

Approximate robust optimal control of nonlinear dynamic systems under process noise*

Dries Telen¹, Mattia Vallerio¹, Lorenzo Cabianca¹, Boris Houska², Jan Van Impe¹, and Filip Logist¹

Abstract—Dynamic optimization techniques for nonlinear systems can provide the process industry with sustainable and efficient operating regimes. These regimes can lie close to the process limits. It is therefore critical that these operating conditions are robust with respect to process noise, i.e., an unmodeled time-varying random disturbance. Besides the uncertainty in the constraints, also uncertainty in the objective function should be considered. However, including robustness in an optimization problem typically leads to semi-infinite optimization problems which are challenging to solve in practice. In this paper several computationally tractable methods are exploited to approximately solve the robust optimal control problem. The presented approaches allow the use of fast deterministic gradient based optimization techniques. The first method is based on a linearization approach while the second method exploits the unscented transformation to construct an estimate of the uncertainty propagation. Both methods yield an approximation of the variance-covariance matrix of the critical constraints and of the objective function. These variance-covariance matrices are employed in the optimization routine. The illustrative case study is a jacketed tubular reactor.

I. INTRODUCTION

Sustainability concerns, market saturation and global competition are a continuous driver for the process industry to increase its performance. Mathematical models and optimization techniques are useful tools to achieve this goal. The optimization of processes described by ordinary differential equations leads to so-called *dynamic optimization* or *optimal control* problems. The solution of these optimal control problems usually pushes the system to its operating limits.

An inherent problem of mathematical models in the process industry is the presence of uncertainty. The considered uncertainty is assumed to be external disturbances which are subsequently also present in the optimization of these processes [19]. The field of *robust optimization* aims to take this uncertainty into account such that critical constraints are met. Generally, uncertainty is modeled as follows. If information regarding the probability distribution is available, it can lead to the formulation of *expected values* for the objective function and *chance constraints* [13], [15], [18], [25]. A different setting arises when the uncertainty is

known to be fully contained within a given set, e.g., a box or ellipsoid. This usually leads to the formulation where all constraints have to be satisfied in the *worst case* scenario and what is the worst possible performance [4], [9], [15]. This last setting gives typically rise to hard-to-solve min max optimization problems. The price to pay for this increased robustness is typically a decreased performance [3], [14]. However, the amount of robustness can often be adjusted based on trade-off or backoff parameters [7], [14].

In the current paper, it is assumed that the uncertainty is present in the model right hand side, i.e., so-called *process noise*. The nature of the uncertainty is assumed to be stochastic. This process noise in the model description is induced by fluctuating process conditions.

Traditionally, the first type of techniques is based on *Taylor series approximations* of the model functions with respect to the uncertainty. Typically a first-order approximation is used. This is justified if the uncertainty is small compared to the model curvature such that higher order terms can be neglected [15]. It yields a linear approximation of the variance-covariance matrix [22] of the states which can be easily taken into account in the subsequent dynamic optimization procedure as single chance constraints. Alternatively, the resulting expected value can be obtained via a computationally expensive *integration over the parameter distribution* [1], [13], [25]. In contrast to these integration based schemes, several efficient sampling schemes for uncertainty quantification have been reported, e.g., using Hammersley sequences [5], using polynomial chaos expansions [16] and the unscented transformation or sigma point approach [12]. But their use in off line optimal control is relatively limited and mainly focussed on parametric uncertainty. Other strategies which exploit the availability of measurements to ensure robustness [10], [17], [22] are not considered in the current paper.

The aims of the current paper are the following. First, it discusses approximation strategies for the uncertainty propagation of through dynamic systems. Two different approaches are exploited: a traditional linearization approach and a novel technique based on the unscented transformation. Second, it presents the different formulations in detail for the resulting robust optimal control problems which include the effect of uncertainty on the objective and/or constraints satisfaction. The link to well-known estimation schemes is highlighted. Both approaches lead to larger optimal

*This work was not supported by any organization

¹Dries Telen, Mattia Vallerio, Lorenzo Cabianca, Jan Van Impe, and Filip Logist are with KU Leuven, Department of Chemical Engineering, Willem de Croylaan 46, B-3001 Leuven-Heverlee, Belgium. Contact: jan.vanimpe@cit.kuleuven.be

²Boris Houska is with Shanghai Tech University, School of Information Science and Technology, No. 8 Building, 319 Yueyang Road, Shanghai 200031, China

control formulation compared with the nonrobust case. Computational details are also illustrated on a benchmark case study.

