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Economic performance analysis in the design of on-line batch optimization systems

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Abstract

In this paper, the on-line optimization of batch reactors under parametric uncertainty is considered. A method is presented that estimates the likely economic performance of the on-line optimizer. The method of orthogonal collocation is employed to convert the differential algebraic optimization problem (DAOP) of the dynamic optimization into a nonlinear program (NLP) and determine the nominal optimum. Based on the resulting NLP, the optimization steps are approximated by neighbouring extremal problems and the average deviation from the true process optimum is estimated dependent on the measurement error and the parametric uncertainty. The true process optimum is assumed to be represented by the optimum of the process model with the true parameter values. A back off from the active path and endpoint inequality constraints is determined at each optimization step which ensures the feasible operation of the process. Based on the analysis results the optimal structure of the optimizer in terms of measured variables and estimated parameters can be determined. The method of the average deviation from optimum is developed for the fixed terminal time case and for time optimal problems. In both cases, the theory is demonstrated on an example.

Keywords: Batch reactor; On-line optimization; Parametric uncertainty; Structural decisions

Notation

A_i	sensitivity matrix of optimal input variables at EOT i
B_i	sensitivity matrix of optimal input variables at EOT i
c	concentration, (mol/l)
C_i	objective function sensitivity matrices
D_i	sensitivity matrix of parameter estimates at EOT i
E_i	sensitivity matrix of parameter estimates at EOT i
f	nonlinear function or probability density function
f	feed rate to semi-batch reactor, (l/min)
F	system of nonlinear equations of collocated dynamic system
F_i	sensitivity matrix of optimal input variables at EOT i
g	nonlinear constraint functions
G_i	constraint sensitivity matrix at EOT i
H_i	constraint sensitivity matrix at EOT i
J_i	measurement sensitivity matrix at EOT i
k	reaction rate constant, (l/(mol min))
n_{SE}	number of super-elements
p	parameter vector
P_i	permutation matrix
P_Q	least squares projection matrix
q	permutation vector to eliminate inputs not applied to the process
Q	least squares objective function weighting matrix (square root of inverse of measurement error covariance matrix)
r	reaction rate, (mol/(l min))
t	time
t_f	final batch time, (min)
u	manipulated variable vector
v_R	holdup in the reactor, (l)
W	least squares objective function weighting matrix (square root of inverse of parameter uncertainty covariance matrix)
x	state variable vector
y	output variable vector
α	probability

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β vector of constraint back offs
δ perturbation variable around nominal optimum
ε vector of normally distributed measurement error
η vector of normally distributed parameter uncertainty
Θ average deviation from optimum
ν vector of approximation coefficients of input variable profiles
ξ vector of approximation coefficients of state variable profiles
σ standard deviation
Φ economic objective function
Ψ constraint covariance matrix

Subscripts

e estimated
i variable or variable sensitivity at EOT i

Superscripts

$-$ variable or variable sensitivity in the past at EOT i
$*$ optimal value
$\hat{}$ estimate, i.e. $\hat{p}$ is an estimate of p

1. Introduction

A wide variety of products in the chemical industries are produced in batch mode. Due to disturbances during operation and uncertainties in process parameters, such as reaction kinetic parameters, there is a danger of producing unsatisfactory batches where the product or safety specifications are not met and path or endpoint constraints are violated. Additionally, it is desired to operate the process maximizing an economic objective function, such as the yield of the desired product. These issues can be tackled using model-based optimization techniques.

One approach is based on robust optimization strategies, where an optimal operating policy is determined off-line, while considering the parameter uncertainty. Alternative strategies include expected value optimization, where the expected value of the objective function under uncertainty is optimized, rather than the objective function dependent on the expected value of the uncertain parameters which is also called nominal optimization [1,2]. This approach improves on the nominal approach but can still be suboptimal or yield unsatisfactory batches if the optimum or the constraints are very sensitive to the uncertain parameters. Another option is risk-conscious optimization, where the risk of making an unsatisfactory product is minimized [2]. Although this approach guarantees satisfactory batches for a high probability, it usually yields an economically suboptimal operating policy [2]. Since all these strategies do not make use of information from the process during its operation, an alternative is the batch-to-batch improvement using tendency models [3,4]. A tendency model is a so-called grey box model where an approximate model is developed using the available information of the process. The process information might not be complete as is the case for rigorous or white models [3]. The process is optimized by collecting process data during the operation of the batch and using this information to improve the modelling of the process. The updated model is then optimized and the optimal input trajectory is applied to the next batch. This batch-to-batch improvement is repeated until a reliable model of the process is obtained. Another approach to the improved operation of batch processes is on-line optimization. Process information is acquired on-line, by measuring one or more process variables, and used to determine an improved operating policy for the rest of the batch. Two approaches can be distinguished. The first option consists of deriving an analytical optimal feedback law, which determines the optimal inputs dependent on the current states of the system, as proposed by Rahman and Palanki [5]. Every time new state estimates are obtained, the new optimal input policy is given by the analytical feedback law. The drawback of this method is that the analytical feedback laws may be quite complex expressions for bigger systems. One alternative is to obtain the improved input profile through numerical reoptimization of the process model, as reported by Ruppen et al. [6]. The state and control variables are parametrized by polynomials, thus transforming the differential optimization problem into an algebraic one, which can be solved using successive quadratic or linear programming methods. This results in the following on-line optimization scheme which consists of two steps, as depicted in Fig. 1. In a first step, the process model is identified or updated by estimating the state variables and/or a set of parameters using past and present process measurements. The updated model is then optimized with respect to the manipulated variables and a new optimal input trajectory over the remaining time horizon is determined. This sequence of an estimation and optimization step is referred to in the following as an Estimation-Optimization-Task, EOT [6]. The first part of the calculated input

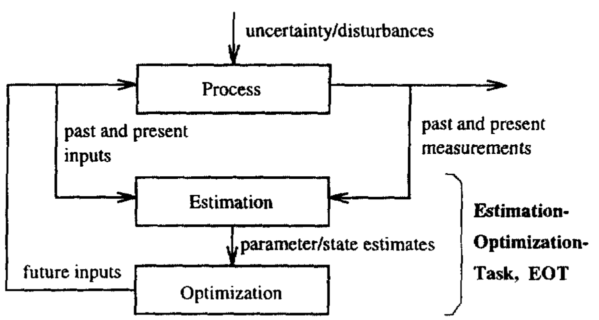

Fig. 1. General structure of an on-line batch optimization system.

trajectory is applied to the process until a new EOT is carried out at some future point in time. Since after each EOT only the first part of the calculated input trajectory is applied to the process, the strategy is similar to the moving or receding horizon principle of model predictive control [7]. The difference is, however, that the size of the prediction horizon during the on-line optimization of the batch process changes at each EOT because the batch process is a discontinuous process and its operation is only considered until the final batch time. Another similarity to model predictive control is the closed-loop feedback structure of the on-line optimizer. On-line optimization as described above can also be referred to as a nonlinear model predictive control. If the EOTs are carried out very frequently, it resembles conventional feedback control [6]. However, this is usually not possible due to the nonlinearity of the models used for estimation and optimization. Their evaluation is in general too time consuming to obtain a frequency of operation similar to linear feedback control or model predictive control algorithms based on linear models.

The purpose of this paper is to analyse the economic performance of a given structure of an on-line optimization system, as shown in Fig. 1, in order to design an on-line optimizer for a particular application. The structure is defined by the estimated parameters and the measurements taken for estimation. Based on the analysis results, the structure with the best economic performance can be chosen for implementation. The nonlinear problem is approximated and an analytical expression is derived, which gives an estimation of how close to the true process optimum the process can be operated in the presence of different error sources. The organization of the paper is as follows. The next section gives a brief description of the solution of dynamic optimization problems using the method of orthogonal collocation. Following that, the theory of the method of the average deviation from optimum is described in some detail for both fixed terminal time and time optimal problems. Thereafter, the method is demonstrated on two examples. Finally, some conclusions complete the paper.

2. Method of orthogonal collocation

Since in batch processes the dynamic behaviour is dominating and usually no steady-state is reached, the objective function needs to be optimized with respect to the dynamic model equations:

$$\begin{aligned} &\min_{u,t_f} \Phi\big(x(t_f), t_f\big) \\ &s.t.\ \ \dot{x} = f(x, u, p, t),\ x(t_0) = x_0 \\ &\quad g(x, u, p, t) \le 0. \end{aligned} \tag{1}$$

The state variables are denoted by x, u are the control inputs and p the uncertain process parameters. The objective is the minimization of some function of the states at the final time, t_f, and/or the final time itself. Since besides the dynamic model equations, f, very often a set of algebraic path and endpoint inequality constraints, g, is present, this problem is called a differential algebraic optimization problem, DAOP.

The solution of this problem via the Hamiltonian [8] results in the solution of a two-point boundary value problem, TPBVP. These problems are numerically expensive to solve due to the explicit integration of the system at every iteration. Algebraic path and endpoint constraints and discontinuities in the input variables complicate the solution of the problem further.

