# Close-Loop Stochastic Dynamic Optimization Under Probabilistic Output-Constraints

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**Summary.** In this work, two methods based on a nonlinear MPC scheme are proposed to solve close-loop stochastic dynamic optimization problems assuring both robustness and feasibility with respect to output constraints. The main concept lies in the consideration of unknown and unexpected disturbances in advance. The first one is a novel *deterministic* approach based on the *wait-and-see* strategy. The key idea is here to anticipate violation of output hard-constraints, which are strongly affected by instantaneous disturbances, by backing off of their bounds along the moving horizon. The second method is a new *stochastic* approach to solving nonlinear chance-constrained dynamic optimization problems under uncertainties. The key aspect is the explicit consideration of the stochastic properties of both exogenous and endogenous uncertainties in the problem formulation (*here-and-now* strategy). The approach considers a *nonlinear* relation between the uncertain input and the constrained output variables.

## 1 Introduction

Due to its ability to directly include constraints in the computation of the control moves, nonlinear model predictive control offers advantages for the optimal operation of transient chemical plants. Previous works on robust MPC have focused on output constrained problems under model parameter uncertainty, in particular, worst-case performance analysis over a specified uncertainty range [4, 8]. The drawback of this worst-case formulation – min-max approach – is that the resulting control strategy will be overly conservative. In this work, we extended our previous work in [3, 5, 7] to a new chance-constrained optimization approach for NMPC. Unlike the linear case, for nonlinear (dynamic) processes the controls have also an impact on the covariane of the outputs. The new approach also involves efficient algorithms so as to compute the probabilities and, simultaneously, the gradients through integration by collocation in finite elements. However, in contrast to all our previous works (see e.g. [7]), the main novelty here is also that the chance-constrained approach is now also applicable for those cases where a monotic relationship between constrained output and uncertain input can not be asurred. In addition, due to the consideration of a first principle model with a several number of uncertain variables, the problem can conditionally become too computationally intensive for an online

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application. Thus, we propose alternatively a dynamic adaptive back-off strategy for a NMPC scheme embedded in an online re-optimization framework. The performance of both proposed approaches is assessed via application to a runaway-safe semi-batch reactor under safety constraints.

## 2 Problem Formulation

A strongly exothermic series reaction conducted in a non-isothermal fed-batch reactor is considered. 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 the desired product.

$$2A \xrightarrow{K_1} B \xrightarrow{K_2} C \tag{1}$$

A detailed first-principles model of the process is given by a set of DAEs based on mass balances:

$$\begin{aligned} \dot{n}_A &= -\nu_a k_{01} \frac{n_A^2}{V} e^{-\frac{E_{A1}}{\mathbb{R}T}} + feed; \quad \dot{n}_B = -k_{02}\, n_B\, e^{-\frac{E_{A2}}{\mathbb{R}T}} + k_{01} \frac{n_A^2}{V} e^{-\frac{E_{A1}}{\mathbb{R}T}}; \\ \dot{n}_C &= +k_{02}\, n_B\, e^{-\frac{E_{A2}}{\mathbb{R}T}}, \end{aligned} \tag{2}$$

the energy balance:

$$\dot{\bar{T}}_{cool} = \frac{\dot{V}_{cool} \cdot \rho_{cool} \cdot c_{p,cool} \cdot (T_{cool,in} - \bar{T}_{cool}) - \dot{Q}_{cool}^{HT}}{V_{cool} \cdot \rho_{cool} \cdot c_{p,cool}}; \; \dot{T} = \frac{\dot{Q}_{reac} + \dot{Q}_{feed} + \dot{Q}_{cool}}{n_S \sum_i (c_{pi} x_i)} \tag{3}$$

and constitutive algebraic equations:

$$\begin{aligned} \dot{Q}_{reac} &= -\sum (h_i \dot{n}_i) = (h_{0A} + c_{pA}(T - T_0))\dot{n}_A + (h_{0B} + c_{pB}(T - T_0))\dot{n}_B \\ &\quad + (h_{0C} + c_{pC}(T - T_0))\dot{n}_C \\ \dot{Q}_{feed} &= (h_{0A} + c_{pA}(T - T_0)) \cdot feed \\ \dot{Q}_{cool}^{HT} &= -k_{HT} A (T - \bar{T}_{cool}) = -k_{HT}(0.25\pi d^2 + 4Vd^{-1})(T - \bar{T}_{cool}) \\ n_S &= n_A + n_B + n_C; \quad n_S \sum_i (c_{pi} x_i) = c_{pA} n_A + c_{pB} n_B + c_{pC} n_C \\ V &= \frac{n_A \tilde{M}_A + n_B \tilde{M}_B + n_C \tilde{M}_C}{n_A \bar{\bar{\rho}}_A + n_B \bar{\bar{\rho}}_B + n_C \bar{\bar{\rho}}_C} n_S. \end{aligned} \tag{4}$$

