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Chance Constrained Process Optimization under Uncertainty

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In this contribution, a generalized optimization framework to solving nonlinear chance-constrained dynamic optimization problems under time-dependent uncertainties is proposed. The time dependent uncertainties are described in discrete stochastic variables in the prediction horizon. Hence, the influence of these uncertain variables on the output constraints will propagate through the nonlinear process from time interval to time interval. The solution of the problem has the feature of prediction, robustness and being closed-loop. The developed approach is applicable to all kinds of operational and control problems of chemical processes, where uncertainties need to be taken into consideration. The main challenge lies in the computation of the probabilities of holding the constraints, as well as their gradients. The applicability and efficiency of the developed approaches will be presented through application to different case studies in operation and control.

1. Introduction

Deterministic optimization approaches have been well developed and widely used in the process industry to accomplish off-line and on-line process optimization. The challenging task for the academic research currently is to address large-scale, complex optimization problems under various uncertainties (Sahinidis, 2004). Therefore, investigations on the development of stochastic optimization approaches are required. 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 operation and control. During the past decades several approaches have been suggested to address these problems in a systematic manner (Samsatli et al., 1998). One method of stochastic programming is the probabilistic or chance-constrained approach which focuses on the reliability of the system, i.e., the system's ability to remain feasible in an uncertain environment. The reliability is expressed as a minimum requirement on the probability of satisfying the system constraints. Specifically in complex dynamic systems there are parameters which are usually uncertain, but may have a large impact on the objective function and the constrained outputs. Thus, the challenge is to make decisions a priori for the future operation. However, the decision is needed to be made before the realization of the uncertain inputs. Consequently, under the consideration of uncertainties, the following questions should be answered: 1) how to achieve an economically optimal operation? 2) How to ensure that the constraints of the output variables are satisfied? 3) How to prevent the propagation of the uncertainties to downstream processes? And 4) how to design a proper feedback control system? A stochastic programming problem has to be defined and solved to answer these questions.

2. Chance Constrained Optimization Approach

A general chance constrained optimization or control problem under uncertainty can be formulated as follows:

$$\begin{aligned}
\min\ & \mathrm{E}\left[f(\mathbf{x},\mathbf{u},\xi)\right]+\omega\, D\left[f(\mathbf{x},\mathbf{u},\xi)\right] \\
\text{s.t.}\ & \mathbf{g}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi)=\mathbf{0},\ \ \mathbf{x}(\mathrm{t}_0)=\mathbf{x}_0 \\
& \Pr\left\{\mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi)\geq\mathbf{0}\right\}\geq\alpha \\
& \mathbf{u}_{\min}\leq\mathbf{u}\leq\mathbf{u}_{\max},\ \ \mathrm{t}_0\leq\mathrm{t}\leq\mathrm{t}_\mathrm{f}
\end{aligned}$$

where f is the objective function, E and D are the operators of expectation and variation, respectively. ω is a weighting factor between the two terms. Here, **x**, **u** and ξ are state, decision and random vectors, respectively. **g** represents the equality constraints (i.e model equations). The reliability or probability of complying with the inequality constraints is given by $\Pr\left\{\mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi)\geq\mathbf{0}\right\}\geq\alpha$. The value α $(0\leq\alpha\leq 1)$ represents the probability level. Since α can be defined by the user, it is possible to select different levels and make a compromise between the objective function value and the risk of constraint violation. However, the values of α are not given by an explicit formula, but rather defined as probabilities of some implicitly defined regions in the space of the random parameter ξ, i.e. the feasible region will shrink if the confidence level is increased, which implies a conservative decision. As shown in Fig. 1, such problems can be classified based on the properties of processes, uncertainties and constraint forms.

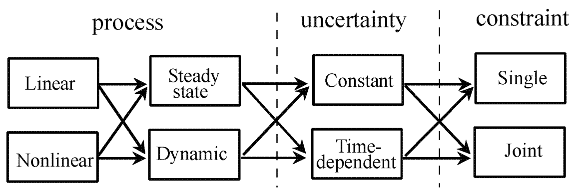


Figure 1. Classification of chance constrained problems

The main challenge in chance constrained programming lies in calculating probability values, the gradients of the probability function to the controls and possibly Hessians

(Arellano-Garcia et al., 2003). The proposed approach uses a two-staged computation framework to decompose the problem (Fig. 2). The upper stage is a superior optimizer following the sequential strategy, where the optimization generates the values of the decision variables and supplies those to a lower stage (simulation stage). This stage gives the values of the objective function, the deterministic and probabilistic constraints, as well as the gradients back to the superior optimizer.

