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PROCESS OPTIMIZATION AND CONTROL UNDER UNCERTAINTY: A CHANCE CONSTRAINED PROGRAMMING APPROACH

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Abstract: A novel chance constrained programming approach for process optimization of large-scale nonlinear dynamic systems and control under uncertainty is proposed. The stochastic property of the uncertainties is explicitly considered in the problem formulation in which some input and state constraints are to be complied with predefined probability levels. This incorporates the issue of feasibility and the contemplation of trade-off between profitability and reliability. The approach considers a nonlinear relation between the uncertain input and the constrained variables. It also involves novel efficient algorithms both to consider time-dependent uncertainties and to compute the probabilities and, simultaneously, their gradients. To demonstrate the performance of the proposed method, a chance constrained NMPC scheme for the online optimization of a batch reactor under safety restrictions, and the optimal operation and control of a coupled two-pressure column system are discussed to show the efficiency and potential for optimization and control under uncertainty.

Keywords: uncertainty, chance constraints, dynamic real-time optimization, NMPC

1. INTRODUCTION

For a quantitative understanding and control of time varying phenomena in process system, it is essential to relate the observed dynamical behaviour to mathematical models. These models usually depend on a number of parameters whose values are unknown or only known roughly. Furthermore, often only a part of the system's dynamics can be measured. Therefore, a plant model unavoidably involves uncertainties. They are either endemic due to the external disturbances or introduced into the model to account for imprecisely known dynamics. However, uncertainty and variability are inherent characteristics of any process system. These arise due to the unpredictable and instantaneous variability of different process conditions, such as temperature and pressure of coupled operating units, market conditions, (recycle) flow rates and/or its composition, or due to certain model parameters such as kinetic constants or equilibrium parameters. These uncertainties or disturbances are often multivariate and correlated stochastic sequences which have a chain-effect to each unit operation of a production line. In industrial practice, uncertainties are usually compensated for by using conservative decisions like an over-design of process equipment and then retrofits to overcome operability bottlenecks, or an overestimation of operational parameters caused by worst case assumptions of the uncertain parameters, which leads to a significant deterioration of the objective function in an optimization problem. In other deterministic approaches, the expected values are used, which most likely leads to violations of the constraints when the decision variables are implemented on site. Moreover, the use of feedback control in order to compensate uncertainty can not ensure constraints on open-loop variables. Consequently, the consideration of uncertainties /disturbances and their stochastic properties in optimization approaches are necessary for robust process operation, and control.

During the past decades several approaches have been suggested to address these problems in a systematic manner (Sahinidis, 2004). These techniques mostly differ in how uncertainty is handled as well as in the objectives that may include process flexibility, profitability, and/or robustness. Nearly 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. In cases where 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. Thus, in this work, we propose a systematic approach to solving chance constrained process optimization and control problems.

Decision making inherently involves consideration of uncertain outcomes. Thus, we are confronted with decisions a priori for the future operation. The decision should be taken before the realization of the random inputs. These uncertain variables can be constant or time-dependent in the future horizon. The stochastic distribution of the uncertain variables may feature different forms. The mean and variance values can be determined based on historical data analysis. However, stochastic optimization with even an approximated distribution is more reliable than a deterministic optimization. In this work, uncertainties are assumed to have a correlated multivariate normal distribution, but the presented approach does not depend on the distribution form.

2. CHANCE CONSTRAINED APPROACH

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

$$\begin{aligned} \min \quad & \mathrm{E}[f(\mathbf{x},\mathbf{u},\xi)] + \omega\, D[f(\mathbf{x},\mathbf{u},\xi)] \\ \text{s.t.} \quad & \mathbf{g}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi) = \mathbf{0},\ \mathbf{x}(t_0) = \mathbf{x}_0 \\ & \Pr\{\mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi) \geq \mathbf{0}\} \geq \alpha \\ & \mathbf{u}_{\min} \leq \mathbf{u} \leq \mathbf{u}_{\max},\ t_0 \leq t \leq t_f \end{aligned} \tag{1}$$