One method that circumvents the numerically expensive integration of the system and allows the easy incorporation of algebraic path and endpoint constraints and discontinuities in the inputs is the method of orthogonal collocation [9,10]. In this method, the system is solved and optimized simultaneously. This is achieved by converting the DAOP into a nonlinear algebraic optimization problem, NLP. The conversion into an NLP consists of two steps: parametrization and discretization. In the first step, the state and input variable profiles, x and u, are approximated by polynomials parametrized by ξ and ν:

$$x(t) = X(\xi, t) = \sum_{i=0}^{K_x} \xi_i \prod_{k=0,i}^{K_x} \frac{t - t_{x,k}}{t_{x,i} - t_{x,k}} \tag{2}$$

$$u(t) = U(\nu, t) = \sum_{i=1}^{K_u} \nu_i \prod_{k=1}^{K_u} \frac{t - t_{u,k}}{t_{u,i} - t_{u,k}} \tag{3}$$

Due to the initial conditions for x, the degree of the polynomial approximating x should be at least one higher than the degree of the polynomial approximating u. In the second step, the dynamic model equations are discretized and the residual equations are enforced on a finite number of collocation points in order to obtain a finite dimensional problem:

$$\begin{aligned} &R\big(\xi, \nu, t_{x,i}\big) = \dot{X}\big(\xi, \nu, t_{x,i}\big) - f\big(\xi, \nu, p t_{x,i}\big) = 0, \\ &i = 1, \ldots, K_x. \end{aligned} \tag{4}$$

The collocation points, $t_{x,i}$, are chosen to be the roots of an orthogonal Legendre polynomial of degree K_x [9]. Together with the algebraic path and endpoint inequality constraints the DAOP (1) is converted into the following NLP in ξ, ν and t_f which can be solved with standard NLP solvers, e.g. sequential quadratic programming (SQP) methods:

$$\min_{\xi,\nu,t_f} \Phi(\xi,\nu,t_f) \tag{5}$$

$$\text{s.t. } R(\xi,\nu,t_{x,i}) = \dot{X}(\xi,\nu,t_{x,i}) - f(\xi,\nu,p,t_{x,i}) = 0, \ \forall t_{x,i}$$
$$g(\xi,\nu,p,t_{u,i}) \le 0, \ \forall t_{u,i}.$$

In this approach, the dynamic model equations are considered as algebraic equality constraints which only need to be satisfied at the final solution, but not at every iteration during the optimization. This is also referred to as an infeasible path method.

Usually the input and state variable profiles are approximated by piecewise polynomials on a number of finite elements. This can be seen in Fig. 2, where the time domain is partitioned into several finite elements denoted by FE. This improves the approximation of sharply changing profiles, where a global approximation would require a very high degree of the approximation polynomial. Furthermore, super-elements (SE) are introduced which allow the definition of discontinuities in the input variables, see Fig. 2. In this case, the continuity conditions for the input and state variable profiles at the boundaries of the finite elements and for the state variable profiles at the boundaries of the super-elements are added to the equations of the NLP (5). A detailed description of the method of orthogonal collocation can be found in the two papers by Cuthrell and Biegler [9,10].

3. Average deviation from optimum

Due to the different error sources which are present during on-line optimization, such as measurement errors and parametric uncertainties, the optimizer will usually not predict the true optimum, but there will be a deviation from the same. Therefore, the performance of an on-line batch optimization system depends on the available measurements together with their quality and the amount of uncertainty in the process parameters. For continuous processes, the method of the average deviation from optimum [11,12] was developed in order to estimate the likely economic performance of a given structure of an on-line optimization system. In this paper, the method of the average deviation from optimum is extended to the dynamic optimization of batch processes under uncertainty. It estimates the economic performance of an on-line optimization system by analysing how close to the true optimum it is possible to operate the process. The plant-model mismatch is assumed to consist only in the uncertain parameter values and no structural mismatch is present. The true process optimum is then assumed to be given by the optimum of the process model with the true parameter values. The performance of on-line optimization can be compared against off-line optimization and the economic benefit of on-line optimization identified. Also, the relative performance of different on-line optimization systems, involving for example different choices of measured and manipulated variables or different estimated parameters, may be compared. The error sources are described by a normally distributed measurement error, ε, with given standard deviation σ_ε and a normally distributed parameter uncertainty around a nominal value, η, with given standard deviation σ_η. The normally distributed error sources η and ε have zero mean and it is assumed that there is no covariance among η and ε. Furthermore, non-random measurement errors such as sensor biases or failures are not considered here.

In the analysis which follows it will be assumed that the optimization using orthogonal collocation is carried out with respect to piecewise constant, equally distributed input variables, see Fig. 3. This implies that the inputs are approximated by a zero order polynomial on equally distributed super-elements with one finite element defined on each super-element. The state variable profiles are approximated by first or higher order polynomials in order to give a good approximation of the system. Furthermore, the different EOTs are carried out at the discontinuities in the input variables. At these points in time, measurements are taken to update the estimates of a set of parameters. With the updated model parameters the process model is optimized and a new optimal input trajectory is determined over the remaining time horizon. The first element of the calculated input moves is then applied to the process until at the next discontinuity another EOT is carried out and

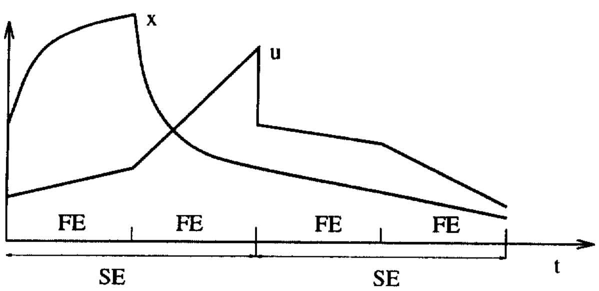

Fig. 2. Piecewise approximation of input and state profiles on finite elements and super-elements.

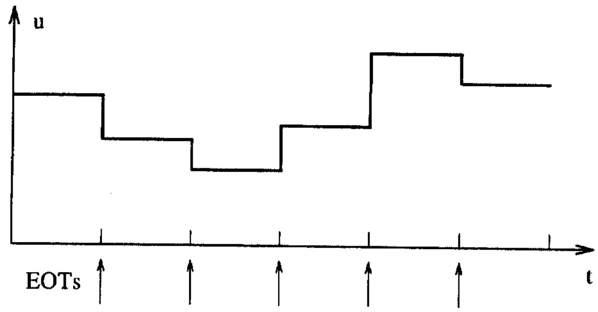

Fig. 3. Input profile and EOTs.

new optimal input variables are determined for the remaining super-elements in the future.

In the following sections, the method of the average deviation from optimum is derived for the optimization of batch reactors with a fixed final time, and for time optimal problems, where the objective is the minimization of the final batch time.

3.1. Fixed terminal time problems

With a specified final batch time and assuming that the dynamic model equations, f, and inequality constraints, g, are not explicitly dependent on the time t, the DAOP (1) reduces to:

$$\begin{aligned} &\min_u \ \Phi(x(t_f)) \\ &s.t.\ \dot{x} = f(x,u,p),\ x(t_0) = x_0 \\ &\quad g(x,u,p) \leq 0 \end{aligned} \tag{6}$$

In a first step towards the analysis, the nonlinear process model is optimized using the nominal parameter values. The nominal parameter values are the parameter values, around which the normally distributed uncertainty in the process parameters is defined. It is assumed that the plant-model mismatch consists only in the uncertain parameters and no structural modelling error is present. The method of orthogonal collocation is employed in order to obtain the nominal optimum.

3.1.1. First and second order approximation

Since the method of the average deviation from optimum is based on an approximation of the nonlinear problem, a first and second order perturbation model around the nominal trajectory is obtained from the collocated system. Due to this representation of the problem, both the estimation and the optimization steps can be solved analytically and the effect of the error sources can be mapped through the estimation and optimization steps in order to analyse their effect on the optimizer performance. The required perturbation model is obtained from a second order Taylor series expansion of the objective function, Φ, with respect to the approximation coefficients of the input variables and the uncertain process parameters after the equality constraints representing the collocated dynamic model equations are met. The set of the active path and endpoint inequality constraints, g, at the nominal optimum is linearized with respect to the inputs and uncertain parameters:

$$\delta\Phi = C_1\delta u + \delta p^T C_2 \delta u + \frac{1}{2}\delta u^T C_3 \delta u + C_4 \delta p + \frac{1}{2}\delta p^T C_5 \delta p \tag{7}$$

$$\delta g = G\delta p + H\delta u = 0 \tag{8}$$

In this formulation, δp is the perturbation variable of the uncertain process parameters around the nominal parameter values. Similarly, δu is the perturbation vector of the piecewise constant input variables around the inputs at the nominal optimum. The process variables which are measured for the parameter estimation at each EOT are linearized with respect to the uncertain process parameters:

$$\delta y = J\delta p \tag{9}$$

More details about the calculation of the first and second order perturbation model are given in Appendix A.1.1.

3.1.2. Least squares parameter estimation

The following minimization problem is solved in order to obtain estimates of the uncertain process parameters:

$$\begin{aligned} \min_{\delta\hat{p}_i}\ & (\delta y_i - \delta\hat{y}_i)^T Q_i^T Q_i (\delta y_i - \delta\hat{y}_i) \\ & + \left(\delta\hat{p}_{i,e} - \delta\hat{p}_{0,e}\right)^T W_e^T W_e \left(\delta\hat{p}_{i,e} - \delta\hat{p}_{0,e}\right) \\ \text{s.t.}\ & \delta\hat{y}_i = J_{i,e}\delta\hat{p}_{i,e} \\ & \delta y_i = J_i \delta p + \varepsilon_i \end{aligned} \tag{10}$$

