ROBUST OPERATIONAL PROCESS DESIGN OPTIMIZATION UNDER UNCERTAINTY

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Abstract

Robust decision making under uncertainty is considered to be of fundamental significance in several discipline and application areas. In dynamic processes, in particular, there are parameters which are usually uncertain, but may have a large impact on the targets like the objective value and the constrained outputs. Thus consideration of the stochastic property of the uncertainties in the optimization approach is necessary for robust process design and operation. In this work we present a novel chance constrained optimization approach to address the problem of optimal process design under uncertainty, in which optimal operational considerations and robustness analysis are simultaneously considered. The formulation of individual pre-defined probability limits of complying with the restrictions incorporates the issue of feasibility and the contemplation of trade-off between profitability and reliability. A two-stage reactor system is investigated in detail to demonstrate the potential of the new approach.

Keywords

Optimal Design, Uncertainty, Chance Constraints, Probabilistic Programming

Introduction

The competitive nature of the market environment imposes reliability in the meeting of product demands and quality specifications. The chemical industry is, therefore, required to make design and operating decisions to satisfy several conflicting goals in an optimal and safe manner. However, uncertainty and variability are inherent characteristics of any process system. These arise due to unpredictable and instantaneous variability of different process conditions, such as temperature or flow rates, or due to uncertain model parameters, such as kinetic constants or equilibrium parameters. The conventional way to compensate for uncertainties at the design stage is an overdesign of process equipment and then retrofits to overcome operability bottlenecks. At the operation stage, processes are normally run with an operating point defined by an overestimation of the uncertainties, consequently, greater costs than necessary will be the cause of these heuristic rules. During the past decades several approaches have been suggested to address the problem of process design under uncertainty (Halemane et al., 1983, Pistikopoulos et al., 1995). Virtually most of these approaches employed the two-stage programming method with the recourse formulation to handle inequality constraints. In this method, violation of the constraints is compensated for by some penalty terms in the objective function. This compensation, however, requires a common measurement to describe the objective function and constraint violations. Alternatively, when this measurement is not available, the formulation of chance constraints with a user pre-defined probability limit of constraint compliance will be the most suitable approach. For the numerical optimization under probabilistic constraints, several methods have been developed. Alternative to efficient sampling techniques (Diwekar et al., 1997), we proposed in a previous work a systematic approach to solving nonlinear chance constrained optimization problems, where the monotony of the constrained output to at least one uncertain input is utilized, so that the feasible

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region (output distribution) is mapped to a region of the uncertain variables (Arellano-Garcia, et al., 2003). However, there are, in fact, some stochastic optimization problems where no monotone relation between constrained output and any uncertain input variable can be assured. Predominantly, such processes which imply complex reaction systems where the question of whether there is a monotony or not are strongly dependent on the policies of the decision variables. To address this problem, a novel efficient approach is proposed to chance constrained programming for nonlinear dynamic processes with no guarantee for monotone relation between constrained output and uncertain input.

New Method for Nonlinear Probabilistic Programming

In this work, a novel optimization framework is proposed for simultaneously solving design and operation problems of systems under uncertainty. To decompose the problem, the proposed approach uses a two-stage computation framework (see Fig. 1). The upper stage is a superior optimizer following the sequential strategy. Inside the simulation layer there is a two-layer structure to compute the probabilistic constraints. One is the superior layer, where the probabilities and their gradients are finally calculated by multivariate integration. The main novelty is contained in the other, the inferior layer, and is the key to the computation of the chance constraints with non-monotonous relation. The main principal is that for the multivariate integration the bounds of the constrained output $\mathbf{y}$ and those for the selected uncertain variables $\boldsymbol{\xi}$ reflecting the feasible area concerning $\mathbf{y}$ are computed at temporarily given values of both the decision and the other uncertain variables. Thus, all local minima und maxima of the function reflecting $\mathbf{y}$ are first detected (see Fig. 2). This computation of the required points of [min $\mathbf{y}(\boldsymbol{\xi})$] and [max $\mathbf{y}(\boldsymbol{\xi})$] is achieved by an optimization step in the inferior layer. With the help of those significant points, the entire space of $\boldsymbol{\xi}$ can be divided into monotonous sections in which the bounds of the subspaces of feasibility can be computed through a reverse projection by solving the model equations in the following step of this inferior layer.