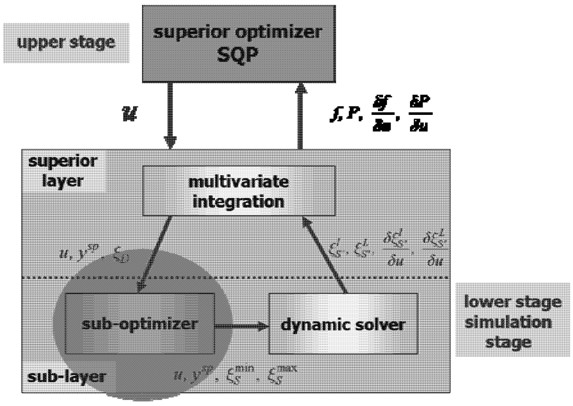


Figure 2. Chance constrained optimization framework

Furthermore, there is a two-layer structure inside the simulation layer to compute the chance constraints. One is the superior layer, where the probabilities and their gradients are finally calculated by multivariate integration. The structure of the inferior layer is the key to the computation of the chance constraints with non-monotonic relation. The main principal of this section is that at temporarily given values of both the decision and uncertain variables the bounds of the constrained outputs **y** and those for the selected uncertain variables ξ reflecting the feasible area concerning **y**, are computed for the multivariate integration (Arellano-Garcia et al., 2004).

Case study: A semi-batch reactor under time-dependent uncertainty

In order to assess the applicability of the presented approach to allowing for dynamic random variables, a simple semi-batch reactor example is considered where a sequential reaction system ($A \rightarrow B \rightarrow C$) takes places (Fig. 3). Both reactions are assumed to be first order. Basically, the aim is to achieve a certain concentration of the desired product B and minimize the batch time by means of manipulating the feed flow rate $F_e(t)$. For the sake of illustration, the cooling system is neglected and thus the reactor temperature is also a time-varying operational degree of freedom. By this means, an energy balance can be omitted and the actual model is simply composed of the component balances, and the equations for the reaction rates. The chance-constrained optimization is formulated as follows

$$\min_{T, F_e, \Delta t} t_f$$

s.t. model equations and

$$\int_{t=0}^{t_f} F_e(t)dt = 162\text{mol}$$

$$N_C(t_f) \le N_C^{max}$$

$$\Pr\{N_B(t_f) \ge N_B^{min}\} \ge 98\%$$

$$T^{min} \le T(t) \le T^{max}$$

$$F_e^{min} \le F_e(t) \le F_e^{max}$$

$$\xi(t) = \{x_{eA}(t), x_{eB}(t)\}$$

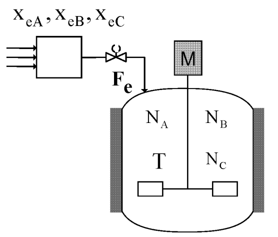


Figure 3. Scheme of the semi-batch reactor

The total feed amount is restricted to 162mol. In addition to the deterministic constraints, the defined single chance constraint corresponds to the end-point restriction on the concentration of B and is to be satisfied with a probability level of 98%. In this case study, the time-varying uncertainties are assumed to be the feed flow concentration $x_{ei}(t)$.

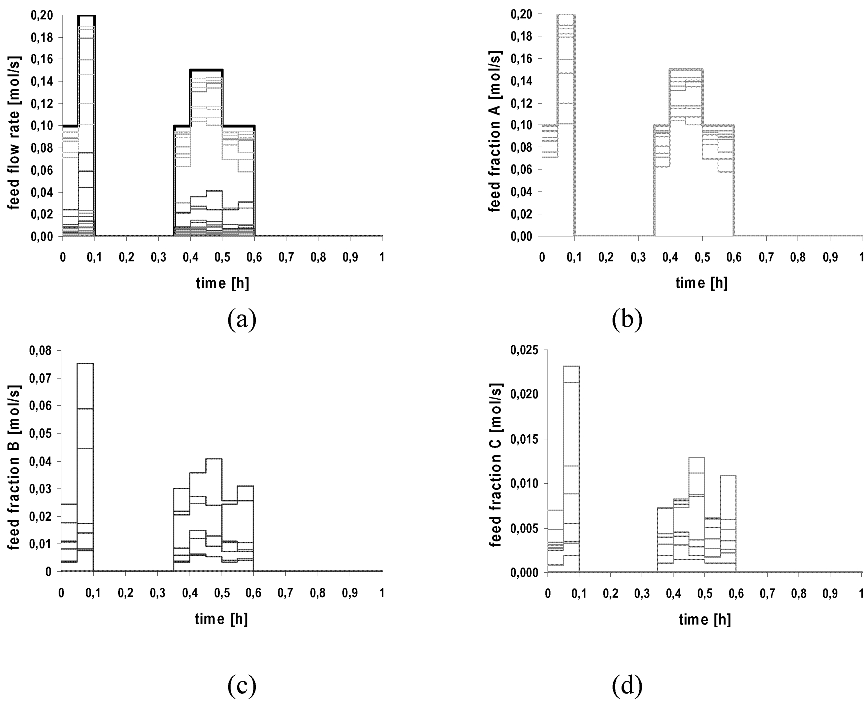
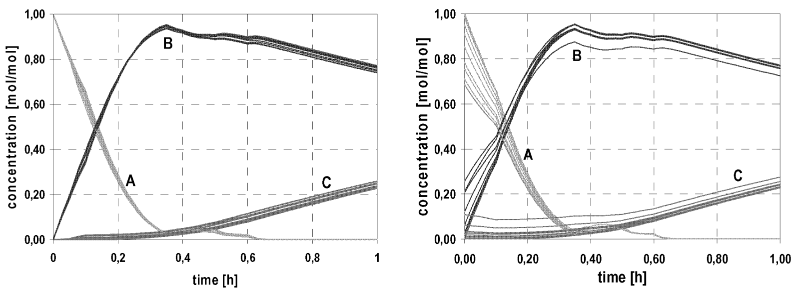


