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Multiobjective batch process design aiming at robust performances

Andrej Mošat', Ulrich Fischer*, Konrad Hungerbühler

ETH Zurich, Institute for Chemical and Bioengineering, 8093 Zurich, Switzerland

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Abstract

The most common batch design approach in practice and literature is a deterministic one. However, given the uncertainties prevailing in early stages of process design, a deterministically calculated productivity is not sufficient to select one of the large number of optional designs. Therefore, we propose a Tabu Search multiobjective optimization framework, which allows to approximate the Pareto-optimal set of designs while considering uncertain variables in the initial recipe. As a novel technique, we include performance robustness as a separate objective function within the multiobjective optimization alongside with productivity of a design, thus obtaining not only designs with high productivity or solely robust designs, but both high productivity and robust designs in one set of solutions. We examined several robustness criteria as a possible quantification of performance deviations under uncertain recipe variables. The implementation of a Tabu Search framework in combination with Monte-Carlo simulation and Latin Hypercube sampling provides a huge flexibility in the problem specification, in particular in the definition of parameter uncertainties. As a result we successfully demonstrate that metaheuristic optimization techniques are capable to approximate the Pareto-optimal set under uncertainty and are able to capture potentially antagonistic solution qualities such as high productivity and robustness by multiobjective optimization. With the help of this approach, parameters can be identified that have to be put into the focus of process research and development efforts in order to obtain high performance batch process designs.

Keywords: Performance robustness; Optimization; Batch process design

1. Introduction

Multipurpose batch processes are particularly suitable for production of fine chemicals in small to medium quantities. The key element to flexible manufacturing is optimized usage of multipurpose equipment and intermediate storage capacities. In the preliminary design stage of such processes the aim is to identify and tackle the problems appearing later in the production phase. In this scope, the opportunities for process optimization must be considered at the early stages of process development before the process is frozen due to regulatory (pharmaceuticals) or safety and quality-assurance (specialty chemicals) reasons. In the process development, the sequence from (a) process research and development (R&D) to (b) small-scale production and (c) full-scale production allows for largest improvements at the beginning of this sequence when, however, only little knowledge is available. If the optimization process starts later, the chances for major improvements in productivity and delivery times are lowered.

The most common batch design approach in practice and literature is a deterministic one, in which fixed inputs are used for rendering fixed outputs (e.g. Wellons and Reklaitis, 1991; Dedieu et al., 2003; Cavin et al., 2004, 2005; Dietz et al., 2006). However, it is often the case that many factors are unknown or uncertain in the early stage of process development, for example reaction time to obtain required conversion, problems with crystallization and filtration time, which is often difficult to predict in the scale-up processing, or solvent volume needed for a given task e.g. in separation tasks or simply in the context of the solubility of a certain compound. Therefore, process design approaches are needed that incorporate the treatment of parameter uncertainties into the model-based optimization of batch processes.

In the literature, the probabilistic batch design problem is mainly cited in the scope of scheduling (e.g. Balasubramanian

* Corresponding author. Tel.: +41 446325668.
E-mail address: ufischer@chem.ethz.ch (U. Fischer).

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and Grossmann, 2003; Bonfill et al., 2005) and production requirement satisfaction, where the allocation of tasks to units or vice versa is considered under uncertain production variables or uncertain per annum production quotas for a number of products (e.g. Wellons and Reklaitis, 1989; Shah and Pantelides, 1992; Straub and Grossmann, 1992; Subrahmanyam et al., 1994).

Usually the production quota is given by customers and the delivery time is a function of the available plant equipment and equipment sizes, etc. The most important factor for delivery time is the productivity measure defined as ratio of batch size over cycle time (CT) which should be maximized. Maximization of the productivity typically leads to inflexibility of a batch design and vulnerability of the design performance by changes in operating conditions. This general trade-off between peak-performance and invariance towards uncertainty, for which a compromise has to be achieved, has been demonstrated by Mulvey et al. (1995) for various problem settings.