The paper is structured as follows. The description of dynamic systems and solution approaches of optimal control problems are presented in Section II. The formulation of (i) the chance constraints and (ii) the uncertainty in the objective function based on the linearization and sigma point technique for the presence of process noise is discussed in Section III. The mathematical formulations are clearly presented in this section, together with a discussion on the computational effort. In Section IV, the employed case study is introduced while the obtained numerical results are described in Section V. The conclusions are presented in Section VI.

II. DYNAMIC SYSTEMS

Consider the following dynamic optimization problem in the interval $\xi \in [0, \xi_f]$:

$$\min_{u(\cdot), x(\cdot), \xi_f} M(x(\xi_f), p, w(\xi_f)) \quad (1)$$

subject to:

$$\dot{x}(\xi) = f(x(\xi), p, u(\xi), w(\xi)), \quad (2)$$

$$0 = b_c(x(0)), \quad (3)$$

$$0 \geq c_p(x(\xi), p, u(\xi)), \quad (4)$$

$$0 \geq c_t(x(\xi_f), p). \quad (5)$$

Here, $x(\xi) \in \mathbb{R}^{n_x}$ denotes the state vector, $p \in \mathbb{R}^{n_p}$ a time-invariant parameter vector, $w \in \mathbb{R}^{n_w}$ is a time-varying white noise signal disturbing the process right hand side, i.e., the process noise and $u(\xi) \in \mathbb{R}^{n_u}$ is the control input. All these variables enter the right hand side function f in a possibly nonlinear way. The function M is called a Mayer term. Without loss of generality it is assumed that problems containing a so-called Lagrange term are rewritten such that only Mayer terms are present. The function b_c denotes the initial conditions of the system while the vectors c_p and c_t describe the path and terminal inequality constraints.

III. COMPUTING THE EFFECT OF PROCESS NOISE

The effect of process noise is quantified in this section. It is assumed that there is a Gaussian, white noise signal $w(\xi)$ present in the process with zero mean and variance-covariance matrix $W(\xi)$. In the first subsection a linearization approach is presented while in the second a novel approach based on the unscented transformation is described. Each time the link with uncertainty propagation in classic estimation algorithms is highlighted.

A. The linearization approach

A linear approximation of the states' variance-covariance matrix can be computed as the solution of the following

equation [14]:

$$\dot{P}_{\text{LIN}}(\xi) = A(\xi)P_{\text{LIN}}(\xi) + P_{\text{LIN}}(\xi)A^\top(\xi) + B(\xi)W(\xi)B(\xi)^\top, \quad (6)$$

$$P(0) = P_0. \quad (7)$$

Here, the matrices $A(\xi)$ and $B(\xi)$ denote:

$$A(\xi) = \frac{\partial f(x(\xi), p, u(\xi), 0)}{\partial x}, \quad (8)$$

$$B(\xi) = \frac{\partial f(x(\xi), p, u(\xi), 0)}{\partial w}. \quad (9)$$

The matrix P_0 is the initial variance-covariance matrix of the states. It has to be noted that the above expression corresponds to the variance prediction without measurements exploited in the classic (continuous) extended Kalman filter (EKF) [11]. Although the EKF is widely known, applications of the variance prediction in view of robust control are still scarce [21].

The total number of additional states for the above approach if symmetry in the variance-covariance matrix is exploited, is $\frac{n_x}{2}(n_x + 1)$.

Formulation 1: the extended Kalman filter approach: The propagation of the states' uncertainty can be used to make the optimal control problem more robust with respect to path constraint violations. The constraints are reformulated as:

$$0 \geq c_p(x(\xi), p, u(\xi))_i + \alpha_c \sqrt{C_i(\xi)P_{\text{LIN}}(\xi)C_i(\xi)^\top} \quad (10)$$

in which $C(\xi)$ is defined as:

$$C(\xi) = \frac{\partial c_p(x(\xi), p, u(\xi))}{\partial x}, \quad (11)$$

where $C_i(\xi)$ denotes the i -th row of the matrix $C(\xi)$. Here i runs over all constraint components. Terminal constraints are reformulated similarly:

$$0 \geq c_t(x(\xi_f), p)_i + \alpha_t \sqrt{D_i(\xi)P_{\text{LIN}}(\xi)D_i(\xi)^\top} \quad (12)$$

in which:

$$D(\xi) = \frac{\partial c_t(x(\xi_f), p, \xi_f)}{\partial x}. \quad (13)$$

An additional term is introduced in the constraints which provides a *backoff* value [7] to cope with the uncertainty in the constraints. The importance of the backoff can be managed by varying α_c and α_t . If the considered constraints can be assumed to be normally distributed, α_c and α_t can be chosen such that a predefined probability level is reached. It can be interpreted as the confidence level that is associated with the single-chance probability of a constraint violation.