In these equations $V$ denotes the varying volume, $n_i$ the molar amount of component $i$, $T$, $T_F$, $\bar{T}_{cool}$, $T_{cool}$, the reactor, dosing, jacket and cooling medium temperatures, respectively. $h_{0i}$ are the specific standard enthalpies, $k_{HT}$ the heat transfer coefficient, $d$ the scaled reactor diameter, $A$ the heat exchange surface, $\tilde{M}_i$ molecular weights, $\rho_i$ densities and $c_{pi}$ are heat capacities. Besides, since the heat removal is limited, the temperature is controlled by the feed rate of the reactant $A(feed)$, and the flow rate of the cooling liquid $\dot{V}_{cool}$ in the nominal operation. The reactor is equipped with a jacket cooling system.

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. The open-loop optimal control is solved first for the successive optimization with moving horizons involved in NMPC. The objective function is to maximize the production of $B$ at the end of the batch $CB_f$ while minimizing the total batch time $t_f$ with $\beta = 1/70$:

$$\min_{\Delta t,\, \dot{V}_{cool},\, feed} \left(-CB_f + \beta \cdot t_f\right) \tag{5}$$

subject to the equality constraints (process model equations (2) – (4)) as well as path and end point constraints. First, a limited available amount of $A$ to be converted by the final time is fixed to $\int_{t_0=0}^{t_f} n_A(t)dt = 500 mol$. Furthermore, so as to consider the shut-down operation, the reactor temperature at the final batch time must not exceed a limit $(T(t_f) \leq 303\, K)$. There are also path constraints for the maximal reactor temperature and the adiabatic end temperature $T_{ad}$. The latter is used to determine the temperature after failure. This is a safety restriction to ensure that even in the exterme case of a total cooling failure no runaway will occur $(T(t) \leq 356\, K; \quad T_{ad}(t) \leq 500\, K)$ [1]. Additionally, the cooling flow rate changes from interval to interval are restricted to an upper bound: $\left\|\dot{V}_{cool}(t+1) - \dot{V}_{cool}(t)\right\| \leq 0.05$. The decision variables are the feed flow rate into the reactor, the cooling flow rate, and the length of the different time intervals. A multiple time-scale strategy based on the orthogonal collocation method on finite elements is applied for both discretization and implementation of the optimal policies according to the controller's discrete time intervals (6 – 12 s; 600 – 700 intervals). The resulting trajectories of the reactor temperature and the adiabatic end temperature (safety constraint) for which constraints have been formulated are depicted in Fig. 1. It can be observed that during a large part of the batch time both states variables evolve along their upper limits i.e. the constraints are active. The safety constraint (adiabatic end temperature), in particular, is an active constraint over a large time period (Fig. 1 right). Although operation at this nominal optimum is desired, it typically cannot be ahieved with simultaneous satisfaction of all contraints due to the influence of uncertainties and/or external disturbances. However, the safety hard-constraints should not be violated at any time point.

## 3 Dynamik Adaptive Back–Off Strategy

Based on the open-loop optimal control trajectories of the critical state variables, in this section, a deterministic NMPC scheme for the online optimization of the fed-batch process is proposed. Furthermore, the momentary criteria on the restricted controller horizon with regard to the entire batch operation is however insufficient. Thus, the original objective of the nominal open-loop optimization