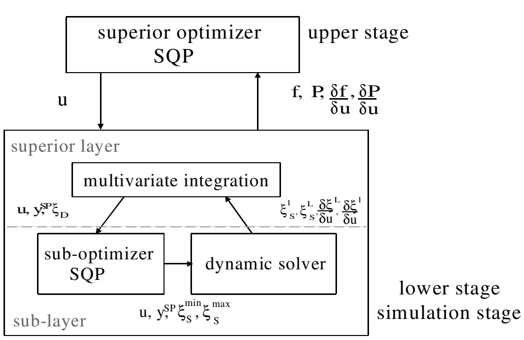

Figure 1. Optimization framework

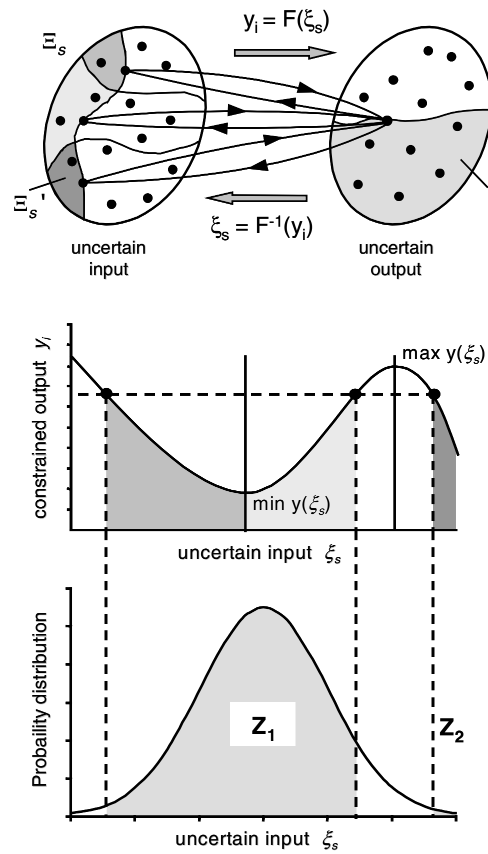

Figure2. Mapping feasible regions

The bounds of feasibility are supplied to the superior multivariate integration layer, where the necessary probabilities (Eq. 1, 2) and the gradients are computed by adding all those feasible fractions together (see Fig. 2).

$$\mathbf{Pr} = \sum \mathbf{Pr}(\mathbf{z_i}) \tag{1}$$

$$\mathbf{Pr}(\mathbf{z_i}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}..\int_{\xi_s^{l,i}}^{\xi_s^{L,i}} \varphi(\boldsymbol{\xi}_i;\mathbf{R})\, d\boldsymbol{\xi}_s d\boldsymbol{\xi}_{s-1}..d\boldsymbol{\xi}_1 \tag{2}$$

Arising changes of the integration limits are consistently verified for every monotone section. In case of variation, a reverse projection of $\mathbf{y}^{SP}$ using the bisectional method leads to new integration limits, which are, then, employed to compute the probability by multivariate integration. For this purpose collocation on finite elements is used with an optimal number of collocation points and intervals.

Application to a Dynamic Reactor Network System

The major challenge of design and operation lies in dealing with the conflicts between the objectives. Moreover, there are uncertainties, that need to be taken into consideration in order to make the results more reliable for practical realization. In this work we consider a reactor network system illustrated as a flowsheet in Figure 3 as a practical example. The reactor network consists of two reactors connected in series, in which two main chain reactions take place. Component B (**CB**), as the middle product, is deemed to be the desired product. It is assumed that the feed flow into the 1st reactor, F_0, is the product stream from an upstream plant, and which is stored previously in a vessel as the middle buffer and can be supplied to the network with a controllable flow rate, but with a given composition and temperature.