The propagation of the states' uncertainty can also be used to account for robustness with respect to the objective function. The uncertainty on the objective function can be computed as:

$$M(x(\xi_f), p, 0) + \alpha_o \sqrt{\frac{\partial M(x(\xi_f), p, 0)}{\partial x} P_{\text{LIN}}(\xi_f) \frac{\partial M(x(\xi_f), p, 0)}{\partial x}^\top}}. \quad (14)$$

The additional term takes the uncertainty on the objective function [22], [14] into account and indicates a performance loss compared to the nominal case. If the Mayer term can be assumed to be normally distributed, α_o can again be chosen such that a predefined probability level is reached. The *robust optimization problem* becomes:

$$\min_{u(\cdot), x(\cdot), P_{\text{LIN}}(\cdot), \xi_f} M(x(\xi_f), p, 0) + \alpha_o \sqrt{\frac{\partial M(x(\xi_f), p, 0)}{\partial x} P_{\text{LIN}}(\xi_f) \frac{\partial M(x(\xi_f), p, 0)}{\partial x}^\top} \quad (15)$$

subject to:

$$\dot{x}(\xi) = f(x(\xi), u(\xi), p, 0), \quad (16)$$

$$0 = b_c(x(0)), \quad (17)$$

$$\dot{P}_{\text{LIN}}(\xi) = A(\xi)P_{\text{LIN}}(\xi) + P_{\text{LIN}}(\xi)A^\top(\xi) + B(\xi)W(\xi)B(\xi)^\top, \quad (18)$$

$$P(0) = P_0, \quad (19)$$

$$0 \geq c_p(x(\xi), p, u(\xi))_i + \alpha_c \sqrt{C_i(\xi)P_{\text{LIN}}(\xi)C_i(\xi)^\top} \quad \text{with } i = 1 \dots, n_{c_p}, \quad (20)$$

$$0 \geq c_t(x(\xi_f), p)_i + \alpha_t \sqrt{D_i(\xi)P_{\text{LIN}}(\xi)D_i(\xi)^\top} \quad \text{with } i = 1 \dots, n_{c_t}. \quad (21)$$

B. The unscented transformation approach

A different, novel strategy is to use the continuous unscented transformation approach or sigma point approach to compute the propagation of the uncertainty due to process noise. This approach is based on the idea that by propagating well chosen points, i.e., the sigma points through a nonlinear function an accurate estimate of the statistical distribution after a nonlinear function can be obtained. It has to be noted that this realization exploits the variance prediction without measurements as used in the unscented Kalman filter (UKF) [21]. This filter can be implemented in its standard form or in its square root form. The problem with the standard form, is that it involves the computation of a matrix square root which can lead to numerical issues for the computation of derivatives, required in the optimal control formulation of this paper. Each of the individual sigma point states can be computed as:

$$\dot{X}_i(\xi) = f(X(\xi), p, u(\xi), 0)w_m + \sqrt{n_x + \kappa} [0 \quad R(\xi)\Phi(T(\xi)) \quad -R(\xi)\Phi(T(\xi))]_i \quad \text{with } i = 0, \dots, 2n_x, \quad (22)$$

$$0 = b_c(X_0(0)), \quad (23)$$

$$X_i(0) = X_0(0) + \sqrt{n_x + \kappa} R_i(0) \quad \text{with } i = 1, \dots, n_x, \quad (24)$$

$$X_i(0) = X_0(0) - \sqrt{n_x + \kappa} R_{i-n_x}(0) \quad \text{with } i = n_x + 1, \dots, 2n_x, \quad (25)$$

here the matrix of the sigma points with dimensions $n_x \times (2n_x + 1)$, is defined as:

$$X(\xi) = [X_0(\xi) \quad X_0(\xi) \quad \dots \quad X_0(\xi) + \sqrt{n_x + \kappa} [0 \quad R(\xi) \quad -R(\xi)], \quad (26)$$

and the term $T(\xi) =$

$$R^{-1}(\xi)[X(\xi)W_m f^\top(X(\xi), p, u(\xi), 0) + f(X(\xi), p, u(\xi), 0)W_m X^\top(\xi) + W(\xi)]R^{-\top}(\xi), \quad (27)$$

while $R(\xi)$ is the lower triangular Cholesky factor of the states' variance-covariance matrix, i.e., $P_{SP}(\xi) = R(\xi)R(\xi)^\top$. The function $\Phi(\cdot)$ is a function that returns the lower diagonal part of the argument [21]. The expression $f(X(\xi), p, u(\xi), 0)$ is the evaluation of the model right hand side for each column of $X(\xi)$, resulting in an expression of dimensions $n_x \times (2n_x + 1)$. The vector w_m is defined as:

$$w_m = \left[\frac{\kappa}{\kappa + n_x} \quad \frac{1}{2(\kappa + n_x)} \quad \dots \quad \frac{1}{2(\kappa + n_x)} \right]^\top \quad (28)$$

while the matrix W_m is:

$$W_m = (I - [w_m \quad w_m \quad \dots \quad w_m]) \text{diag}(w_m) (I - [w_m \quad w_m \quad \dots \quad w_m])^\top. \quad (29)$$

The columns of $R(\xi)$ can be easily computed as:

$$R_i(\xi) = \frac{1}{\sqrt{n_x + \kappa}} (X_i(\xi) - X_0(\xi)) \quad \text{with } i = 1, \dots, n_x. \quad (30)$$

The states X_0 are the non-convex weighted sum average evolution of the states. In the following formulation the predicted variance-covariance matrix is used to obtain a robust optimal control formulation.

Formulation 2: the unscented Kalman filter approach:
The *robust optimization problem* becomes:

$$\min_{u(\cdot), X(\cdot), \xi_f} M(X_0(\xi_f), p, 0) + \alpha_o \sqrt{\frac{\partial M(X_0(\xi_f), p, 0)}{\partial X_0} P_{\text{SP}}(\xi_f) \frac{\partial M(X_0(\xi_f), p, 0)}{\partial X_0}^\top} \quad (31)$$

subject to:

$$\dot{X}_i = f(X(\xi), p, u(\xi), 0)w_m + \sqrt{n_x + \kappa} [0 \quad R(\xi)\Phi(T(\xi)) \quad -R(\xi)\Phi(T(\xi))]_i \quad \text{with } i = 0, \dots, 2n_x, \quad (32)$$

$$0 = b_c(X_0(0)), \quad (33)$$

$$X_i(0) = X_0(0) + \sqrt{n_x + \kappa} R_i(0) \quad \text{with } i = 1, \dots, n_x, \quad (34)$$

$$X_i(0) = X_0(0) - \sqrt{n_x + \kappa} R_{i-n_x}(0) \quad \text{with } i = n_x + 1, \dots, 2n_x, \quad (35)$$

$$T(\xi) = R^{-1}(\xi) \left[X(\xi)W_m f^\top(X(\xi), p, u(\xi), 0) + f(X(\xi), p, u(\xi), 0)W_m X^\top(\xi) + W(\xi) \right] R^{-\top}(\xi), \quad (36)$$

$$X(\xi) = [X_0(\xi) \ X_0(\xi) \ \cdots \ X_0(\xi)] + \sqrt{n_x + \kappa} [0 \ R(\xi) \ -R(\xi)], \quad (37)$$

$$R_i(\xi) = \frac{1}{\sqrt{n_x + \kappa}} (X_i(\xi) - X_0(\xi)) \text{ with } i = 1, \dots, n_x, \quad (38)$$

$$P_{\text{SP}}(\xi) = R(\xi)R^\top(\xi), \quad (39)$$

$$0 \geq c_{p,i} + \alpha_c \sqrt{\frac{\partial c_{p,i}}{\partial X_0} P_{\text{SP}}(\xi) \frac{\partial c_{p,i}}{\partial X_0}^\top} \text{ with } i = 1 \dots, n_{c_p}, \quad (40)$$

$$0 \geq c_{t,i} + \alpha_c \sqrt{\frac{\partial c_{t,i}}{\partial X_0} P_{\text{SP}}(\xi_f) \frac{\partial c_{t,i}}{\partial X_0}^\top} \text{ with } i = 1 \dots, n_{c_t}. \quad (41)$$