The past model outputs are represented by $\delta\hat{y}_i$, while δy_i is the vector of all the measurements collected in the past with normally distributed measurement errors ε_i. The matrix $J_{i,e}$ is the appropriate submatrix of J_i according to the estimated parameters, $\delta\hat{p}_{i,e}$. The objective function is weighted with the covariances of the a priori parameter uncertainty and the measurement error. Since it is assumed that there is no covariance among η and ε, the matrices W_e and Q_i have the inverse of the standard deviations of the parametric uncertainty and the measurement error on the main diagonal, $W_e = \text{diag}(\sigma_{\eta_e}^{-1})$ and $Q_i = \text{diag}(\sigma_{\varepsilon_i}^{-1})$. In contrast to the parameter estimation of continuous processes, where prior information about the uncertain parameters is usually neglected, the a priori estimate of the uncertain parameters, $\delta\hat{p}_{0,e}$, is taken into account in the estimation objective function. Due to the linearization in Eq. (9), $\delta\hat{p}_0$ is zero as it represents the perturbation variable around the nominal parameter value, which is equal to the a priori estimate of the uncertain parameters. Because of this incorporation of a priori knowledge of the uncertain parameters into the parameter estimation problem, the covariance of the error in the parameter estimates can never be bigger than the covariance of the a priori uncertainty, regardless of the quality of the measurements. By considering the vector of all past measurements, this formulation allows the representation of the parameter estimates dependent on the measurement error and the a priori parameter uncertainty, which is necessary for the analysis of the average deviation from optimum. Introducing the normally distributed parameter uncertainty, $\delta p = \eta$, gives the following solution for the parameter estimate at EOT i:

$$\delta\hat{p}_i = D_i W^{\eta} + E_i Q_i \varepsilon_i \tag{11}$$

with

$$P_{Qi,e} = \left((Q_i J_{i,e})^T Q_i J_{i,e} + W_e^T W_e \right)^{-1} (Q_i J_{i,e})^T$$
$$D_i = \begin{bmatrix} P_{Qi,e} Q_i J_i \\ \hline 0 \end{bmatrix} W^{-1}$$
$$E_i = \begin{bmatrix} P_{Qi,e} \\ \hline 0 \end{bmatrix}$$

The location of the zeros in the matrices D_i and E_i indicates the parameters that are not estimated. The estimation problem can be equivalently reformulated in a recursive manner which can also be interpreted as a special case of the state estimation problem using a Kalman filter [13]. This is necessary in an on-line implementation of the algorithm, where it is not desired to store all past measurements, but update the current parameter estimate with every new measurement coming in during the operation of a batch. This also represents a main difference to the 'one-shot' strategy of the steady-state parameter estimation of continuous processes, where each set of measurements at different times contains the same amount of information and only the current set of measurements is used to estimate the uncertain parameters [12,14].

3.1.3. Optimization and back off from active inequality constraints

At every point in time, where an EOT is carried out, the optimal piecewise constant input variables over the remaining time horizon until the end of the batch are calculated using the current parameter estimates. In order to prevent the process constraints from being violated, once the calculated inputs have been applied to the process, some conservatism is introduced into the optimization in the form of a back off from the active inequality constraints.

For the analysis, the optimization step at each EOT is approximated by the solution of the following neighbouring extremal problem. It is obtained from the first and second order perturbation model of the objective function (7) and active inequality constraints (8) by considering the remaining degrees of freedom for optimization in the future at EOT i:

$$\begin{aligned} &\min_{\delta u_i} C_{i1}\delta u_i + \delta\hat{p}_i^T C_{i2}\delta u_i + \delta\bar{u}_i^T \bar{C}_{i2}\delta u_i + \frac{1}{2}\delta u_i^T C_{i3}\delta u_i \\ &\text{s.t. } \delta g_i(\delta u_i, \delta\bar{u}_i, \delta\hat{p}_i) = G_i\delta\hat{p}_i + \bar{H}_i\delta\bar{u}_i \\ &\qquad\qquad + H_i\delta u_i + \beta_i = 0 \end{aligned} \tag{12}$$

The vector δu_i is the vector of the remaining piecewise constant inputs in the future at EOT i and $\delta\bar{u}_i$ is the vector of the inputs, that were applied to the process in the past:

$$\delta u_i = [\delta u(i+1), \ldots, \delta u(n_{SE})]^T$$
$$\delta\bar{u}_i = [\delta u(1), \ldots, \delta u(i)]^T$$

Since the estimation of the state variables of the process is not considered in the parameter estimation step, the deviation of the state variables from their nominal values at EOT i is taken into account implicitly by including the past input variables, $\delta\bar{u}_i$, as a constant parameter vector into the optimization problem at EOT i. The sensitivity matrices $C_{i1}, C_{i2}, \bar{C}_{i2}$ and C_{i3} are the appropriate submatrices of the sensitivity matrices of the objective function in perturbation model (7), C_1, C_2 and C_3, according to the remaining piecewise constant inputs in the future and the applied inputs in the past, see Appendix A.1.2. Constant terms in the objective function which do not give a contribution to the optimization are ignored. A back off, β_i, from the active inequality constraints is introduced into the optimization at every EOT to ensure the feasible operation of the process.

This QP can be solved analytically in the reduced space and gives the following optimal inputs, dependent on the back off introduced, the current parameter estimates and the past inputs applied to the process:

$$\delta u_i^* = A_i\beta_i + B_i\delta\hat{p}_i + F_i\delta\bar{u}_i \tag{13}$$

Choosing a partition of $H_i = [H_{i1}\, H_{i2}]$ such that H_{i1} is square and nonsingular gives the following matrix definitions:

$$Z_i = \left[I - H_{i1}^{-1}H_{i2}\right]$$
$$S_i = -Z_i\left(Z_i^T C_{i3} Z_i\right)^{-1} Z_i^T$$
$$A_i = -(I + S_i C_{i3})\begin{bmatrix} H_{i1}^{-1} \\ 0 \end{bmatrix}$$
$$B_i = \left(S_i C_{i2}^T + A_i G_i\right)$$
$$F_i = \left(S_i \bar{C}_{i2}^T + A_i \bar{H}_i\right)$$

There is no contribution from the first order quantities, C_{i1} to δu_i^* since the perturbation model was obtained around the nominal optimum. Note that only the first element of δu_i^* is applied to the process, since at the next discontinuity in the inputs a further EOT is carried out and the input profile is recomputed over the remaining time horizon. This implies that the vector of the inputs applied to the process in the past, $\delta\bar{u}_i$, consists of the first elements of each solution vector of the past EOTs.

Each of the past inputs is itself dependent on the previous inputs, corresponding to Eq. (13). This expression can be rearranged in terms of past back offs and parameter estimates considering Eq. (11). Thus, the input moves, that are applied to the process during on-line optimization with n EOTs, are a function of the set of back offs at the different EOTs, β, and the set of parameter estimates, $\delta\hat{p}$:

$$\delta u^* = \delta u^*(\beta_0, \ldots, \beta_n, \delta\hat{p}_0, \ldots, \delta\hat{p}_n) = \delta u^*(\beta, \delta\hat{p}) \tag{14}$$

The derivation of the last equation and the corresponding matrix definitions are given in Appendix A.1.2.

The back off, β_i, in Eq. (12) is introduced in order to try to ensure that the process constraints are not violated when the calculated input moves are applied to the process. The basic idea of the back off is shown in Fig. 4. The true process optimum often lies on a boundary of the feasible region defined by one or more active path or endpoint inequality constraints. Due to the uncertainty in the parameters and the measurement errors it is unlikely that the optimization will predict the true optimal input variables which would operate the process exactly on this set of active constraints. Dependent on the error sources the suboptimal input variables might cause a violation of the process constraints once they are applied to the process. Therefore, some conservatism is introduced into the optimization by considering a back off from the active inequality constraints. This back off tries to accommodate all the possible error sources and keep the variation of the process constraints due to uncertainty and measurement errors inside the feasible region of the process, while still operating as closely to the constraints as possible, Fig. 4.

As opposed to the concept of back off for the steady-state optimization of continuous processes, where the necessary back off remains constant for a fixed set of active constraints [11,12], the back off during batch on-line optimization is time-varying due to the inherent dynamics of the estimation and optimization of the batch process, see Fig. 4. It is recomputed at every EOT and decreases, the more confidence in the uncertain parameters is gained. Its size is determined by examining the variation of the process constraints when the inputs calculated during the optimization are applied to the process:

$$G_i\delta p + \bar{H}_i\delta\bar{u}_i + \bar{H}_i\delta u_i^*(\beta_i, \delta\hat{p}_i, \delta\bar{u}_i) \le 0 \tag{15}$$

Using the expressions for the optimal inputs, Eq. (13) and the corresponding matrix definitions, the back off may be calculated as a function of the confidence in the uncertain parameters:

$$G_i(\delta p - \delta\hat{p}_i) \le \beta_i \tag{16}$$

Since the a priori parameter uncertainty and the parameter estimates are normally distributed and the dependencies are all linear, the variation in the active process constraint functions is also normally distributed. Introducing the equation for the parameter estimates (11), the variance of the process constraints can be determined dependent on the standard deviations of the a priori parametric uncertainty and the measurement error:

$$\Psi_{g,i} = G_i\left(W^{-1} - D_i\right)\left(W^{-1} - D_i\right)^T G_i^T + G_i E_i E_i^T G_i^T \tag{17}$$

The variance of the individual constraint functions is given by the diagonal elements of the covariance matrix $\Psi_{g,i}$. For a probability of α% of not violating an individual constraint, the vector of back offs is given by the following expression, dependent on the vector of variances of the individual constraints, $\mathrm{diag}(\Psi_{g,i})$:

$$\beta_i = \sqrt{2}\sqrt{\mathrm{diag}(\Psi_{g,i})}\,\mathrm{erf}^{-1}(2\alpha - 1) \tag{18}$$

It should be noted that there is an α% probability of not violating each individual constraint, but a smaller probability of not breaking any constraint.