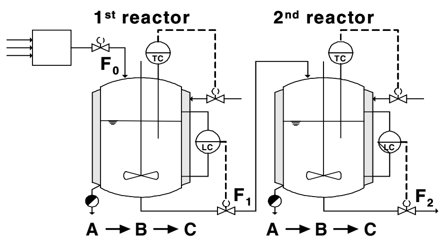

Figure 3. Reactor network flowsheet

First of all, the potential for optimization needs to be investigated through preliminary simulation studies. The dynamic behavior of the process is computed through discretization by the collocation method on finite elements. The results of the simulation studies are illustrated in figure 4, where the necessity for design and operational optimization can be demonstrated.

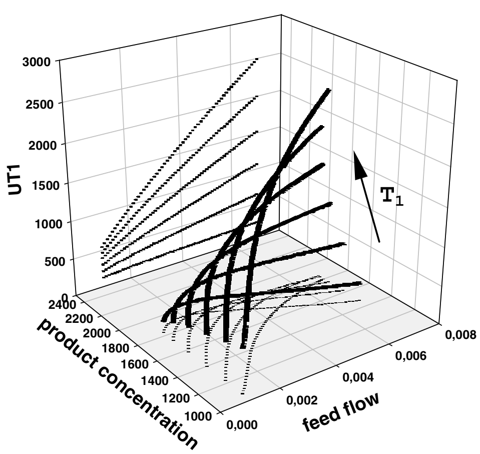

Figure 4. Optimization potential analysis

As expected, the product concentration of component B depends on the reaction kinetics of both reactors, which actually depends on both the residence time and the temperature. Figure 4 is created for fixed volumes and thus F_0 can roughly be seen as a reciprocal measurement for the residence time. It can also be seen that an increasing temperature allows lower residence times for fulfilling the purity restriction concerning **CB**, which allows either higher feed flow rates and thus higher product flow rates or lower design costs related to the volumes. On the other hand, it induces higher utility costs (**UT**). With regards to the residence time, a decision is required between higher flow rates or smaller volumes. Those facts lead to the conclusion that, for cost minimization, overall trade-off decisions need to be made between the temperatures, the flow rates and the volumes. Due to the process dynamic a high degree of flexibility concerning the time-dependence of temperatures and flow rates will lead to better optimal results. In reality, however, the design optimization is often realized first, before optimal operation policies are computed based on the previously optimized design parameters. The analysis of Figure 4 leads to the conclusion that better results are expected when design and dynamic operational optimization are both realized simultaneously in one optimization scheme.

Problem Definition

The aim of the optimization is the minimization of total costs. Thus the objective function includes both the design which implies material costs of the reactor depending on the volumes (V_i) and operational costs (utilities UT_i) during the time period, minus a term indicating the total amount of the desired product (**PB**), which is assumed to be profitable. The objective function of the optimization problem can be written as follows with A, B and C as specific price factors:

$$\min f = \min \left(\sum_{i=1}^{2} A_i \cdot V_i^{2/3} - B \cdot PB + \sum_{i=1}^{2} C_i \cdot UT_i \right)$$

Additionally, there are lower bounds for the amount of the converted Product (**PB**) and upper bounds of utility supply for both reactors (UT_1 and UT_2) necessary to realize the desired trajectories of reactor temperatures in closed control loops. To achieve the optimization goal, the design parameters such as volumes (V_1 and V_2) of both reactors, as well as operational parameters such as flow rates and temperatures are used as free decision variables. The latter ones can be seen as time-dependent, which leads to greater improvement in the dynamic optimization problem.

It should be noted that utility costs are caused by both hot utility supply for sudden increase and cold utility supply for sudden decrease of reactor temperatures. Thus, the utility costs are proportional to the absolute value of the current temperature deviation. This may lead to complications concerning the gradient computation around the value of the current temperature, which could be critical for the implementation of NLP solvers such as SQP. To overcome this problem, the relation of the utility costs to the reactor temperature deviation is approximated by a self formulated exponential function, which is smooth also around the point of the current temperature and thus easy to differentiate, and on the other hand close to the original curve.