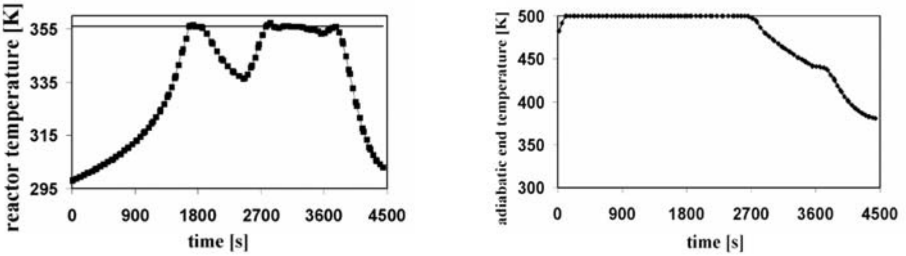


**Fig. 1.** Path constraints: Optimal reactor temperature (left) and adiabatic end temperature (right)

problem is substituted by a tracking function which can then be evaluated on the local NMPC prediction horizon:

$$\min_{\dot{V}_{cool}} J(N_1,\ N_2,\ N_U) = \sum_{j=N_1}^{N_2} \delta(j) \cdot [\hat{y}(t+j \mid t) - w(t+j)]^2 + \sum_{j=1}^{N_U} \lambda(j) \cdot [\Delta u(t+j-1)]^2 \tag{6}$$

The first term of the function stands for the task of keeping as close as possible to the calculated open loop optimal trajectory of the critical variables $\hat{y}$ (e.g. the reactor temperature, which can easily be measured online), whereas the second term corresponds to control activity under the consideration of the systems restriction's described above. $N_1$, $N_2$ denote the number of past, and future time intervals, respectively. $N_U$ stands for the number of controls. The prediction $T_P$ and control horizon $T_C$ comprises 8 intervals, respectively. Furthermore, $\lambda = 3000$ and $\delta(j) = 0.7^{(T_P - j)}$ are the variation and offset weighting factor, respectively. In order to guarantee robustness and feasibility with respect to output constraints despite of uncertainties and unexpected disturbances, an adaptive dynamic back-off strategy is introduced into the optimization problem to guarantee that the restrictions are not violated at any time point, in particular, in case of sudden cooling failure [1]. For this purpose, it is necessary to consider the impact of the uncertainties between the time points for re-optimization and the resulting control re-setting by setting, in advance, the constraint bounds much more severe than the physical ones within the moving horizon. Thus, as shown in Fig. 2 left, the key idea of the approach is based on backing-off of these bounds with a decreasing degree of severity leading then to the generation of a trajectory which consist of the modified constraint bounds along the moving horizon. For the near future time points within the horizon, these limits (bounds) are more severe than the real physical constraints and will gradually be eased (e.g. logarithmic) for further time points. The trajectory of these bounds is dependent on the amount of measurement error and parameter variation including uncertainty.

As previously illustrated in Fig. 1, the true process optimum lies on the boundary of the feasible region defined by the active constraints. Due to the uncertainty in the parameters and the measurement errors, the process optimum and

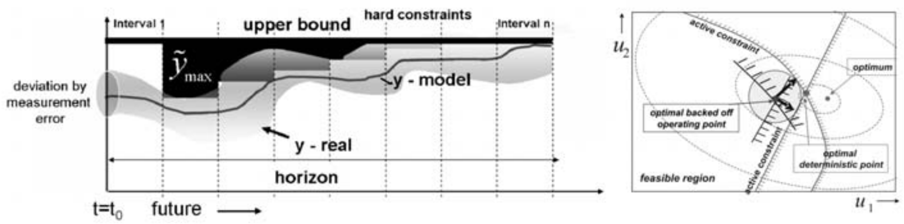


**Fig. 2.** Back-off strategy within moving horizon; back-off from active constraints

the set-point trajectory would be infeasible. By introducing a back-off from the active constraints in the optimization, the region of the set-point trajectory is moved inside the feasible region of the process to ensure, on the one hand, feasible operation, and to operate the process, on the other hand, still as closely to the true optimum as possible. By this means, the black-marked area in Fig. 2 illustrates the corrected bounds $\tilde{y}_{max}$ of the hard constraints. Here, it should however be noted that due to the severe bound at the computation of the previous horizon, the initial value at $t_0$ is rather far away from the constraint limit in the feasible area. Thus, in the first intervall of the current moving horizon, the bound is set at the original physical limit to avoid infeasibility. The back-off adjustment starts from the second interval, i.e. from the time point on, where the next re-optimization begins. The size of $\tilde{y}_{max}$ strongly depends on parametric uncertainty, disturbances, and the deviation by measurement errors. Thus, the constraints in (8) within the moving horizon (8 intervals) are now reformulated as follows with $j = 2, ..., 8$, $\alpha = 0.5$, $\tilde{T}_{max} = 4\,K$ and $\tilde{T}_{ad,\,max} = 3\,K$:

$$T(j) \leq 356\,K - \tilde{T}_{max} \cdot \alpha^{(j-2)}; \quad T_{ad}(j) \leq 500\,K - \tilde{T}_{ad,\,max} \cdot \alpha^{(j-2)} \tag{7}$$