During on-line optimization of continuous processes the number of degrees of freedom for optimization (i.e. the set points for the regulatory structure) remains constant. This is not the case for the optimization of the batch process, since at each EOT the process is optimized with respect to the remaining piecewise constant inputs in the future and this number decreases towards the end of the batch. If at a particular EOT there are more active path and/or endpoint inequality constraints than there are degrees of freedom for optimization, the process cannot be reoptimized. Instead, it needs to be run in open loop until enough degrees of freedom are available again or the end of the batch is reached. Otherwise, the optimization does not have enough degrees of freedom to back off from all active path/

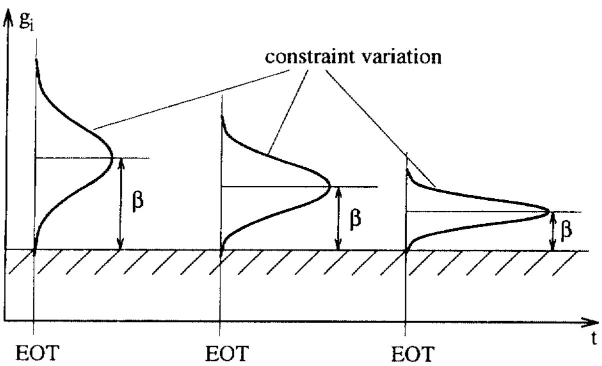

Fig. 4. Back off from active inequality constraints.

endpoint inequality constraints and the necessary back off cannot be determined for all the active inequality constraints. This means in particular for the case with more than one endpoint constraint, that the process is run in open loop with respect to the last few inputs and the actual benefit of on-line optimization is gained as long as the number of remaining inputs in the future is higher than the number of active endpoint inequality constraints.

3.1.4. Integration of the deviation from optimum

Similar to the calculation of the inputs during the on-line optimization, the true optimum input variables can be determined by minimizing Eq. (7) subject to Eq. (8) dependent on the normally distributed parametric uncertainty, $\delta p = \eta$:

$$\delta u^*(\delta p) = B\delta p = B\eta \tag{19}$$

Partitioning $H = [H_1\, H_2]$ with H_1 being a square and nonsingular matrix, B is given as:

$$Z = \begin{bmatrix} -H_1^{-1}H_2 \\ I \end{bmatrix}$$
$$S = -Z(Z^T C_3 Z)^{-1} Z^T$$
$$B = \left(SC_2^T - (I + SC_3)\begin{bmatrix} H_1^{-1} \\ 0 \end{bmatrix} G\right)$$

The expressions for the inputs calculated during the on-line optimization at each EOT, Eq. (14) and the true optimum inputs, Eq. (19) can be introduced into the second order perturbation model of the process objective function, $\delta\Phi$, Eq. (7) and the deviation of the calculated from the true process optimum can be determined:

$$\delta\Phi(\delta u^*(\delta p), \delta p) - \delta\Phi(\delta u^*(\beta, \delta\hat{p}), \delta p) \tag{20}$$

This deviation is then integrated with respect to the distribution functions of the parametric uncertainty and the measurement error and an analytical expression for the average deviation from optimum for the on-line optimization with n EOTs is obtained:

$$\Theta = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \left[\delta\Phi(\delta u^*(\delta p), \delta p) - \delta\Phi(\delta u^*(\beta, \delta\hat{p}), \delta p)\right] f(\eta) f(\varepsilon)\, d\varepsilon\, d\eta \tag{21}$$

$$= \Theta(\beta, \sigma_\varepsilon, \sigma_\eta, n) \tag{22}$$

The average deviation from optimum for off-line optimization, where the optimal input profile and the necessary back off are determined off-line considering the a priori uncertainty in the process parameters, is dependent only on the a priori parameter uncertainty and the necessary back off at the beginning of the batch, β_0:

$$\Theta_{\text{off-line}} = \Theta(\beta_0, \sigma_\eta) \tag{23}$$

The exact expressions for the average deviation from optimum for on-line and off-line optimization are given in Appendix A.1.3.

3.2. Time optimal problems

Time optimal problems, where the only objective is the minimization of the final batch time, have the following form:

$$\begin{aligned} &\min_{u, t_f} t_f \\ &\text{s.t. } \dot{x} = f(x, u, p),\ x(t_0) = x_0 \\ &\quad g(x, u, p) \le 0 \end{aligned} \tag{24}$$

In this case, one or more conditions which are represented by a subset of the inequality constraints g need to be reached in the minimum possible time. This subset of the constraints represents the so-called terminal conditions, which define the moment when the terminal time t_f is reached.

3.2.1. First and second order approximation

The time optimal problem (24) is solved with the nominal parameter values, in order to obtain the nominal optimum, and a first and second order perturbation model around the nominal trajectory is derived. However, the perturbation model needs to be obtained in a different manner than in the fixed terminal time case. The reason is that the input variables u do not directly affect the terminal time, t_f. The terminal time is only affected by changes in the terminal conditions, i.e. the appropriate subset of the constraints g, which are in turn dependent on the input variables, u. Therefore, a second order Taylor series expansion of the objective function with respect to the piecewise constant inputs and the uncertain parameters can only be obtained through the terminal constraints.

In a first step, the entire set of path and endpoint inequality constraints, which are active at the nominal optimum, is linearized with respect to the piecewise constant inputs, u, the uncertain parameters, p, and the final batch time, t_f:

$$\delta g = [H\, H_{t_f}]\begin{bmatrix} \delta u \\ \delta t_f \end{bmatrix} + G\delta p = 0 \tag{25}$$

While the matrices G and H are obtained as in the fixed terminal time case, the calculation of H_{t_f} is not as straightforward. The reason is that with changing t_f the locations of the discontinuities in the input variables, t_i, change, since the piecewise constant inputs were assumed to be equally distributed, see Fig. 5. The calculation of the sensitivity matrix of the active constraints with respect to the final time, H_{t_f}, is described in Appendix A.2.1.

In the case of more than one active constraint, the vector of the piecewise constant inputs, δu, and the matrix H need to be partitioned according to the dimension of δg, such that $[H_2\, H_{t_f}]$ is a square matrix:

$$\begin{bmatrix} \delta u_2 \\ \delta t_f \end{bmatrix} = -[H_2\, H_{t_f}]^{-1}(H_1 \delta u_1 + G\delta p) \tag{26}$$

The second order sensitivities of the final time, t_f, are determined from the last row of the previous equation by perturbing δu_1 and δp and calculating the finite differences of the perturbed first order quantities. The result is the following second order approximation of the objective function:

$$\begin{aligned} \delta t_f = {} & C_1 \delta u_1 + \delta p^T C_2 \delta u_1 + \frac{1}{2}\delta u_1^T C_3 \delta u_1 \\ & + C_4 \delta p + \frac{1}{2}\delta p^T C_5 \delta p \end{aligned} \tag{27}$$

Note that the minimization of δt_f represents an unconstrained QP in the reduced space of the remaining degrees of freedom δu_1, after the active inequality constraints including terminal conditions are met. This is due to the fact that the dependence of the terminal time on the input variables can only be obtained through the terminal constraints. After solving Eq. (27) with respect to δu_1, the remaining input variables can be determined from Eq. (26).

As in the fixed terminal time case, the measurements are linearized with respect to the uncertain parameters, $\delta y = J\delta p$. This implies that the parameter estimates are obtained in the same way as for fixed terminal time problems.

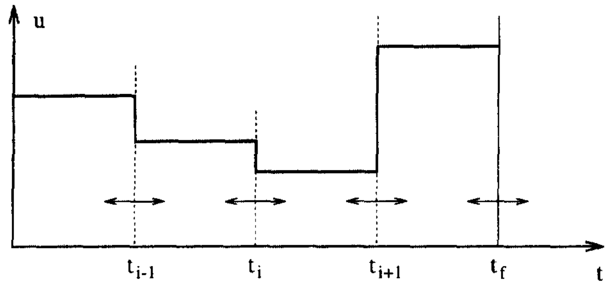

Fig. 5. Change of the switching times in the inputs with changing final time.

3.2.2. *Optimization and back offs from active inequality constraints*

Since it is not always possible to obtain full information about the state of a system, it is very difficult to decide when the terminal conditions of the batch are reached and the batch can be stopped. Additionally, measurement errors represent an error source, even with all the states measured. Therefore, also in the time optimal case, a back off from the active inequality constraints is introduced into the optimization at each EOT, which ensures that the batch reaction is not stopped before the endpoint specifications are met.

The minimization of Eq. (27) represents an unconstrained QP which is due to the fact that the objective function was obtained through the terminal constraints. This implies that the back off needs to be considered at an earlier stage during the derivation of the second order objective function. For that purpose, the back off, β, is introduced into the linearized equation of the constraints, Eq. (25):

$$\delta g = [H\, H_{t_f}]\begin{bmatrix} \delta u \\ \delta t_f \end{bmatrix} + G\delta p + \beta \tag{28}$$

This equation is then rewritten according to Eq. (26):

$$\begin{bmatrix} \delta u_2 \\ \delta t_f \end{bmatrix} = -[H_2\, H_{t_f}]^{-1}(H_1 \delta u_1 + G\delta p + \beta) \tag{29}$$

The second order sensitivities are determined according to the approach that was taken previously, and the following second order perturbation model of the problem including back off from the active inequality constraints is obtained:

$$\begin{aligned} \delta t_f = {} & C_1 \delta u_1 + \delta p^T C_1 \delta u_1 + \frac{1}{2}\delta u_1^T C_3 \delta u_1 + C_4 \delta p \\ & + \frac{1}{2}\delta p^T C_5 \delta p + C_6 \beta + \beta^T C_7 \delta u_1 + \beta^T C_8 \delta p \\ & + \frac{1}{2}\beta^T C_9 \beta \end{aligned} \tag{30}$$