A literature review and a discussion of examples on uncertainty, flexibility and robustness in chemical process has been presented by Bernardo et al. (2003). In the extensive review by Sahinidis (2004), probabilistic batch design problems solved by mathematical programming methods are enlisted. The author recognizes, among many sub-problems in the stochastic optimization of batch processes, that the most important topics are minimizing deviation from goals, robustness as a quantified criterion of process quality, and flexibility of a design.

In all cases the terms 'flexible' or 'flexibility' and 'robust' or 'robustness' are related to uncertainty, but definitions of the terms differ substantially. We will use the distinction between 1. *flexible design problem* and 2. *robust design problem* both defined as follows:

(1) *The flexible design problem*: The flexibility criterion's goal is to provide quantitative measures of ensuring feasible performance of a design under all considered uncertain conditions. In this sense, a flexible design is a reliable design, which even under unfavorable conditions is still operable. This definition of flexibility is also known under probability of feasible operation (Straub and Grossmann, 1990, 1992, 1993), operational flexibility (Swaney and Grossmann, 1985), and design reliability (Kubic and Stein, 1988).
(2) *The robust design problem*: The robust design criterion's goal is to provide a quantitative measure of process stability under uncertain conditions so that the performance/profit variance is minimized. The aim of the robust design method is to identify a design in which the influence of all uncertain input parameters in all possible combinations is minimized. Applications of robustness concepts in the context of chemical process design include work by Bernardo et al. (2001), who identified and incorporated quality costs and robustness criteria in chemical process design problems under uncertainty within a single-level stochastic optimization formulation delivering an optimal design, together with a robust operating policy that maximizes average process performance; Ahmed and Sahinidis (1998), who defined robustness as a goal programming approach to balance trade-offs between expectation and variability of the recourse cost in the batch process development; Wen and Chang (1968), who introduced a mono-objective measure determining a minimum average normalized deviation of the objective from the optima over the range of uncertainty; Nishida et al. (1974), who defined robustness as a mono-objective measure of attaining the min–max performance structure of a design, which should minimize the effect of the worst variations in the uncertain parameters; Painton and Diwekar (1995), who defined a robustness penalty in the mono-objective cost optimization of a chemical process with uncertain inputs; and Samsatli et al. (1998), who considered robustness as a measure of reasonable performance over a wide range of uncertainty.

Another approach combines both flexibility and robustness into one criterion for obtaining both flexible and robust designs. Rooney and Biegler (2003) formulated the combination of feasibility problem (model parameter uncertainty) and robust design problem, where robustness is a quantifier to the operating parameters response. Mulvey et al. (1995) defined the term robust optimization (RO) and differentiated between model robustness, which measures constraint violations, and solution robustness. They combine both measures into a single objective by the way of a goal programming weight.

One of the successful methods for handling optimization under uncertainty is programming with recourse, a *two-stage here-and-now programming* (e.g. Ahmed and Sahinidis, 1998; Bernardo et al., 2001; Sahinidis, 2004), where the first-stage variables are those that have to be decided before the actual realization of the uncertain parameters. Subsequently, once the random events have presented themselves, further design or operational policy improvements can be made by selecting, at a certain cost, the values of the second stage, or recourse, variables.

We use the *two-stage here-and-now programming method* in connection with a metaheuristic multiobjective Tabu Search algorithm for solving the *multiobjective robust design problem*. The implementation of the Tabu Search algorithm guarantees that only feasible designs are created. The aim of this method is to complement industrial decision making in the early process development stage in order to obtain a set of high productivity and highly robust designs, which, if compared to high peak productivity and low robustness designs, yield stable production quotas under varying conditions. We approach the problem as a *single product batch design optimization*, where the single product is to be manufactured in a given *multipurpose plant*. The uncertain recipe variables can be for instance operation time and operation volume. As a novel technique, we include performance robustness as a separate objective function within the multiobjective optimization alongside with productivity of a design, thus obtaining not only designs with high productivity or solely robust designs, but both high productivity and robust designs in one set of solutions. We examined several robustness criteria as a possible quantification of performance deviations under uncertain recipe variables.