Here $c_{p,i}$ and $c_{t,i}$ denote the path and terminal constraints evaluated at X_0 , i.e., $c_{p,i}(X_0(\xi), p, u(\xi))$ and $c_{t,i}(X_0(\xi_f), p)$. The total number of additional differential equations for the extended Kalman filter approach is $n_x \frac{n_x+1}{2}$ if the symmetry is exploited while the unscented Kalman filter approach results in $n_x(2n_x)$ additional equations. The overview of the number of required states is presented in Table I. Both approaches significantly increase the size of the optimization problem to account for the uncertainty. Remark that the sigma point approach leads to a larger optimization problem where all sigma points are influencing the average state profile while in the linearization, the variance-covariance matrix does not influence the state profile. An advantage of the two presented methods is that they enable the use of fast deterministic gradient based optimization schemes.

TABLE I
OVERVIEW OF THE NUMBER OF STATES REQUIRED FOR THE
LINEARIZATION AND SIGMA POINT APPROACH.

	Nonrobust	Linearization	Sigma point
Original	n_x	n_x	n_x
Added	0	$\frac{n_x}{2}(n_x + 1)$	$2n_x^2$
Total	n_x	$\frac{n_x}{2} + \frac{3}{2}n_x$	$2n_x^2 + n_x$

Remark

Parametric uncertainty, i.e., uncertainty in the model parameters, can also be tackled using the aforementioned linearization and sigma point approaches. To this extent, uncertain parameters p with a given variance-covariance matrix are reformulated as additional trivial differential states ($\dot{p} = 0$ with $p(0) = p$ [24]). This will increase the computational effort but allows for an elegant formulation to incorporate the parametric uncertainty. A similar approach for optimal experiment design has been successfully illustrated in [23].

IV. CASE STUDY

A. Model description

The case study involves a jacketed tubular reactor under steady-state conditions. Inside the reactor an irreversible first-order reaction takes place. The mass and energy balances give rise to two coupled ordinary differential equations. However, the steady-state scenario is described by an ordinary differential equation in the spatial coordinate z denoting the position along the reactor, as the time-dependence is eliminated [14].

$$\frac{dx_1}{dz} = \frac{\alpha_{\text{kin}}}{v} (1 - x_1) e^{\frac{\gamma x_2}{1+x_2}} + w_1, \quad (42)$$

$$\frac{dx_2}{dz} = \frac{\alpha_{\text{kin}} \delta}{v} (1 - x_1) e^{\frac{\gamma x_2}{1+x_2}} + \frac{\beta}{v} (u - x_2) + w_2, \quad (43)$$

and with initial conditions:

$$x(0) = (0, 0)^\top, \quad (44)$$

and constraints:

$$\frac{T_{\text{min}} - T_{\text{in}}}{T_{\text{in}}} \leq x_2(z) \leq \frac{T_{\text{max}} - T_{\text{in}}}{T_{\text{in}}}, \quad (45)$$

$$\frac{T_{w,\text{min}} - T_{\text{in}}}{T_{\text{in}}} \leq u(z) \leq \frac{T_{w,\text{max}} - T_{\text{in}}}{T_{\text{in}}}. \quad (46)$$

The states are the dimensionless reactant concentration $x_1 = (C_{\text{in}} - C)/C_{\text{in}}$ and the dimensionless reactor temperature $x_2 = (T - T_{\text{in}})/T_{\text{in}}$. The symbols w_1 and w_2 denote the process noise present in the model equations. Here, T_{in} and C_{in} are the temperature and the reactant concentration of the feed stream, respectively. The control $u = (T_w - T_{\text{in}})/T_{\text{in}}$ is a dimensionless version of the jacket temperature T_w . Bounds are imposed on the reactor and jacket temperatures (Equations (45) and (46)) while the length of the reactor L is fixed to 1, i.e., the differential equations are regarded on the interval $z \in [0, 1]$. The objective is to minimize the following function which relates to the maximization of the conversion:

$$C_{\text{in}}(1 - x_1(L)). \quad (47)$$

The number of equidistant control intervals is set to 100. The assumed variance-covariance matrix for the process noise is:

$$W = \begin{pmatrix} 0.001 & 0 \\ 0 & 0.001 \end{pmatrix}. \quad (48)$$

For the remaining expressions and parameter values, the reader is referred to [14].

