): a given set of specifications of a simple distillation column, can be fulfilled by different combinations of the choice of the number of theoretical stages N and the reboiler duty Q, cf. Figure 1. The feed stage is optimized for all choices of N and Q. N and Q are conflicting objectives reflecting investment and operational costs of a column. The N,Q-curve divides the solution space in two regions: one in which the design (choice of N,Q, and the corresponding number for the feed stage) does not allow meeting the specifications and one in which the design allows overfulfilling them, i.e., lower numbers for N,Q would be sufficient to meet the specifications. Hence, the choice of N, Q in that region would not be Pareto optimal. Furthermore, any other choice of the number of the feed stage than the one resulting from the optimization would lead to an increase in Q and would, hence, also not be Pareto optimal. Therefore, the N,Q-curve is a true Pareto front and choosing the operating point on the N,Q-curve is a true Pareto navigation.

2. Decision Support System

The general problem in process engineering is that we are usually working with certain process parameters $\boldsymbol{x}$, e.g., temperatures, pressures and concentrations which will result in different outcomes for the objectives $\boldsymbol{f}$ like variable and fixed costs. The projection from the parameter space to the objective space is usually a nonlinear transformation so that the outcome for the objectives upon a variation of $\boldsymbol{x}$ is hard to predict. It is also in general not easy to solve the inverse problem, i.e. to fix the objectives $\boldsymbol{f}$ and to determine the process parameters $\boldsymbol{x}$ so that the desired $\boldsymbol{f}$ is obtained. Multiobjective optimization using Pareto-navigation helps fulfilling this task.

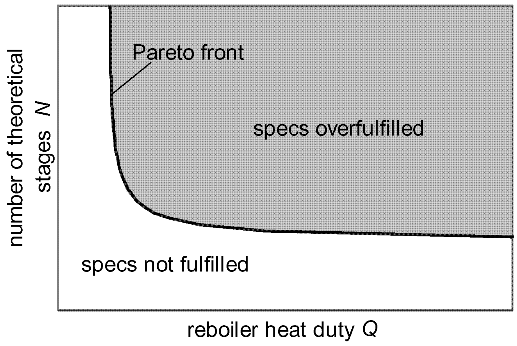

Fig. 1: N,Q-curve for a simple distillation with given specifications: The N,Q-curve is a Pareto front and choosing the operating point on the N,Q-curve is a Pareto navigation.

Multiobjective optimization especially with a large number of objectives is often very time-consuming. Therefore, efficient strategies for exploring the Pareto front are necessary (e.g. Ruzika and Wiecek 2005). In the following the sandwiching approach and the Pareto-Navigation will be briefly presented.

2.1 Sandwiching

Experience shows that within one process concept and with continuous objectives, it is reasonable to assume that most Pareto fronts in chemical engineering are convex (like e.g. *N,Q*-curves). That assumption helps to considerably reduce the effort for constructing the Pareto front. In case of non-convex Pareto fronts it can be shown that these can be sub-divided in convex parts (Monz, 2006).

First the extreme compromises (i.e. the solutions with optimized single objectives) are estimated in the given parameter range. With an inner and outer convex hull the uncertainty region of the Pareto front can be estimated. The Pareto front will be explored until a certain accuracy is reached.

In the first step the inner convex hull is defined by the already known Pareto points, which are the vertexes of the convex hull. For the two-dimensional case the inner convex hull connects adjacent Pareto points by straight lines, which is shown in Fig. 2a. The outer convex hull can be determined by the normal vectors to the Pareto front at the estimated Pareto points, which are also results of the optimization. The normal vectors are defining tangential hyperplanes of the Pareto front. Besides the extreme compromises the intersections of these hyperplanes are the vertexes of the outer convex hull. For the two-dimensional case the hyperplanes are straight lines as can be seen in Fig. 2a.

In the sandwiching approach always the region with the largest difference between the inner and the outer convex hull is explored. To determine this thickest part the inner convex hull is elongated until this elongated hull includes the complete outer hull (Fig.