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, $\mathbf{x}$, $\mathbf{u}$ and $\boldsymbol{\xi}$ are state, decision and random vectors, respectively. $\mathbf{g}$ represents the equality constraints (i.e model equations). The reliability or probability of complying with the inequality constraints is given by $\Pr\{\mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi) \geq \mathbf{0}\} \geq \alpha$. 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. The proposed approach relies on formulating output constraints as chance constraints which can be formulated in two different forms: single chance constraint where individual probabilities of ensuring each inequality will be held. In this form, different confidence levels can be assigned to different outputs based on their specifications. Another form is the joint chance constraint, where all inequalities are included in the probability computation i.e. they have to be satisfied simultaneously with the unique given confidence (probability) level.

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. It has, however, the advantage of keeping a more stable operation, but it may be not flexible to the variations required. Thus, the main difference between single and joint constraints consists in their reliability. However, as shown in Fig. 1, such problems can be classified based on the properties of processes, uncertainties and constraint forms.

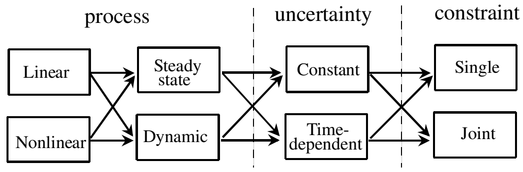

Fig. 1. Classification of chance constrained problems

The main challenge in chance constrained programming lies in calculating probability values, the gradients of the probability function to the controls and possibly Hessians. Different problems have different degrees of complexity for computing these values, which will be discussed in the next sections.

2.1 Monotonic relationship between constrained output and uncertain input

In systems where the relation between uncertain and constrained variables is nonlinear, the type of the probability distribution function of the uncertain input is not the same as the one of the constrained output. Thus, it is difficult to obtain the stochastic distribution of output variables. For this reason, nonlinear chance constrained programming remains an unresolved problem. Recently, a promising optimization framework for dynamic systems under uncertainty was introduced for the off-line optimization under probabilistic constraints and successfully applied to a large-scale nonlinear dynamic chemical process (Arellano-Garcia et al. 2003). The basic idea is to avoid directly computing the output probability distribution. Instead, an equivalent representation of the probability is derived by mapping the probabilistic constrained output region back to a bounded region of the uncertain inputs. Hence, the output probabilities and, simultaneously, their gradients can be calculated through multivariate integration of the density function of the uncertain inputs by collocation in finite elements (2). Since multiple time intervals are considered, the reverse projection of the output feasible region is not trivial. Thus, the approach also involves efficient algorithms for the computation of the required (mapping) reverse projection. The method relies upon the case of a monotonic relationship between the constrained output variables $y_i \in Y_i$ and at least one of the uncertain input variables $\xi_s \in \Xi_s$ where Ξ_s is a subspace of Ξ. So, for instance if $\xi_S \uparrow \Rightarrow y_i \uparrow$, then

$$\begin{aligned} \Pr\{y_i(\mathbf{u},\boldsymbol{\xi}) \leq y_i^{\max}\} &= \Pr\{\xi_S \leq \xi_S^{\max},\ \forall \xi_1, \cdots \xi_{S-1}\} \\ &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\xi_S^{\max}} \rho(\xi_1, \cdots, \xi_S)\, d\xi_S \cdots d\xi_1 \end{aligned} \tag{2}$$