The decision variable is the cooling flow rate. In order to test robustness characteristics of the controler, the performances of the open-loop nominal solution, the nominal NMPC, and the NMPC with the proposed adaptive back-off approach are compared under different disturbances, 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% and temperature 2%.

### 3.1 Dynamik Real–Time Optimization

The size of the dynamic operating region around the optimum (see Fig. 2 right) is affected by fast disturbances. These are, however, efficiently buffered by the proposed regulatory NMPC-based approach. On the other hand, there are, in fact, slowly time-varying non-zero mean disturbances or drifting model parameters which change the plant optimum with time. Thus, a online re-optimization i.e. dynamic real-time optimization (D-RTO) may be indispensable for an optimal operation. When on-line measurement gives access to the system state,

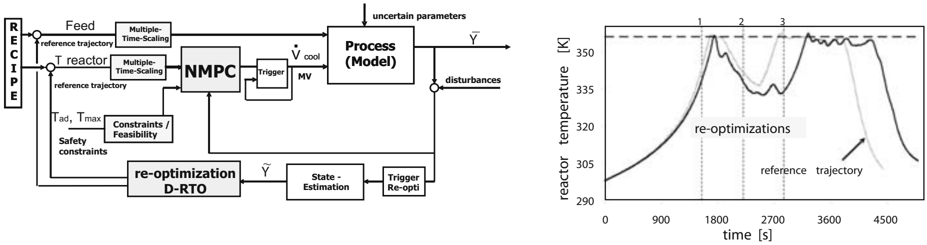


**Fig. 3.** Integration of NMPC and D-RTO; On-line re-optimization

its promises considerably improvement. Moreover, additional constraints can be integrated. Simulation results are shown in Fig. 3 right.

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 (Fig. 3 right). 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 [6]. As a result, the total batch time increases. But, despite the large plant mismatch and the absence of reliable kinetic knowledge a very good control is accomplished. Thus, 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. The proposed scheme yields almost the same profit as the one of the off-line optimization operational profiles (see Tab. 1) where $CB_f$ and $CC_f$ are the final total amount of $B$ and $C$.

**Table 1.** Simulation results

| | $CB_f$ [mol] | $CC_f$ [mol] | $t_f$ [s] |
|---|---|---|---|
| Nominal open-loop optimization | 152.5 | 37.8 | 4297 |
| NMPC w. uncertainty + dyn. back-off | 127.9 | 12.8 | 4297 |
| NMPC w. uncertainty + dyn. back-off + D-RTO | 148.8 | 36.8 | 4892 |

## 4 Robust NMPC Under Chance Constraints

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 explicit into the output constraints of the online optimization is needed. Thus, in this work, a robust NMPC that uses a close-loop model considering the uncertainty in future process outputs due to stationary and non-stationary stochastic disturbances is presented. The new controller solves a chance-constrained nonlinear dynamic problem at each execution in order to determine the set of control moves that will optimize the expected performance of the system while complying with the constraints. The controller deals with the model uncertainty and disturbances by replacing deterministic constraints in the NMPC formulation of the form $y_{min} \leq y \leq y_{max}$, here Eq. (8), with chance constraints of the form:

$$\boldsymbol{Pr}\left\{y_{min} \leq y \leq y_{max}\right\} \geq \boldsymbol{\alpha} \tag{8}$$

The main challenge lies in the computation of the probability and its gradients. To address this problem, we propose in [7] an inverse mapping approach where the monotonic relationship of the constrained output $y^{bound}$ to at least one uncertain input $\xi_S$ is employed. Due to the monotony, the constrained bound value $y^{bound}$ in the output region corresponds to a limit value $\xi_S^L$ for $\xi_S$ in the uncertain input region. The basic idea is to map 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 on finite elements with an optimal number of collocation points and intervals.