2b). It can be shown that the thickest part is always at a vertex of the outer convex hull. This vertex is than the starting point for a one-dimensional optimization. The direction of the optimization is in the direction of the thickest part (method of Pascoletti-Serafini (Monz, 2006, see for example Fig. 2b). The convex hull has to be recalculated in the neighborhood of this new Pareto point only (Fig. 2c), which means the effort is relatively small.

Compared to other techniques like evolutionary algorithms or the ε-constraint method (kind of optimization with enumeration, Miettinen, 1999) the sandwiching approach has a superior performance due to the controllability of progress and the estimation of errors.

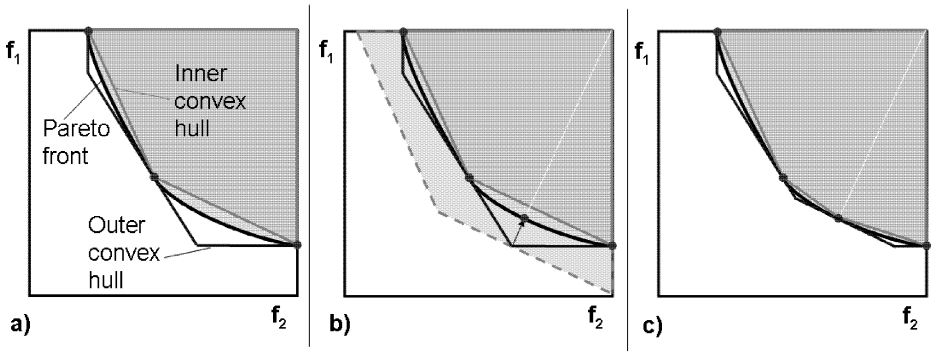

Fig. 2: Sandwiching approach for determining the Pareto front: a) determine convex hulls, b) indentify thickest part of the sandwich and calculate Pareto point in this direction, c) update convex hulls

2.2 Pareto-Navigation

The goal of the sandwiching approach is to estimate the Pareto front only on a few points which allow an interpolation as well in the objectives as in the parameter space. Usually the Pareto front will be estimated in an off-line mode and the results of each simulation will be stored. This allows to load the results afterwards in a navigation tool and to navigate in the Pareto front. Here the different objectives together with certain process parameters will be shown. For example one might change the outcome of one objective and will see the impact on the other objectives and the parameters. It is also possible to change parameters and to see the influence on the objectives. The navigation tool gives the possibility to compare Pareto fronts of different process configurations or sites. One can use it also for comparison of different absorption or extraction solvents. From a chosen solution a simulation with the model can be restarted.

The sandwiching approach gives a good estimate of the uncertainty in the Pareto front. So it is possible to start a multiobjective optimization with a lower accuracy and as soon as the parameter region with the interesting solutions in the navigation tool is identified to perform a second multiobjective optimization with tighter limits for the parameters and higher accuracy in the Pareto front. Furthermore it is possible to add additional parameters and objectives and to explore the new Pareto fronts.

3. Example

For the preliminary study which is reported here, the ε-constraint method (Miettinen, 1999) was used for constructing the Pareto front. In a later project phase the computational effort will be reduced by using the sandwiching approach and interpolation as presented above.

In this study the separation of an acetone/chloroform mixture by a pressure swing distillation was investigated, cf. Fig. 3.

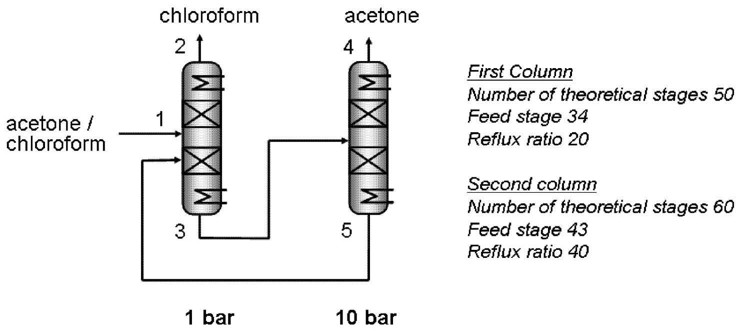

Fig. 3: Separation of an acetone/chloroform mixture by pressure swing distillation