B. Implementation details

Optimal control problems are infinite dimensional as an optimal value for the controls has to be found at almost every point in time. To convert the infinite dimensional optimization problem to a finite dimensional problem and to cope with a large number of states, a first discretize then optimize approach is selected in the current paper [2].

For the optimal control problems a single shooting approach is employed. The main reason to do so, is to

avoid numerical problems in the unscented Kalman filter as a matrix inverse is present. This means that only the control action is discretized [20] and the states are obtained through numerical integration. The problem is formulated in ACADO [8], which is an open source self-contained software tool for formulating and solving optimal control problems using single or multiple shooting schemes. Due to its symbolic implementations exact second order derivatives are obtained. The resulting nonlinear programming problem is solved using a SQP algorithm [6]. The integrator tolerances are set to 10^{-6} while the KKT tolerance is set to 10^{-5} .

V. SIMULATION RESULTS

The following constraints are added for the robust approaches:

$$x_2(z) - 1.96\sqrt{P_{x_2x_2,LIN}(z)} \geq \frac{T_{\min} - T_{\text{in}}}{T_{\text{in}}}, \quad (49)$$

while for the sigma point approach the following constraints are considered:

$$X_{20}(z) + 1.96\sqrt{P_{22,SP}(z)} \leq \frac{T_{\max} - T_{\text{in}}}{T_{\text{in}}}, \quad (50)$$

$$X_{20}(z) - 1.96\sqrt{P_{22,SP}(z)} \geq \frac{T_{\min} - T_{\text{in}}}{T_{\text{in}}}, \quad (51)$$

where α_c is chosen to be equal to 1.96 which reflects that if the constraint profile is normally distributed, a 95% confidence region should be obtained. The number of required states and variables in addition to the computational time for the different approaches are given in Table II. Note that the robust approaches require more computational time compared with the nonrobust case. The sigma point approach requires even more time as all states are influencing each other, while in the linearization method the states influence the variance-covariance matrix but not vice versa.

TABLE II

OVERVIEW OF THE NUMBER OF STATES AND VARIABLES REQUIRED FOR EACH APPROACH.

Process noise	Nonrobust	Linearization	Sigma point
Original	2	2	2
Added	0	3	4
Total states	2	5	6
Total variables	100	100	100
Total CPU time	1.98 s	5.3 s	24.0 s

The obtained reactor and temperature profiles for both nonrobust and robust cases are depicted in Figures 1 and 3. The predicted confidence region for the linearization and sigma point approach is also provided in Figure 1. Note that for the nominal temperature profile the temperature constraint is active in 70% of the reactor length while the robust cases clearly back off from the temperature upper bound as the confidence region is considered. The difference between the nonrobust and robust control actions is also clear from Figure 3. The nominal case leads to a longer

heating period with a singular arc for the remaining part of the integration interval to maintain the reactor temperature at the upper bound. It can, however, be observed that both robust approaches lead to similar control actions and predicted state evolutions. They both have a shorter heating period and the remaining control aims to keep to upper confidence bound at the temperature upper bound.

The three approaches are also compared by a Monte Carlo simulation. In total 200 process noise realizations are drawn with the assumed statistical distribution and applied to the system. The number of constraint violations are given in Table III. The nominal control action violates the constraints in 93% of the cases, while the linearization and unscented transformation approach perform better with 16-19% of violations. This is significantly more than the 5% which is the target aim. A closer investigation of the obtained state profiles, reveals that they cannot be assumed to be normally distributed. This means that the chosen quantile value does not necessarily lead to only 5% of violations. The empirical confidence regions are illustrated in Figure 2. These are violating the bounds in several places illustrating the challenging aspect of accounting for process noise. The objective function value for the two robust approaches are 0.066 for the linearization and 0.070 for the unscented transformation approach, which is remarkably worse compared with the nominal case, i.e., 0.006.

TABLE III

OVERVIEW OF THE NUMBER OF CONSTRAINT VIOLATIONS FOR EACH APPROACH OUT OF 200 PROCESS NOISE REALIZATIONS.