So as to make the optimization more robust and the results more reliable, uncertainties of several parameters need to be taken into consideration. For this example the kinetic parameters and the reaction enthalpies are considered to be uncertain. Since all constraints are affected by the uncertain parameters, they should be reformulated to chance constraints. The uncertain parameters also have an impact on the objective function. The usual way is to reformulate it to its expected value. However, for practical application, it is more convenient to assure a certain reliability of the realization of the calculated objective value. This can be achieved by minimizing an upper bound β and the compliance of it can be guaranteed with a certain reliability by formulating an additional chance constraint. Thus, the entire dynamic stochastic optimization problem will be formulated as follows with p_i as the probability levels:

$$\min \beta$$

$$\Pr\{f \le \beta\} \ge p_1$$

$$\Pr\{CB \ge CB^{sp}\} \ge p_2$$

$$\Pr\left\{\left(PB - \int_0^{t_e} F_0 c_{B0}\, dt\right) \ge M_B^{sp}\right\} \ge p_3$$

$$\Pr\{UT_1 \le UT_1^{sp}\} \ge p_4$$

$$\Pr\{W_2 \le W_2^{sp}\} \ge p_5$$

$$t_e \le t^{sp}$$

This formulation allows the user greater flexibility to control the reliability of certain bounds of the objective value. With this formulation, it is also possible to analyze the impact on the optimized value of β with a variation of the probability limit p_1. The created curve of β as a function of p_1 can be a base for trade-off decisions between the upper bound of costs and the reliability. For instance, the end of a section, where this curve is rather flat, could be an interesting point for the user, since a high increase of p_1 induces only a low increase of the cost limit.

Numerical results

Figures 5 illustrate the reliability of both the deterministic optimization results and the stochastic optimization results concerning the compliance of the upper bounds of the utility costs through variation of the uncertain parameters by Monte Carlo simulations. For the stochastic results only less than 5 % of the samples exceeded the bounds of feasibility as claimed in the formulation of the chance constraints, while for the deterministic results the exceeding samples are close to 50%. Moreover, it is interesting to observe the difference concerning the distribution shapes of the utility costs in the second reactor caused by different values of the decision variables. This is due to the non-monotonous relation between the activation energy E_{A1} and that constrained output. While the simulation with deterministically optimized controls induces one minimum of the utility costs, the one with stochastically optimized controls induces at least two minima and one maximum. The fact that the shape of the curves and the number of peaks strongly depend on the values of the decision variables is illustrated in the two graphics at the bottom of the figure 5 as the main reason why the development of this new approach has become necessary.

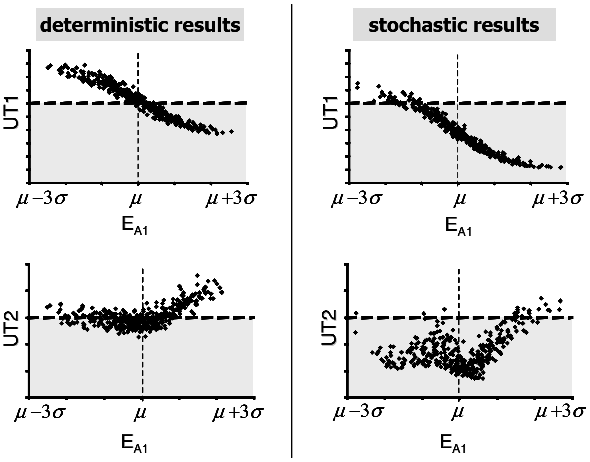

Figure 5. Optimization results

Moreover, the relationship between the probability levels and the corresponding values of the objective function can be used for a suitable trade-off decision between *profitability* and *robustness*. Tuning the value of P_i is also an issue of the relation between *feasibility* and profitability. The solution of a defined problem, however, is only able to arrive at a maximum value **Pmax** which is dependent on the properties of the uncertain inputs and the restriction of the controls.

Conclusions and Acknowledgments

In this work, a new optimization framework via probabilistic programming for simultaneously solving design and operation problems of systems under uncertainty and process variability is proposed. In fact, the approach is relevant to all cases when uncertainty can be described by any kind of joint correlated multivariate distribution function. The authors gratefully acknowledge the financial support of the Deutsche Forschungs-gemeinschaft (DFG) under the contract WO 565/12-2.

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