The following three objectives were chosen: purity of the chloroform product (Stream 2), purity of the acetone product (Stream 4) and the amount of recycle (Stream 5). Here the basic assumption was: minimizing the recycle will give the most profit. For simplicity, the columns in the rigorous simulation had a fixed but reasonably chosen number of stages and a fixed reflux ratio and were operated at the pressure given in Fig. 3. Therefore the only parameters of this optimization were the reboiler duties of both columns. An optimization of the column design could straightforwardly be included in the procedure. In the simulation a short-cut tool for apparatus design of the columns, investment and variable cost estimates as well as prices for the products were included, so that it was possible to estimate the profit (here given without currency).

4. Results

In Fig. 4 a snapshot from the navigation tool is shown which also includes a visualization of the Pareto front obtained from the rigorous simulations (with BASF's inhouse steady-state simulation tool CHEMASIM using the NRTL model). As can be seen, interestingly, the highest profit is not achieved at low recycle rates as one could assume, but rather at high recycle rates. Furthermore, the highest profit is achieved for the lowest tolerable purity of chloroform (98%), but the highest purity of acetone (99.95%). All this is not obvious at a simple glance and such solutions could well be missed when the presently still common intuitive design procedures are applied. Of course, these findings can be explained: the reason is the higher price of chloroform compared to acetone. Due to increasing purity of acetone the yield of chloroform increases and, furthermore, the recycle gets further from the azeotrope at 1 bar, so that the separation in the first column becomes easier (i.e. less variable costs).

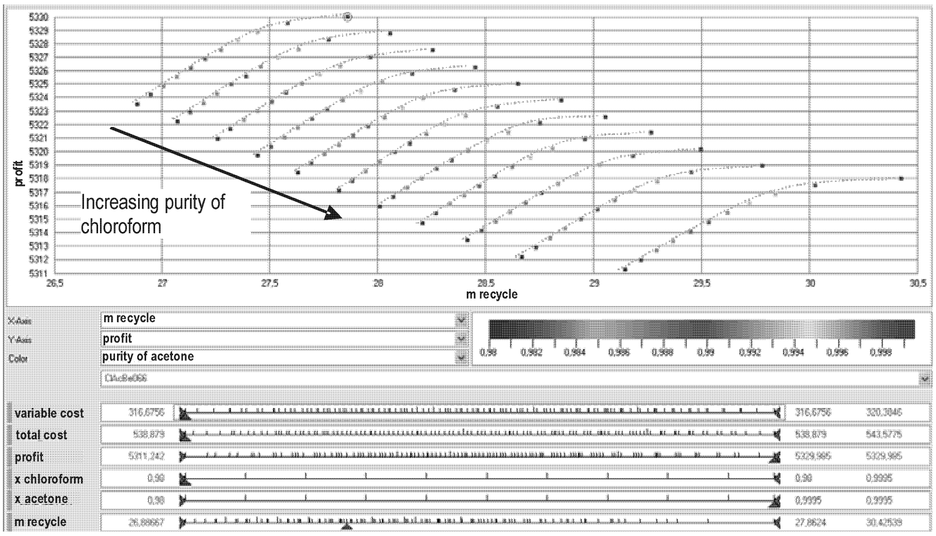

Fig. 4: Pareto-navigation tool applied to the separation of an acetone/chloroform mixture as shown in Figure 2

5. Conclusion and Outlook

This very simple example of a pressure swing distillation shows that a manual optimization in chemical engineering will be sub-optimal, since some cases will be omitted due to certain expectations – especially when the flow sheets are complex and recycles are present. Pareto navigation helps to understand the influence of design parameters, carrying out a rational and efficient multiobjective optimization, and finally finding economically superior designs for chemical processes

In the presentation the approach will be described, results of the application of the Pareto navigation tool will be presented. The examples will be extended and will include the comparison of a pressure swing distillation to an entrainer distillation.

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