At each EOT the process is reoptimized and the optimal inputs are determined over the remaining time horizon. The sensitivity matrices in Eq. (30) are partitioned according to the remaining degrees of freedom for optimization until the end of the batch, $\delta u_{i1} = [\delta u_1(i+1), \ldots, \delta u_1(n_{u1})]^T$, and the inputs applied to the process in the past, $\delta \bar{u}_{i1} = [\delta u_1(1), \ldots, \delta u_1(i)]^T$. The subsequent, unconstrained QP is obtained at EOT i, where the necessary back off from the process constraints appears in the objective function:

$$\begin{aligned} \min_{\delta u_{i1}} \; & C_{i1} \delta u_{i1} + \delta \hat{p}_i^T C_{i2} \delta u_{i1} + \delta \bar{u}_{i1} \bar{C}_{i2} \delta u_{i1} \\ & + \frac{1}{2}\delta u_{i1}^T C_{i3} \delta u_{i1} + \beta_i^T C_{i7} \delta u_{i1} \end{aligned} \tag{31}$$

The definitions of the sensitivity matrices in the neighbouring extremal problem (31) at EOT i are given in Appendix A.2.2. The analytical solution of the above unconstrained QP is:

$$\delta u_{i1}^* = A_i\beta_i + B_i\delta\hat{p}_i + F_i\delta\bar{u}_{i1} \tag{32}$$

with

$$A_i = -C_{i3}^{-1}C_{i7}^T$$
$$B_i = -C_{i3}^{-1}C_{i2}^T$$
$$F_i = -C_{i3}^{-1}\bar{C}_{i2}^T$$

The contribution of the first order quantities C_{i1} is zero, since the perturbation model was determined around the nominal optimum. Similar to the fixed terminal time case, the expression for the optimal inputs, δu_{i1}^*, can be rearranged dependent on the past back offs and parameter estimates:

$$\delta u_1^* = \delta u_1^*(\beta_0, \ldots, \beta_n, \delta\hat{p}_0, \ldots, \delta\hat{p}_n) = \delta u_1^*(\beta, \delta\hat{p}) \tag{33}$$

The derivation of the last equation and the necessary matrix definitions are given in Appendix A.2.2. The corresponding optimal values for δu_2^* and δt_f^* can be obtained from Eqs. (29) and (30), respectively.

The size of the necessary back off at EOT i is determined by analysing the variation of the active process constraints, when the calculated inputs are applied to the process:

$$\delta g = H_{i1}\delta u_{i1}^* + \bar{H}_{i1}\delta\bar{u}_{i1} + \left[H_2\ H_{t_f}\right]\begin{bmatrix}\delta u_2^* \\ \delta t_f^*\end{bmatrix} + G\delta p \leq 0 \tag{34}$$

The corresponding optimal values of δu_2^* and δt_f^* are both obtained from the linearized constraints, Eq. (29):

$$\begin{bmatrix}\delta u_2^* \\ \delta t_f^*\end{bmatrix} = -\left[H_2\ H_{t_f}\right]^{-1}\left(H_{i1}\delta u_{i1}^* + \bar{H}_{i1}\delta\bar{u}_{i1} + G\delta\hat{p}_i + \beta_i\right) \tag{35}$$

Introducing Eq. (35) into Eq. (34), the back off from the active inequality constraints at EOT i is dependent on the confidence in the uncertain parameters, as it is in the fixed terminal time case, Eq. (16):

$$G_i(\delta p - \delta\hat{p}_i) \leq \beta_i \tag{36}$$

The calculation of the size of the necessary constraint back off is then along the lines of Eqs. (17) and (18).

3.2.3. Integration of the deviation from optimum

In order to calculate the average deviation from optimum, the true optimum input variables need to be determined by minimizing Eq. (27) dependent on the normally distributed parametric uncertainty, $\delta p = \eta$:

$$\delta u_1^*(\delta p) = B\delta p = B\eta \tag{37}$$

The matrix B is given by $B = -C_3^{-1}C_2^T$. The true minimum final batch time is then obtained from Eq. (27) with the true optimum input variables introduced. The final batch time that is achieved in reality is given by Eq. (30) with the predicted optimal inputs $\delta u_1^*(\beta, \delta\hat{p})$ introduced:

$$\delta t_f^* = C_1\delta u_1^* + \delta p^T C_2\delta u_1^* + \frac{1}{2}\delta u_1^{*T}C_3\delta u_1^* + C_4\delta p + \frac{1}{2}\delta p^T C_5\delta p + C_6\beta_n + \beta_n^T C_7\delta u_1^* + \beta_n^T C_8\delta p + \frac{1}{2}\beta_n^T C_9\beta_n \tag{38}$$

The back off, β_n, in the objective function represents the necessary back off at the last EOT n. The deviation of the achieved final batch time from the true minimum final time is integrated with respect to the distribution functions of the parametric uncertainty and the measurement error. This gives an analytical expression for the average deviation from optimum for the on-line optimization with n EOTs, dependent on the set of back offs, β, and the standard deviations of the parameter uncertainty, σ_η, and the measurement error, σ_ε:

$$\Theta = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left[\delta t_f^*(\delta u_1^*(\delta p), \delta p) - \delta t_f^*(\delta u_1^*(\beta, \delta\hat{p}), \delta p, \beta_n)\right]f(\eta)f(\varepsilon)\mathrm{d}\varepsilon\mathrm{d}\eta \tag{39}$$

$$= \Theta(\beta, \sigma_\eta, \sigma_\eta, n) \tag{40}$$

The average deviation from optimum for off-line optimization is only dependent on the a priori parameter uncertainty and the necessary back off from the active path and endpoint inequality constraints at the start of the batch:

$$\Theta_{\text{off-line}} = \Theta(\beta_0, \sigma_\eta). \tag{41}$$

The exact expressions for the average deviation from optimum for on-line and off-line optimization are given in Appendix A.2.3.

4. Examples

In this section, the method of the average deviation from optimum is demonstrated on two examples. The first example is a second order dynamic system with fixed final time. After that, the time optimal operation of a semi-batch reactor is considered.

4.1. Fixed terminal time case

In a batch reactor, the substance P is produced from the raw material R with an undesired side reaction to byproduct W:

$$R \xrightarrow{k_1} P,\ R \xrightarrow{k_2} W$$

The temperature dependence of the reaction rates is described by an Arrhenius type equation: $k_i = k_{i0}\exp\left(-\frac{E_i}{RT}\right)$ The objective is to find a temperature profile such that the product yield is maximized at the end of a given reaction time [15]. With a constraint on the concentration of the component R, the optimization problem can be formulated using the following dimensionless model:

$$\begin{aligned} &\max_u x_2(t_f = 1) \\ &\text{s.t. } \dot{x}_1 = -(u + pu^2)x_1,\ x_1(0) = 1 \\ &\quad \dot{x}_2 = ux_1,\ x_2(0) = 0 \\ &\quad x_1(t) \geq 0.2. \end{aligned} \tag{42}$$

The dimensionless variables are given by $x_1 = c_R/c_{R0}$, $x_2 = c_P/c_{R0}$ and $u = k_1$. The ratio of the activation energies of the two reactions is $E_2/E_1 = 2$. The only uncertain parameter is k_{02}, or in the dimensionless formulation $p = k_{02}/k_{01}^2$ with a nominal value of $p_0 = 0.5$.

4.1.1. Nominal optimum

Since the method of the average deviation from optimum is based on a perturbation model around the nominal optimum, the problem is optimized with the nominal parameter value using the method of orthogonal collocation. In order to be able to carry out enough EOTs during on-line optimization without having a too high frequency of execution, the time axis is divided into four super-elements with one finite element on each super-element. The inputs are piecewise constant on the four super-elements. An accurate representation of the dynamic system is obtained by approximating the state variable profiles by quadratic polynomials on each finite element. The optimal input profile is shown in Fig. 6. Fig. 7 shows the approximated state variable profiles at the nominal optimum together with the collocation points. In the same graph, the state variable profiles of the system are plotted, where the dynamic model equations are integrated with the optimal input variables. As can be seen, the approximation is quite accurate. The nominal optimum gives a product yield of $x_2(t_f) = 0.5349$. The inequality constraint on the first state variable becomes active at the final time.

4.1.2. Optimization analysis

In the following, the method of the average deviation from optimum is employed in order to estimate the performance of an on-line optimizer and compare this performance against off-line optimization. The parameter uncertainty is assumed to have a standard deviation of $\sigma_\eta = 0.2$. Two on-line optimization scenarios will be analysed, where either the first or the second state variable is measured, each with a standard variation of the measurement error of $\sigma_\varepsilon = 0.01$.

The average deviation from optimum gives the results shown in Table 1. Both on-line optimization schemes perform significantly better than off-line optimization, which shows an average deviation from optimum of $\Theta = -0.0524$. Thus, there exists an economic benefit of employing an on-line optimizer. However, when comparing the two on-line optimization scenarios, it can be seen that the process can be operated closer to its true optimum when the first state variable is measured. In this case, the on-line optimization shows an average deviation from optimum of $\Theta = -0.0069$, compared to $\Theta = -0.0198$ with the second state measured. This is

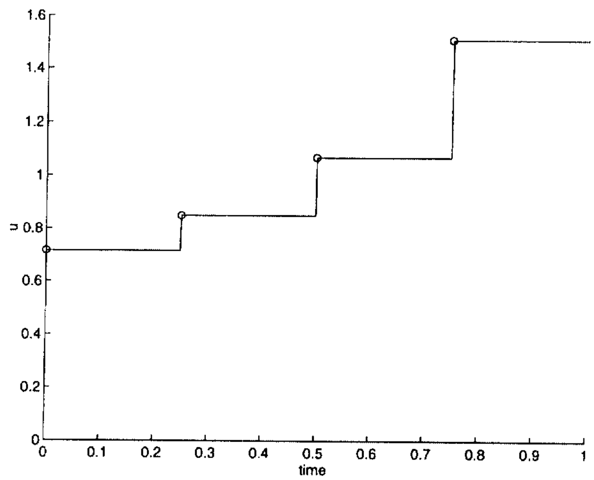

Fig. 6. Input variable profile at nominal optimum.