where $\rho(\boldsymbol{\xi})$ is the joint distribution function of ξ. The input boundary ξ_S^{max} is computed through reverse projection based on the output value of y_i^{max}. The boundaries of the infinite integrals in (2) are chosen as $[-3\sigma, 3\sigma]$. In principle, the solution approach can be used to solve problems under uncertainties with any kind of joint correlated multivariate distribution function, provided that the density function is available or it can be approximated. However, the solution of a chance-constrained problem is only able to arrive at a maximum value α^{max} which is dependent on the properties of the uncertain inputs and the restriction of the controls and outputs. To address this issue, a preceding probability maximization step to find out the maximum probability value is set up. For this purpose, the original objective function is substituted and redefined as maximization of the achievable probability. The problem is then solved for the value of α^{max}. In some processes, where the control variable is strictly monotone w.r.t the constrained variable, α^{max} can be obtained through simulation, then α^{max} corresponds to the confidence level with the lower or upper bound of this control variable. This approach can basically be extended to multiple single probabilistic constraints. The application of the approach to a joint chance constrained problem is only related to those cases where an uncertain variable can be found, which is monotone to the joint probability. The approach has been applied to static and large-scale nonlinear dynamic processes. However, this approach can only be employed if the required monotony between constrained output and uncertain input exists.

2.2 Non-monotonic relationship between constrained output and uncertain input

There are, in fact, some stochastic optimization problems where no monotone relation between constrained output and any uncertain input variable can be assured. Especially, for those process systems where the decision variables are strongly critical to the question of whether there is a monotony or not. To address this problem, a novel efficient approach is proposed to chance constrained programming for process optimization and control under uncertainty with no warranty for a monotonic relation between constrained output and uncertain input. Thus, chance constrained nonlinear dynamic optimization can now also be realized efficiently even for those cases where the monotony can not be guaranteed.

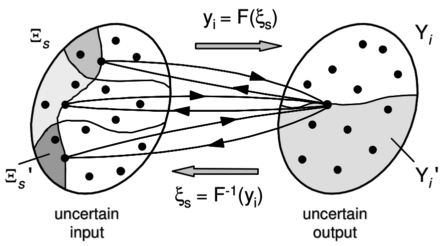

Fig. 2. Mapping feasible regions

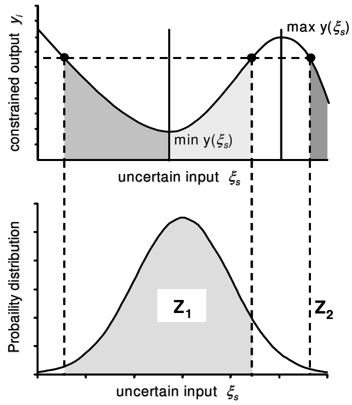

Fig. 3. Non-monotonous sections

The proposed approach uses a two-staged computation framework to decompose the problem. 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.

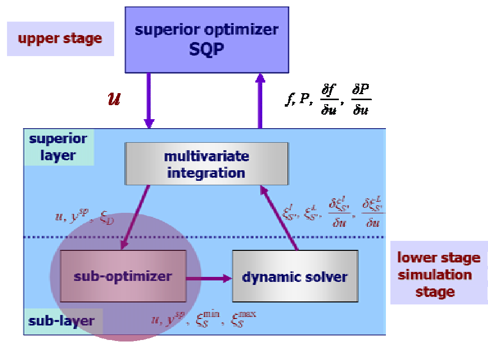

Fig. 4. Chance constrained optimization framework

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 $\mathbf{y}$ and those for the selected uncertain variables $\boldsymbol{\xi}$ reflecting the feasible area concerning $\mathbf{y}$ (Fig. 3), are computed for the multivariate integration. For this purpose, all local minima und maxima of the function reflecting $\mathbf{y}$ are first detected. 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 (in case monotony exists, this optimization step can be neglected). However, with the help of those significant points, the entire space of $\boldsymbol{\xi}$ can be divided into 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. The bounds of feasibility are supplied to the superior multivariate integration layer, where the necessary probabilities (Eq. 3, 4) and the gradients are computed by adding all those feasible fractions together (Fig. 3).

$$\Pr = \sum \Pr(z_i) \tag{3}$$

$$\Pr(z_i) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{\xi_s^{\min,i}}^{\xi_s^{\max,i}} \varphi\left(\xi_i ; \mathbf{R}\right) d\xi_s d\xi_{s-1} .. d\xi_1 \tag{4}$$

In this work, a chance constrained programming framework and its applications to process optimization and control under uncertainty are discussed to demonstrate its potential.