Figure 4. Feed flow and molar flow disturbance profiles.

Since in the nominal optimization is assumed that the feed flow only consist of A, the bold lines in Figure 4a-b represent the deterministic problem solution of with regards to the feed flow rate and the corresponding molar flow of A. Furthermore, the thin lines in all illustrations in Figure 4 characterize the time-dependent behaviour of the molar flow of all components in (a) and for each of them in (b)-(d), respectively.



(a) (b)

Figure 5. Concentration profiles in the reactor for (a) nominal and (b) uncertain initial composition.

Based on the outcomes in Figure 5, the influence of the uncertainties on the composition during the batch operation is pointed up. In Figure 5b, in particular, the concentration changes due to the uncertain initial operating conditions underscore the fact that a classical open-loop implementation of off-line calculated nominal outputs may not lead to the optimal performance. Furthermore, constraint complying can not be assured unless a conservative strategy is implemented such as an extended reaction time, lower feed rate or temperature in order to force the reaction to fully consume the reactant.

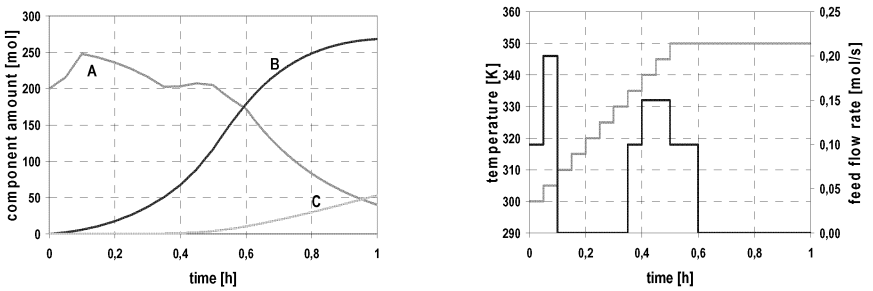


Figure 6. Robust optimal profiles: reactors component amount (left); temperature and feed flow rate policies (right).

The resulting robust optimal trajectories of the operational degree of freedom and the state variables are illustrated in Figure 6. A piecewise constant profile of the reactor temperature is determined. It can be seen that the desired product B is initially converted relatively slow. Towards the end of the batch process both restrictions for B and C, respectively, are however fulfilled. Moreover, the feed flow rate is high in the beginning in order to assure a fast ignition of the reaction. During this period A is accumulated in the reactor. Afterwards the feed flow rate is decreased drastically due to the static potential in the reactor. In order to achieve the desired conversion of B, the remaining feed is again supplied to the reactor. The developed strategies are robust and may be particularly effective for meeting path and terminal constraints under time-varying uncertainties.

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5. Conclusions

This work presents a novel contribution to the research of optimization under uncertainty and provides theoretical developments and practical applications of chance-constrained programming. A number of example problems will be discussed including the application of the optimization framework to large-scale problems. The different solution strategies are mainly applied to transient processes. The solution provides a robust operation strategy in the future time horizon. 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. Thus, one of the main contributions is also that the solution of such problems based on the developed approaches can offer both optimal and reliable decisions such that the analysis of the outcomes allows for identifying the critical constraint which cuts off the largest part of the feasible region. This information is important for decision makers in order to relax the constraint, if necessary, so as to arrive at a meaningful decision. It will be clearly demonstrated that probabilistic programming is a promising technique in solving optimization problems under uncertainty in process system engineering.

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