Number of violations	Nonrobust	Linearization	Sigma point
Normally distributed	186 [93.0%]	38 [19.0%]	32 [16.0%]

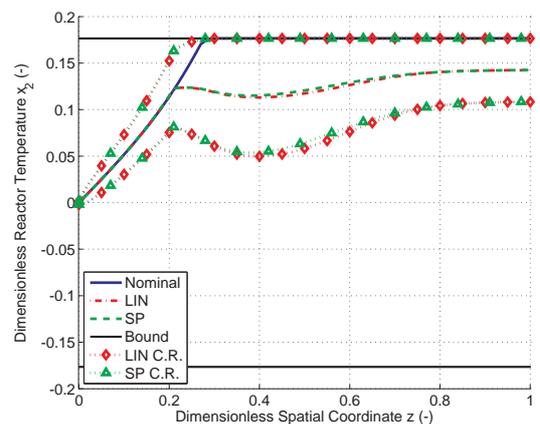


Fig. 1. Evolution of the reactor temperature profile x_2 with predicted 95% confidence bounds for the nonrobust case and both the linearization and sigma point approach.

VI. CONCLUSIONS

In this paper two different approaches for approximate robust nonlinear optimal control are discussed in the presence

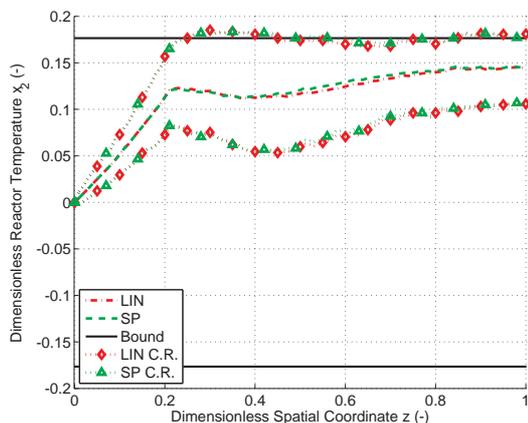


Fig. 2. The empirically observed 95% confidence bound for the reactor temperature x_2 for the two robust approaches.

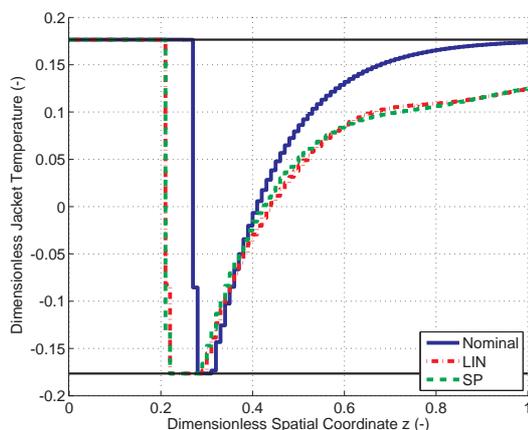


Fig. 3. Control action for the nonrobust case and both the linearization and sigma point approach.

of process noise. Both methods allow a tractable computation of an approximation of the variance-covariance matrix of the constraints and/or the objective function. This variance-covariance matrix allows the formulation of single chance constraints such that critical constraints are satisfied in a stochastic way. Both approaches lead to a larger optimization problems which is more challenging to solve. To assess the quality of the approximate robust optimal control profiles, Monte Carlo simulations can be used to check whether a desired probability level is reached without the need of using Monte Carlo simulations explicitly in the optimization routine. The presented approaches are illustrated with a jacketed tubular reactor.

ACKNOWLEDGMENT

DT and MV each hold an IWT-PhD grant. JVI holds the chair Safety Engineering sponsored by essenscia. The research was supported by: PFV/10/002 (OPTEC), OT/10/035, FWO KAN2013 1.5.189.13, FWO-G.0930.13 and BelSPO: IAP VII/19 (DYSCO).

REFERENCES

[1] S.P. Asprey and S. Macchietto. Designing robust optimal dynamic experiments. *Journal of Process Control*, 12(4):545 – 556, 2002.

[2] L.T. Biegler. An overview of simultaneous strategies for dynamic optimization. *Chemical Engineering and Processing: Process Intensification*, 46:1043–1053, 2007.

[3] I. Datskov, G. Ostrovsky, L. Achenie, and Y. Volin. An approach to multicriteria optimization under uncertainty. *Chemical Engineering Science*, 61:2379 – 2393, 2006.

[4] M. Diehl, J. Gerhard, W. Marquardt, and M. Mönnigmann. Numerical solution approaches for robust nonlinear optimal control problems. *Computers and Chemical Engineering*, 32:1287–1300, 2008.