3. CHANCE CONSTRAINED OPTIMAL PROCESS OPERATION

In the daily production of chemical industry numerous plant and units are operated to satisfy product requirements. Following the optimal operation planning, predefined steady-state operating points (point A in Fig. 5) for continuous processes are assigned to a process control system. The objective of a feedback control system is then to reject known or unknown disturbances so that the a priori setpoints can be pursued. For several processes, however, productivity is optimal close to the inherent limitations or boundary of the equipment capacities. In the neighbourhood of such inherent limitations the process dynamics often exhibit a highly nonlinear behaviour. Furthermore, the constrained variables are often monitored for safety considerations but not close-loop controlled. The disturbances behave randomly and even measured disturbances are stochastic variables since their values can not be predicted for a future time point. Thus, it may be necessary to back off from the nominal optimal value of the constraints which are difficult to measure or to control due to the poor dynamics (Fig. 5). Since multivariate disturbances often exist in a large plant it is difficult to decide a proper value. However, the back off values are usually overestimated and thus leading to a conservative operation. For instance, it is well known that compositions are often non online measurable. Thus, temperatures are selected as reference variables for composition control. However, the specified points of temperature control does not necessarily guarantee the purity specifications (e.g. if the pressure of the plant swings). Consequently, because of the conservative decisions concerning the temperature setpoints (point B in Fig. 5), a much purer product than specified will be achieved which causes much more operating costs than needed.

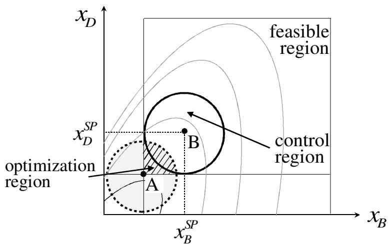

Fig. 5 Operating setpoints by feedback control

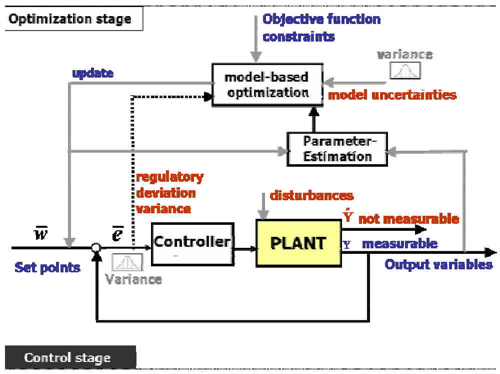

Fig. 6. Open-closed Framework

To overcome these problems, the chance constrained optimization approach is proposed in which the objective function will be improved while satisfying constraints to enforce product quality restrictions with a desired confidence level. This results in a new concept of control: to control open-loop processes by closed-loop control. Unlike the definition where controls are decision variables, in the proposed closed framework the set-points of the measurable outputs are defined as decision variables. Moreover, the controller performance based on the minimum variance control can be regarded as a random input, and thus is also included in the chance constrained formulation of the model-based stochastic optimization problem. The result is a cyclic adjustment of the operating point which guarantees the compliance with the product quality restrictions and assures the controller performance under parametric uncertainty, uncertain boundary conditions, and the random regulatory deviation.

The novel approach is applied to the optimal operation and control of one column embedded in a coupled two-pressure column system for the separation of an azeotropic mixture. The operating point is defined by the distillate and bottom product specifications, cooling outlet temperature limitations, as well as the maximum pressure of the considered high-pressure column. The expected disturbances and implementation errors concern the maximal allowable system pressure, the sensitive tray in the stripping column section as well as the feed flow rate and its composition. However, the values of the setpoints and controls are adjusted so that the target area in Fig. 7 will be tailored to the changing disturbances.

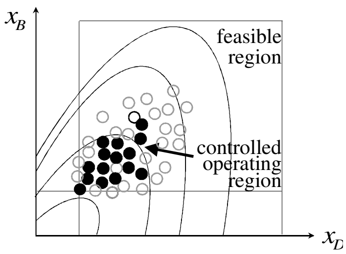

Fig. 7. Operating points of the high-pressure column by the open-closed framework based on the chance constrained approach

In Fig. 7 the black points represent the implemented operating points by feedback control with the open-closed framework. In comparison to the conventional feedback control shown in Fig. 5, the operating points are closer to the nominal point A which leads to a higher profit.