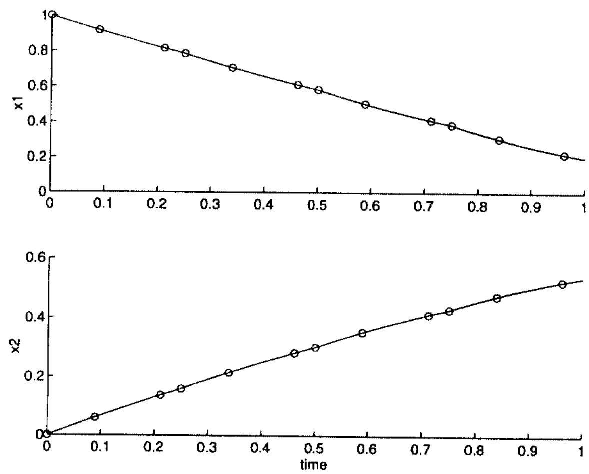

Fig. 7. Approximated and integrated state variable profiles at nominal optimum.

Table 1
Analysis results

Optimization	Measurement	σ_ε	Θ
Off-line	—	—	−0.0524
On-line	x_1	0.01	−0.0069
On-line	x_2	0.01	−0.0198

also illustrated in Fig. 8, where the necessary back offs from the active endpoint inequality constraint at each EOT for the two on-line optimization schemes are shown. Measuring x_1 gives more accurate parameter estimates, so that the back off at each EOT decreases more than in the case when x_2 is measured. Thus, the process can be operated closer to the constraint and therefore closer to the optimum.

4.2. Time optimal case

The average deviation from optimum for the time optimal case is demonstrated on the production of 2-acetoacetyle pyrrole from pyrrole and diketene in a semi-batch reactor in the minimum possible time [6].

Ruppen et al. [6] investigated both a simple and a detailed model of the reaction system. However, for the case of continuous feed addition, the simple model proved to be adequate and the performance was at least as good as the performance of the more detailed model [6].

Therefore, the simple model with the following reactions is considered here:

$$P + D \xrightarrow{K} PAA$$
$$D + D \xrightarrow{K} DHA$$
$$D \xrightarrow{K} \text{oligomers}$$
$$PAA + D \xrightarrow{K} F$$
$$(DHA + D \xrightarrow{K} G)$$

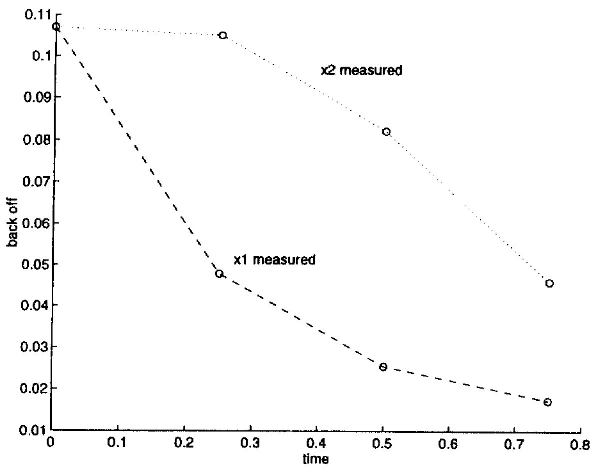

Fig. 8. Necessary back off at different EOTs.

In this reaction system, pyrrole is denoted by P, diketene by D, pyridine which acts as catalyst by K, 2-acetoacetyl pyrrole by PAA and dehydroacetic acid by DHA. The substances F and G stand for by-products. The reaction rates are:

$$r_{PAA} = k_A c_D c_P$$
$$r_{DHA} = k_D c_D^2$$
$$r_O = k_O c_D$$
$$r_F = k_F c_{PAA} c_D$$

Assuming constant density of the components and isothermal operation results in the following reaction model, where the last side reaction producing by-product G is neglected. The dilution of catalyst is considered by normalizing the rate constants with respect to the reaction volume. This is not implemented for the rate constant k_O, since the rate of oligomerization is also promoted by other intermediate products [6]:

$$\frac{dc_D}{dt} = -\frac{k_A}{v_R} c_P c_D - 2\frac{k_D}{v_R} c_D^2 - k_O c_D - \frac{k_F}{v_R} c_{PAA} c_D + \frac{f}{v_R}(c_{Df} - c_D) \tag{43}$$

$$\frac{dc_P}{dt} = -\frac{k_A}{v_R} c_P c_D - \frac{f}{v_R} c_P \tag{44}$$

$$\frac{dc_{PAA}}{dt} = \frac{k_A}{v_R} c_P c_D - \frac{k_F}{v_R} c_{PAA} c_D - \frac{f}{v_R} c_{PAA} \tag{45}$$

$$\frac{dc_{DHA}}{dt} = \frac{k_D}{v_R} c_D^2 - \frac{f}{v_R} c_{DHA} \tag{46}$$

$$\frac{dv_R}{dt} = f \tag{47}$$

The concentration of diketene D in the feed stream is represented by c_{Df}. The manipulated input variable is the feed rate, f (l/min), of diluted diketene. The nominal values of the kinetic parameters and the initial conditions are given in Table 2. These values are taken from Ruppen et al. [6] and are used here for the theoretical analysis.

With the necessary endtime specifications and a path constraint on the feed rate, the optimization problem can be written as follows:

Table 2
Nominal model parameter values and initial conditions

Parameters		Initial conditions	
k_A	0.053 l/(mol min)	c_{D0}	0.09 mol/l
K_D	0.128 l/(mol min)	c_{P0}	0.72 mol/l
k_O	0.028 1/min	c_{PAA0}	0.1 mol/l
k_F	0.003 l/(mol min)	c_{DHA0}	0.02 mol/l
c_{Df}	5.82 mol/l	v_{R0}	1.0 l

$$\min_{f, t_f} t_f$$
$$\text{s.t. dynamic model equations (43) – (47)}$$
$$c_{PAA}(t_f) v_R(t_f) \geq 0.42 \text{ mol} \quad (48)$$
$$c_{DHA}(t) \leq 0.15 \text{ mol/l}$$
$$c_D(t_f) \leq 0.025 \text{ mol/l}$$
$$f(t) \geq 0$$

A detailed description of the diketene chemistry, the modelling of the reactor and the experimental set up of on-line optimization can be found in the work of Ruppen et al. [6].

4.2.1. Nominal optimum

The first step towards the analysis is the determination of the nominal optimum. The dynamic model equations in DAOP (48) are collocated on eight equally distributed super-elements with one finite element per super-element. Thus, a sufficient number of EOTs can be carried out at the input discontinuities in order to obtain satisfactory economic benefit during on-line optimization. The state variables are approximated with quadratic polynomials, while the input variables are specified as piecewise constant. The resulting NLP is then solved using the nominal parameter values and initial conditions given in Table 2. The input and state variable profiles at the nominal optimum are shown in Figs. 9 and 10 respectively. Due to the high number of super-elements, the approximation of the system is quite accurate, as can be seen in Fig. 10, where both the approximated and integrated state variables profiles are plotted. The terminal time at the nominal optimum is $t_f = 138.62$ min. Besides the endpoint constraints, the path constraint on the feed rate becomes active in the last super-element.

4.2.2. Optimization analysis

In order to demonstrate the analysis of the on-line optimization, it is assumed that the uncertain process parameters are the two rate constants k_A and k_D. The uncertainty is described as normally distributed with the standard deviations $\sigma_{\eta,k_A} = 0.003$ and $\sigma_{\eta,k_D} = 0.007$. In the following, three different structures of the on-line optimizer are analysed and their performance is compared against off-line optimization. The different structures are characterized by the selection of the measurement which is used to update the estimates of the uncertain parameters. For that purpose, it is assumed that one or more state variables can be measured on-line. The alternatives consist of measuring either one of the concentrations c_P, c_D or c_{PAA}. The standard deviation of the measurement error is assumed to be 1% of the approximate average nominal value of the corresponding state variable, see Fig. 3. Since the three terminal constraints and the lower bound on the feed rate in the last super-element are active at the nominal optimum, the process has to be run in open loop with respect to the last four inputs. This is necessary for the optimization to have enough degrees of freedom at the last EOT to back off from the four active inequality constraints. The system is collocated on eight super-elements which implies that four EOTs are carried out during on-line optimization.

The analysis results are shown in Table 3. Off-line optimization shows an average deviation from optimum of $\Theta = -47.56$ min. Implementing an on-line optimizer, where the diketene concentration, c_D, is measured, does not improve this result significantly. In this case, the average deviation from optimum is $\Theta = -39.05$ min. However, a much better operation of the reactor can be obtained when either the pyrrole concentration, c_P, or the acetoacetyle pyrrole concentration, c_{PAA}, is measured. Both options show a substantial improvement

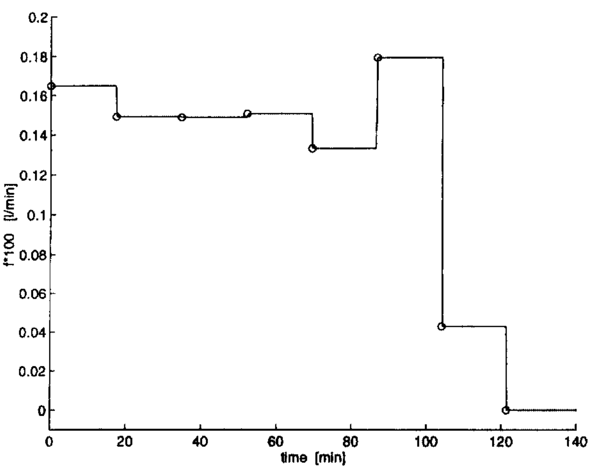

Fig. 9. Input variable profile at nominal optimum.