[5] U.M. Diwekar and Kalagnanam. Efficient sampling technique for optimization under uncertainty. *Chemical Engineering and Processing*, 43:440–447, 1997.

[6] H.J. Ferreau, C. Kirches, A. Potschka, H.G. Bock, and M. Diehl. qpOASES: a parametric active-set algorithm for quadratic programming. *Mathematical Programming Computation*, DOI 10.1007/s12532-014-0071-1, 2014.

[7] F. Galvanin, M. Barolo, F. Bezzo, and S. Macchietto. A backoff strategy for model-based experiment design under parametric uncertainty. *AIChE Journal*, 56:2088–2102, 2010.

[8] B. Houska, H.J. Ferreau, and M. Diehl. ACADO Toolkit - an open-source framework for automatic control and dynamic optimization. *Optimal Control Applications and Methods*, 32:298–312, 2011.

[9] B. Houska, F. Logist, J. Van Impe, and M. Diehl. Robust optimization of nonlinear dynamic systems with application to a jacketed tubular reactor. *Journal of Process Control*, 22:1152–1160, 2012.

[10] J.V. Kadam, M. Schlegel, B. Srinivasan, D. Bonvin, and W. Marquardt. Dynamic optimization in the presence of uncertainty: From off-line nominal solution to measurement-based implementation. *Journal of Process Control*, 17(5):389 – 398, 2007.

[11] R.E. Kalman and R.S. Bucy. New results in linear filtering and prediction theory. *Journal of Basic Engineering*, 83:95–108, 1961.

[12] M. Kawohl, T. Heine, and R. King. A new approach for robust model predictive control of biological production processes. *Chemical Engineering Science*, 62:5212 – 5215, 2007.

[13] P. Li, H. Arellano-Garcia, and G. Wozny. Chance constrained programming approach to process optimization under uncertainty. *Computers and Chemical Engineering*, 32:25 – 45, 2008.

[14] F. Logist, B. Houska, M. Diehl, and J.F. Van Impe. Robust multi-objective optimal control of uncertain (bio)chemical processes. *Chemical Engineering Science*, 66(20):4670 – 4682, 2011.

[15] Z.K. Nagy and R.D. Braatz. Open-loop and closed-loop robust optimal control of batch processes using distributional and worst-case analysis. *Journal of Process Control*, 14:411–422, 2004.

[16] Z.K. Nagy and R.D. Braatz. Distributional uncertainty analysis using power series and polynomial chaos expansions. *Journal of Process Control*, pages 229–240, 2006.

[17] M. Podmajersky, M. Fikar, and B. Chachuat. Measurement-based optimization of batch and repetitive processes using an integrated two-layer architecture. *Journal of Process Control*, 23(7):943 – 955, 2013.

[18] S. Recker, P. Kühl, M. Diehl, and H.G. Bock. Sigmamethod approach for robust optimization of nonlinear dynamic systems. In *Proceeding of SIMULTECH 2012*, pages 199–207, 2012.

[19] N.V. Sahinidis. Optimization under uncertainty: state-of-the-art and opportunities. *Computers and Chemical Engineering*, 28:971–983, 2004.

[20] R.W.H. Sargent. Optimal control. *Journal of Computational and Applied Mathematics*, 124:361–371, 2000.

[21] S. Särkkä. On unscented kalman filtering for state estimation of continuous-time nonlinear systems. *IEEE Transactions on automatic control*, 52:1631–1641, 2007.

[22] B. Srinivasan, D. Bonvin, E. Visser, and S. Palanki. Dynamic optimization of batch processes II. Role of measurements in handling uncertainty. *Computers and Chemical Engineering*, 27:27–44, 2003.

[23] D. Telen, B. Houska, F. Logist, E. Vanderlinden, M. Diehl, and J. Van Impe. Optimal experiment design under process noise using Riccati differential equations. *Journal of Process Control*, 23:613–629, 2013.

[24] J. Valappil and Ch. Georgakis. Accounting for batch reactor uncertainty in the nonlinear MPC of end-use properties. *AIChE Journal*, 49(5):1178–1192, 2003.

[25] M. Wendt, P. Li, and G. Wozny. Nonlinear chance-constrained process optimization under uncertainty. *Industrial and Engineering Chemistry Research*, 41:3621–3629, 2002.