4. CHANCE CONSTRAINED NONLINEAR MODEL PREDICTIVE CONTROL

Since the prediction of future process outputs within an NMPC moving horizon is based on a process model involving the effects of manipulated inputs and disturbances on process outputs, the compliance with constraints on process outputs is more challenging than these on process inputs. Moreover, as the model involves uncertainty, process output predictions are also uncertain. This results in output constraints violation by the close-loop system, even though predicted outputs over the moving horizon might have been properly constrained. Consequently, a method of incorporating uncertainty into the output constraints of the online optimization is needed (Schwarm and Nikolau, 1999; Li et al., 2000).

In most of the previous work, successively updating of the control strategy based on actual measured values has commonly been applied in order to reject disturbances or to compensate for uncertainties. However, since the model mismatch is supposed to be unaltered within the prediction horizon, the control strategy will most likely lead to constraint violations. Another approach in robust MPC represents the assumption that uncertainty is bounded, or equivalently that it is random und uniformly distributed, and then to adopt a worst case contemplation (*min-max* approach) (Lee and Yu, 1997). In this work we propose a chance constrained nonlinear model predictive control. The general chance constrained NMPC problem which is solved at each sampling time k can be formulated as follows:

$$
\begin{aligned}
&\text{Min} \quad J = E\{f\} + \omega D\{f\} \\
&s.t. \\
&\mathbf{x}(k+i+1 \mid k) = \mathbf{g}_1(\mathbf{x}(k+i \mid k), \mathbf{u}(k+i \mid k), \xi(k+i)) \\
&\mathbf{y}(k+i \mid k) = \mathbf{g}_2(\mathbf{x}(k+i \mid k), \mathbf{u}(k+i \mid k), \xi(k+i)) \\
&\mathbf{Pr}\{\mathbf{y}_{\min} \le \mathbf{y}(k+i \mid k) \le \mathbf{y}_{\max}\} \ge \boldsymbol{\alpha}, i = 1, \ldots, n \\
&\mathbf{u}_{\min} \le \mathbf{u}(k+i \mid k) \le \mathbf{u}_{\max}, i = 0, \ldots, m-1. \\
&\Delta\mathbf{u}_{\min} \le \Delta\mathbf{u}(k+i \mid k) = \mathbf{u}(k+i \mid k) - \mathbf{u}(k+i-1 \mid k) \le \Delta\mathbf{u}_{\max}
\end{aligned}
$$

The solution of the above problem, however, is only able to arrive at a maximum value $\boldsymbol{\alpha}^{\mathbf{max}}$ which is dependent on the properties of the uncertain inputs and the restriction of the controls. The value of $\boldsymbol{\alpha}^{\mathbf{max}}$ can be computed through a previous probability maximization step. For this purpose, the original objective function is replaced and the following optimization problem will then be solved:

$$
\begin{aligned}
&\max \ \alpha \\
&\text{s.t.} \quad \mathbf{g}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{y}, \mathbf{u}, \xi) = 0, \ \mathbf{x}(t_0) = \mathbf{x}_0 \\
&\qquad \Pr\left\{ y_j \le y_j^{SP}, \ j = 1, \cdots, m \right\} \ge \alpha \\
&\qquad \mathbf{u}_{\min} \le \mathbf{u} \le \mathbf{u}_{\max}, \ t_0 \le t \le t_f
\end{aligned}
$$

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 α is also an issue of the relation between feasibility and profitability. The resulting NMPC scheme is embedded in the on-line optimization framework (Fig. 8).