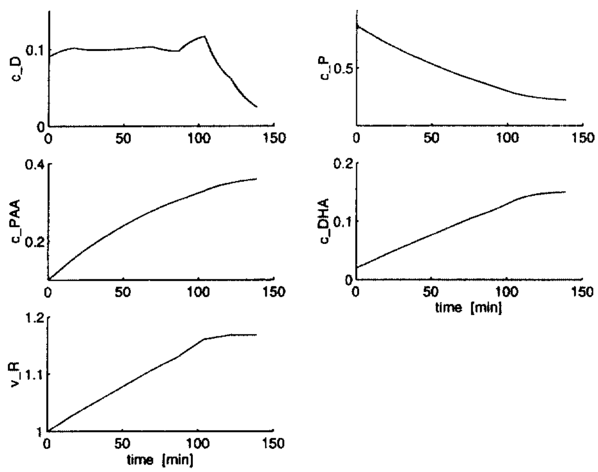

Fig. 10. Approximated and integrated state variable profiles at nominal optimum.

Table 3
Analysis results

Optimization	Measurement	σ_ε	Θ
Off-line	—	—	−47.56 min
On-line	c_D	0.001	−39.05 min
On-line	c_P	0.005	−23.22 min
On-line	c_{PAA}	0.003	−17.72 min

against the off-line optimization result, where measuring c_{PAA} gives the least average deviation from optimum with $\Theta = -17.72$ min, compared to $\Theta = -23.22$ min when c_P is measured.

5. Conclusions

The method of the average deviation from optimum allows the estimation of the economic performance of a given on-line batch optimization system. This performance can be compared against off-line optimization and the economic benefit of on-line optimization identified. Different on-line optimizer structures can be compared and the structure with the best performance can be chosen for implementation. Furthermore, the analysis method returns the necessary back off from the active path and endpoint inequality constraints at each Estimation Optimization Task EOT in order to ensure the feasible operation of the process.

The method of the average deviation from optimum has been developed for two classes of problems. In the first case, the terminal batch time was fixed, while the theory was also derived for time optimal problems. In both cases, the theory has been demonstrated on an example.

Appendix A. Mathematical derivations and matrix definitions

In this section, some details of the mathematical derivation of the method of the average deviation from optimum are presented, both for fixed terminal time and time optimal problems.

A.1. Fixed terminal time problems

A.1.1. First and second order approximation

The linearization of the objective function, Φ, and the active inequality constraints, g, in Eq. (6) is performed at the nominal optimum of the collocated dynamic system. With the approximation coefficients of the input profile, ν, and the state variable profile, ξ, (see Section 2) the linearization of the objective function is given by:

$$\delta\Phi = \frac{\partial\Phi}{\partial\nu}\delta\nu + \frac{\partial\Phi}{\partial\xi}\delta\xi \tag{49}$$

The objective function is a function of the state variables at the final time and is not directly affected by the approximation coefficients of the state and input variables in the first finite and super-elements. They affect the objective function at the final time only through the dynamic system equations, $\dot{x} = f(x, u, p)$ which appear as equality constraints in the NLP after the discretization of the problem. Therefore, all the information about the dynamic system in the collocated problem is given by the equality constraints, namely the discretized dynamic system equations and the continuity conditions at the boundaries of the finite elements and super-elements. For a perturbation in the piecewise constant input variables the following relationship must hold, where F represents the equality constraints corresponding to the discretized system equations and continuity conditions:

$$\frac{\partial F}{\partial\nu}\delta\nu + \frac{\partial F}{\partial\xi}\delta\xi = 0 \tag{50}$$

Since the number of equations in F is equal to the dimension of the vector ξ (the behaviour of the dynamic system is determined for given input variables), the last two equations can be combined to give the linearization of the objective function with respect to the piecewise constant inputs:

$$\delta\Phi = \left(\frac{\partial\Phi}{\partial\nu} - \frac{\partial\Phi}{\partial\xi}\left[\frac{\partial F}{\partial\xi}\right]^{-1}\frac{\partial F}{\partial\nu}\right)\delta\nu \tag{51}$$

The linearization of the objective function with respect to the uncertain parameters and the linearization of the active algebraic path and endpoint inequality constraints are performed in the same way. The second order quantities are obtained by taking finite differences from the perturbed first order sensitivities. This gives the following first and second order perturbation model of the collocated problem around the nominal optimum:

$$\delta\Phi = C_1\delta u + \delta p^T C_2\delta u + \frac{1}{2}\delta u^T C_3\delta u + C_4\delta p + \frac{1}{2}\delta p^T C_5\delta p \tag{52}$$

$$\delta g = G\delta p + H\delta u = 0 \tag{53}$$

In this formulation, δp is the perturbation variable of the uncertain process parameters around the nominal parameter values. Similarly, δu is the perturbation vector of the approximation coefficients of the piecewise constant input variables around the inputs at the nominal optimum, where n_{SE} is the number of super-elements defined on the time horizon:

$$\delta v = \delta u = \left[\delta u(1)^T \delta u(2)^T \cdots \delta u(n_{SE})^T\right]^T \tag{54}$$

A.1.2. Optimization at EOT i

The neighbouring extremal problem at EOT i approximating the optimization step has the following form:

$$\begin{aligned}&\min_{\delta u_i} C_{i1}\delta u_i + \delta\hat{p}_i^T C_{i2}\delta u_i + \delta\bar{u}_i^T \bar{C}_{i2}\delta u_i + \frac{1}{2}\delta u_i^T C_{i3}\delta u_i \\ &\text{s.t. } \delta g_i(\delta u_i, \delta\bar{u}_i, \delta\hat{p}_i) = G_i\delta\hat{p}_i + \bar{H}_i\delta\bar{u}_i + H_i\delta u_i + \beta_i = 0\end{aligned} \tag{55}$$

The sensitivity matrices of the objective function are obtained from C_1, C_2 and C_3 (see Eq. (7)) in the following manner where n_p is the dimension of the uncertain process parameter vector, $n_p = \dim(\delta p)$:

$$\begin{aligned}C_{i1} &= [C_1(1,k)]_{k=i+1,\ldots,n_{SE}} \\ C_{i2} &= [C_2(j,k)]_{j=1,\ldots,n_p;k=i+1,\ldots,n_{SE}} \\ \bar{C}_{i2} &= [C_3(j,k)]_{j=1,\ldots,i;k=i+1,\ldots,n_{SE}} \\ C_{i3} &= [C_3(j,k)]_{j,k=i+1,\ldots,n_{SE}}\end{aligned}$$

Assuming that the $n_{pc,i}$ active path constraints, which are in the past at EOT i, correspond to the first $n_{pc,i}$ rows of δg (with $n_c = \dim(\delta g)$), the sensitivity matrices of δg_i can be written as:

$$\begin{aligned}G_i &= [G(j,k)]_{j=n_{pc,i}+1,\ldots,n_c;k=1,\ldots,n_p} \\ H_i &= [H(j,k)]_{j=n_{pc,i}+1,\ldots,n_c;k=i+1,\ldots,n_{SE}} \\ \bar{H}_i &= [H(j,k)]_{j=n_{pc,i}+1,\ldots,n_c;k=1,\ldots,i}.\end{aligned}$$

The analytical solution of the neighbouring extremal problem at EOT i is given by the following expression, see Eq. (13):

$$\delta u_i^* = A_i\beta_i + B_i\delta\hat{p}_i + F_i\delta\bar{u}_i \tag{56}$$

Note that only the first element of δu_i^* is applied to the process, since at the next discontinuity in the inputs a further EOT is carried out and the input profile is recomputed over the remaining time horizon. This implies that the vector of the inputs applied to the process in the past, $\delta\bar{u}_i$, consists of the first elements of each solution vector of the past EOTs:

$$\delta u_i^* = A_i\beta_i + B_i\delta\hat{p}_i + F_i\begin{bmatrix} q_0\delta u_0^* \\ q_1\delta u_1^* \\ \vdots \\ q_{i-1}\delta u_{i-1}^*\end{bmatrix} \tag{57}$$

This is accomplished by multiplying each solution vector of past inputs with a vector q_j which deletes the input moves not applied to the process. The vectors $q_j, j = 0, \ldots, i-1$, have the following form, where the dimensions of q_j are a function of j, $\dim(q_j) = n_{SE} - j$:

$$q_j = \underbrace{[1 \quad 0 \quad \cdots \quad 0]}_{n_{SE-j}} \tag{58}$$

Note that each of the past inputs is itself dependent on the previous inputs, corresponding to Eq. (57). This expression can be rearranged in terms of past back offs and parameter estimates considering Eq. (11):

$$\begin{aligned}\delta u_i^* &= \sum_{j=0}^{i} K_{ij}\beta_j + \sum_{j=1}^{i} L_{ij}\delta\hat{p}_j \\ &= \sum_{j=0}^{i} K_{ij}\beta_j + \sum_{j=1}^{i} L_{ij}D_jW\eta + \sum_{j=1}^{i} L_{ij}F_jQ_j\varepsilon_j\end{aligned} \tag{59}$$