$$\begin{aligned} P\left\{y \leq y^{bound}\right\} &= P\left\{\xi_S \leq \xi_S^L,\ \xi_k \subseteq \mathbb{R}^K, s \neq k\right\} \\ &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\xi_S^L} \cdots \int_{-\infty}^{\infty} \rho(\xi)\, d\xi_l \cdots d\xi_S \cdots d\xi_K \quad l = 1, ..., n \end{aligned} \tag{9}$$

where the $\rho(\xi)$ is the unified distribution function of $\xi$. The solution strategy is however not dependent on the distribution of the uncertain variables. The probability computation procedure can straightforwardly be extended to multiple single probabilistic constraints with different confidence levels. To compute the probability values of (13), a multivariate integration in the region of uncertain inputs is required. Numerical integration is needed, especially in cases of correlated uncertain variables. We refer to Wendt et al. (2001) for a method based on orthogonal collocation for correlated uncertain variables with normal distributions. Following this idea, we extend the approach to dealing with nonlinear dynamic optimization problems [2, 3]. In this contribution, a new framework is proposed also for such stochastic dynamic optimization problems where *no monotonic* relation between constrained output and any uncertain input variable can be guaranteed. This approach also involves efficient algorithms for the computation of the required (mapping) reverse projection. To decompose the problem, the proposed approach uses a two-stage computation framework(see Fig. 4 left). 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 sub-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 $y$ and those for the selected uncertain variables $\xi$ reflecting the feasible area concerning $y$ 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 $y$ are first detected (see Fig. 4 right). The computation of the required points of $[\min y(\xi)]$ and $[\max y(\xi)]$ is achieved by an optimization step in the sub-layer. With the help of those significant points, the entire space of $\xi$ 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. The bounds of feasibility are supplied to the superior multivariate integration layer, where the necessary probabilities (Eqs. 14) and the gradients are computed by adding all those feasible fractions together (Fig. 4 right).

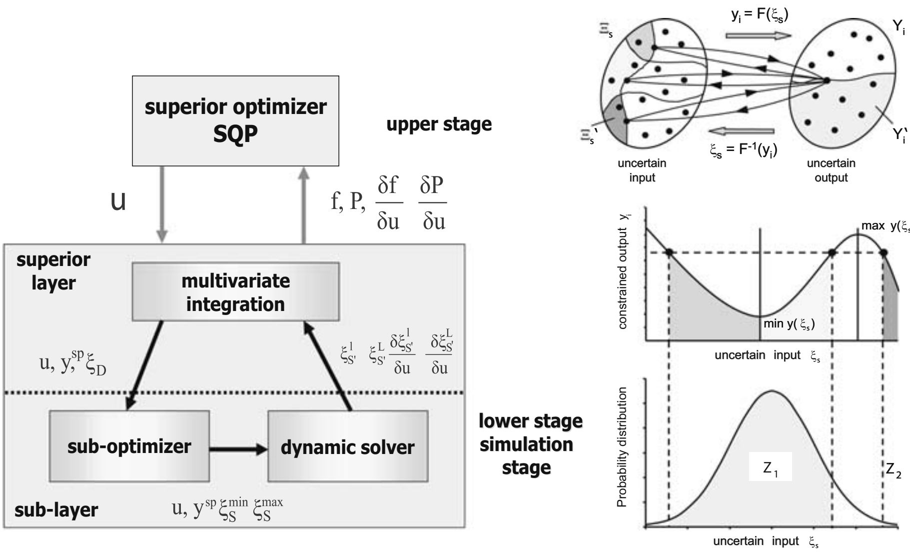


**Fig. 4.** Structure of optimization framework (left) and mapping of feasible reagions (right)

$$\boldsymbol{Pr} = \sum \boldsymbol{Pr}(z_i); \quad \boldsymbol{Pr}(z_i) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\xi_S^{l,i}}^{\xi_S^{L,i}} \varphi\,(\xi_i,\ R) d\xi_S\, d\xi_{S-1} \cdots d\xi_1 \tag{10}$$

where R denotes the covariance matrix. Arising changes of the integration limits are verified for every monotone section. In case of variation, a reverse projection of the constrained output leads to new integration limits, which are, then, employed to compute the probability by multivariate integration. The general chance constrained NMPC problem which is solved at each sampling time $k$ can be formulated as follows:

$$\begin{aligned} &\min \sum_{i=1}^{N_u} [\boldsymbol{u}(k+i) - \boldsymbol{u}(k+i-1)]^2 \\ s.t.\ &\boldsymbol{x}(k+i+1 \mid k) = \boldsymbol{g}_1[\boldsymbol{x}(k+i \mid k),\ \boldsymbol{u}(k+i \mid k),\ \boldsymbol{\xi}(k+i)] \\ &\boldsymbol{y}(k+i \mid k) = \boldsymbol{g}_2[\boldsymbol{x}(k+i \mid k),\ \boldsymbol{u}(k+i \mid k),\ \boldsymbol{\xi}(k+i)] \\ &\boldsymbol{Pr}\,\{\boldsymbol{y}_{min} \le \boldsymbol{y}(k+i \mid k) \le \boldsymbol{y}_{max}\} \ge \alpha; \quad i = 1, ..., n \\ &\boldsymbol{u}_{min} \le \boldsymbol{u}(k+i \mid k) \le \boldsymbol{u}_{max}; \quad i = 0, ..., m-1 \\ &\Delta \boldsymbol{u}_{min} \le \Delta \boldsymbol{u}(k+i \mid k) = \boldsymbol{u}(k+i \mid k) - \boldsymbol{u}(k+i-1 \mid k) \le \Delta \boldsymbol{u}_{max} \end{aligned} \tag{11}$$

Where $\boldsymbol{g}_1$ are the first-principle model equations describing the dynamic changes of the state variables $\boldsymbol{x}$, while $\boldsymbol{g}_2$ describe the state of the constrained variables $\boldsymbol{y}$ depending on the control variables $\boldsymbol{u}$ and the uncertain parameters $\boldsymbol{\xi}$, and $\alpha = 96.7\%$. The efficiency of the chance-constrained approach is proved through application to the same scenario of the fed-batch reactor under safety constraints. The resulting NMPC scheme is also embedded in the same on-line optimization framework. 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 $\boldsymbol{\alpha}$ is also an issue of the relation between *feasibility* and profitability. The solution of a defined problem (Eq. 15), however, is only able to arrive at a maximum value $\alpha^{max}$ which is dependent on the properties of the uncertain inputs and the restriction of the controls. The value of $\alpha^{max}$ can be computed through a previous probability maximization step. The use of this strategy with the consideration of uncertainties in advance has for those NMPC-Problems a great impact in those periods, where the reference trajectory is very close to a defined upper bound of the constraint output. However, a comparison between the stochastic approach and the deterministic dynamic adaptive back-off strategy is meaningful in order to find further improvement of operation policies due to the stochastic approach. Thus, the reference trajectory of the reactor temperature in Equation (10) is set as a constant which is close to the upper bound of the reactor temperature.

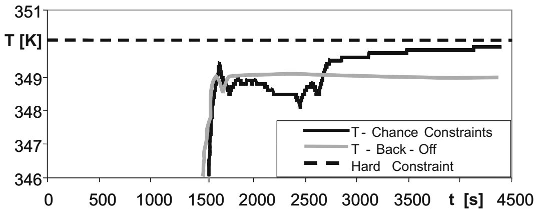


**Fig. 5.** Comparison back-off strategy and chance constraints

The resulting trajectories of the reactor temperature concerning both strategies are illustrated in Fig. 5. The figure shows, that the reactor temperature resulted by the back-off strategy reaches very early a stationary value caused by fixed bounds of the temperature formulated in the corresponding optimization problem. The temperature curve of the stochastic approach shows more drastical changes with lower values of temperatures in earlier parts of the diagram and higher values later. This is caused by the fact, that with the consideration of uncertainties in advance, also the change of sensitivities of uncertain parameters towards the reactor temperature can be taken into consideration by the stochastic approach. At the beginning in the diagram, the stochastic approach realizes the matching of a more conservative strategy to higher sensitivities, and thus the operation achieves more robustness than the one achieved by the back-off strategy. At the end of the curves, the decrease of sensitivities is used for a closer approach to the maximum temperature and thus leads to a better objective value. Therefore, the strategy leads to an improvement of both, robustness and the objective value.

## 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. Thus, the solution of the problem has the feature of prediction, robustness and being closed-loop. The resulting NMPC scheme embedded in the on-line re-optimization framework is viable for the optimization of the 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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