However, a strongly exothermic series reaction conducted in a non-isothermal batch reactor under safety restrictions is considered to demonstrate the efficiency of the proposed approach. The reaction kinetics are second-order for the first reaction producing B from A, and an undesirable consecutive first-order reaction converting B to C. The intermediate product B is deemed to be the desired product. Since the heat removal is limited, the temperature is controlled by the feed rate of the reactant A and the flow rate of the cooling liquid in the nominal operation. The reactor is equipped with a jacket cooling system. At the start, the reactor partly contains the total available amount of A. The remainder is then fed and its feed flow rate is optimized to maximize the yield. However, the accumulation of A at the start of the batch time must be prevented, otherwise, as the batch proceeds exhaustion of the cooling system capacity can not be avoided. Furthermore, whilst the reaction proceeds, the reactor's volume diminishes so that the computation of the corresponding cooling capacity is adapted according to the remaining cooling jacket area. The developed model considers both the reactor and the cooling jacket energy balance. Thus, the dynamic performance between the cooling medium flow rate as manipulated variable and the controlled reactor temperature is also included in the model equations. Thereby, it can be guaranteed that later the computed temperature trajectory can be implemented by the controller. Moreover, by this means the limitations of the cooling system (pump capacity) can explicitly be taken into account for the optimization.

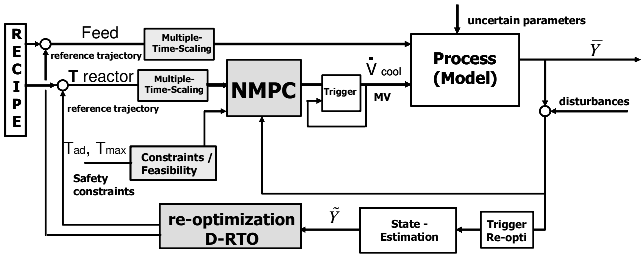

Fig. 8. On-line framework: integration of chance constrained NMPC and dynamic re-optimization.

There are path and end point constraints for the reaction process: first, a limited available amount of A to be converted by the final time is fixed. Furthermore, so as to consider the shut-down operation, the reactor temperature at the final batch time must not exceed a temperature limit. Additionally, there are path constraints for the reactor temperature, and the adiabatic end temperature which is used to determine the temperature after failure.

The decision variable is the cooling flow rate. In order to compare the performances of the open-loop nominal solution and the nominal NMPC with the proposed on-line framework under uncertainty, different disturbances have been considered, namely: catalyst activity mismatch and fluctuations of the reactor jacket cooling fluid temperature. Additionally, all measurements are corrupted with white noise e.g. component amount 8%, Temperature 2%.

While fast disturbances are efficiently rejected by the proposed regulatory NMPC-based approach, there are, on the other hand, in fact, slowly time-varying non-zero mean disturbances or drifting model parameters which change the plant optimum with time. Thus, a re-optimization i.e. dynamic real-time optimization (D-RTO) may be indispensable for an optimal operation (Fig. 8). When on-line measurement gives access to the system state, on-line re-optimization promises considerably improvement. Moreover, additional constraints can be formulated. In this work, we assume that the state information is available.

In order to compensate slow disturbances, the on-line re-optimization problem is automatically activated three times along the batch process time according to a trigger defined as the bounded above difference between the reactor temperature and the temperature reference trajectory. New recipes resulting from this are then updated as input to the on-line framework. Due to the different trigger time-points the current D-RTO problem progressively possesses a reduced number of variables within a shrinking horizon (Nagy and Braatz, 2003). As a result of this, and a catalyst contamination the total batch time increases. But, despite the large plant mismatch and the absence of kinetic knowledge nearly perfect control is accomplished.

5. CONCLUSIONS

The chance constrained optimization framework has been demonstrated to be promising to address optimization and control problems under uncertainties. Feasibility and robustness with respect to input and output constraints have been achieved by the proposed approach. The resulting NMPC scheme embedded in the on-line re-optimization framework is viable for the optimization of the semi-batch reactor recipe while simultaneously guaranteeing the constraints compliance, both for nominal operation as well as for cases of large disturbances e.g. failure situation. 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 Forschungsgemeinschaft (DFG).

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