The matrices K_{ij} and L_{ij} are obtained in the following iterative manner:

$$K_{ii} = A_i \tag{60}$$

$$\bar{K}_{i(i-1)} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ q_{i-1}A_{i-1}\end{bmatrix} \tag{61}$$

$$\bar{K}_{ij} = \begin{bmatrix} \bar{K}_{(i-1)j} \\ q_{i-1}F_{i-1}\bar{K}_{(i-1)j}\end{bmatrix}, \; j < i, \; j \neq i-1 \tag{62}$$

$$K_{ij} = F_i\bar{K}_{ij}, \; j < i \tag{63}$$

The matrices L_{ij} can be determined in the same way with A_i replaced by B_i. Thus, the input moves, that are applied to the process during on-line optimization with n EOTs, are a function of the set of back offs at the different EOTs, β, and the set of parameter estimates, $\delta\hat{p}$:

$$\begin{aligned}\delta u^* &= \begin{bmatrix} q_0\delta u_0^* \\ q_1\delta u_1^* \\ \vdots \\ q_n\delta u_n^*\end{bmatrix} = \delta u^*(\beta_0, \ldots, \beta_n, \delta\hat{p}_0, \ldots, \delta\hat{p}_n) \\ &= \delta u^*(\beta, \delta\hat{p})\end{aligned} \tag{64}$$

A.1.3. Average deviation from optimum

The deviation of the predicted from the true process optimum is integrated with respect to the distribution functions of the parametric uncertainty and the measurement error in order to obtain the average deviation from optimum. The expression for the average deviation from optimum for on-line optimization with n EOTs is given below:

$$\Theta = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \left[\delta\Phi(\delta u^*(\delta p), \delta p) - \delta\Phi(\delta u^*(\beta, \delta\hat{p}), \delta p)\right] f(\eta) f(\varepsilon) \mathrm{d}\varepsilon \mathrm{d}\eta \tag{65}$$

$$\begin{aligned} &= tr\left(W^{-T}C_2BW^{-1}\right) + \frac{1}{2}tr\left(W^{-T}B^TC_3BW^{-1}\right) \\ &- \sum_{i=0}^{n}\Big[C_1P_iR_i + \frac{1}{2}R_i^TP_i^TC_3P_iR_i + tr\left(W^{-T}C_2P_iN_i\right) \\ &+ \frac{1}{2}tr\left(N_i^TP_i^TC_3P_iN_i\right) + \sum_{j=1}^{i}\frac{1}{2}tr\left(M_{ij}^TP_i^TC_3P_iM_{ij}\right) \\ &+ \sum_{j=1}^{i}\sum_{k=j+1}^{i} tr\left(M_{ij}^TP_i^TC_3P_iM_{ik}\right)\Big] \\ &- \sum_{i=0}^{n}\sum_{j=i+1}^{n}\Big[R_i^TP_i^TC_3P_jR_j + tr\left(N_i^TP_i^TC_3P_jN_j\right) \\ &+ \sum_{k=1}^{i}\sum_{l=1}^{j} tr\left(M_{ik}^TP_i^TC_3P_jM_{jl}\right)\Big] \end{aligned} \tag{66}$$

with

$$R_i = \sum_{j=0}^{i} K_{ij}\beta_j$$

$$N_i = \sum_{j=0}^{i} L_{ij}D_j$$

$$M_{ij} = L_{ij}E_j, \; j \leq i$$

The summations start at $i = 0$ indicating the beginning of the batch before the first EOT is carried out, because also in the first time interval, a back off needs to be introduced due to the uncertainty in the process parameters. This implies of course that $D_0 = E_0 = 0$. The permutation matrices P_i are introduced to account for the fact that only the first element of the calculated input vector at EOT i, $\delta u_i^*(\beta_i, \delta\hat{p}_i, \delta\bar{u}_i)$, is applied to the process.

The average deviation from optimum for off-line optimization, where the optimal input profile and the necessary back off are determined off-line considering the a-priori uncertainty in the process parameters, is given by the following expression.

$$\begin{aligned} \Theta_{\text{off-line}} &= \mathrm{tr}\left(W^{-T}C_2BW^{-1}\right) + \frac{1}{2}\mathrm{tr}\left(W^{-T}B^TC_3BW^{-1}\right) \\ &- C_1A_0\beta_0 - \frac{1}{2}\beta_0^TA_0^TC_3A_0\beta_0 \end{aligned} \tag{67}$$

Since no reoptimization is carried out, the whole input profile calculated off-line is applied to the process and no permutation matrix is necessary, i. e. $P_0 = I$.

A.2. Time optimal problems

A.2.1. First and second order approximation

In order to obtain a first and second order perturbation model of the time optimal problem (24) at its nominal optimum, the entire set of path and endpoint inequality constraints, which are active at the nominal optimum, is linearized with respect to the piecewise constant inputs, u, the uncertain parameters, p, and the final batch time, t_f:

$$\delta g = \left[H \; H_{t_f}\right]\begin{bmatrix}\delta u \\ \delta t_f\end{bmatrix} + G\delta p = 0 \tag{68}$$

While the matrices G and H are obtained as in the fixed terminal time case, the calculation of H_{t_f} is not as straightforward. The reason is that with changing t_f the locations of the discontinuities in the input variables, t_i change, since the piecewise constant inputs were assumed to be equally distributed, see Fig. 5. The sensitivity matrix of the active constraints with respect to the final time, H_{t_f}, can be obtained as follows (note that $t_{i+1} - t_i$ is strictly speaking independent of i due to the equal distribution of the super-elements):

$$H_{t_f} = \frac{\mathrm{d}g}{\mathrm{d}t_f} = \frac{t_{i+1} - t_i}{t_f}\left[\sum_i \frac{\partial g}{\partial t_i} + \frac{\partial g}{\partial t_f}\right] \tag{69}$$

where

$$\frac{\partial g}{\partial t_i} = \frac{\partial g}{\partial x(t_i)}\frac{\partial x(t_i)}{\partial t_i} \tag{70}$$

and

$$\frac{\partial g}{\partial t_f} = \frac{\partial g}{\partial x(t_f)}\frac{\partial x(t_f)}{\partial t_i} \tag{71}$$

The sensitivities $(\partial x)/(\partial t)$ are obtained from the model equations $f(x, u, p)$, while the sensitivities $(\partial g)/(\partial x)$ can be determined from the collocated problem using the appropriate approximation coefficients of the state variables.

In the case of more than one active constraint, the vector of the piecewise constant inputs, δu, and the matrix H need to be partitioned according to the dimension of δg, such that $[H_2 H_{t_f}]$ is a square matrix:

$$\delta g = [H_1\ H_2\ H_{t_f}] \begin{bmatrix} \delta u_1 \\ \delta u_2 \\ \delta t_f \end{bmatrix} + G\delta p = 0 \quad (72)$$

Assuming that $[H H_{t_f}]$ is of full row rank, there always exists a partition such that $[H_2 H_{t_f}]$ is nonsingular and the last equation can be rewritten as shown below:

$$\begin{bmatrix} \delta u_2 \\ \delta t_f \end{bmatrix} = -[H_2\ H_{t_f}]^{-1}(H_1\delta u_1 + G\delta p) \quad (73)$$

If $[H H_{t_f}]$ is not of full row rank, then two or more of the constraints are linearly dependent. In this case, the linearly dependent constraints are affected by the inputs in the same way. The singular rows which correspond to the linearly dependent constraints can be removed until $[H H_{t_f}]$ has full row rank. Taking the last row of the previous equation gives the following linear expression for the final time with respect to the inputs and the uncertain parameters:

$$\delta t_f = C_1\delta u_1 + C_4\delta p \quad (74)$$

The second order sensitivities are determined by perturbing δu_1 and δp and calculating the finite differences of the perturbed first order quantities. This gives the following second order approximation of the objective function:

$$\delta t_f = C_1\delta u_1 + \delta p^T C_2 \delta u_1 + \frac{1}{2}\delta u_1^T C_3 \delta u_1 + C_4\delta p + \frac{1}{2}\delta p^T C_5 \delta p \quad (75)$$

A.2.2. Optimization at EOT i

In order to obtain the neighbouring extremal problem at EOT i, the sensitivity matrices C_1, C_2, C_3 and C_7 in Eq. (30) are partitioned according to the remaining degrees of freedom for optimization until the end of the batch, $\delta u_{i1} = [\delta u_1(i+1), \ldots, \delta u_1(n_{u1})]^T$ and the inputs applied to the process in the past, $\delta \bar{u}_{i1} = [\delta u_1(1), \ldots, \delta u_1(i)]^T$.

$$\begin{aligned} C_{i1} &= [C_1(1,k)]_{k=i+1,\ldots,n_{u1}} \\ C_{i2} &= [C_2(j,k)]_{j=1,\ldots,n_p;k=i+1,\ldots,n_{u1}} \\ \bar{C}_{i2} &= [C_3(j,k)]_{j=1,\ldots,i;k=i+1,\ldots,n_{u1}} \\ C_{i3} &= [C_3(j,k)]_{j,k=i+1,\ldots,n_{u1}} \\ C_{i7} &= [C_7(j,k)]_{j=1,\ldots,n_c;k=i+1,\ldots,n_{u1}} \end{aligned}$$

The subsequent, unconstrained QP approximates the optimization step at EOT i:

$$\min_{\delta u_{i1}} C_{i1}\delta u_{i1} + \delta\hat{p}_i^T C_{i2}\delta u_{i1} + \delta\bar{u}_{i1}\bar{C}_{i2}\delta u_{i1} + \frac{1}{2}\delta u_{i1}^T C_{i3}\delta u_{i1} + \beta_i^T C_{i7}\delta u_{i1} \quad (76)$$

The analytical solution is:

$$\delta u_{i1}^* = A_i\beta_i + B_i\delta\hat{p}_i + F_i\delta\bar{u}_{i1} \quad (77)$$

$$= A_i\beta_i + B_i\delta\hat{p}_i + F_i \begin{bmatrix} q_0\delta u_{01}^* \\ q_1\delta u_{11}^* \\ \vdots \\ q_{i-1}\delta u_{(i-1)1}^* \end{bmatrix} \quad (78)$$

The vectors $q_j, j = 0, \ldots, i-1$, are defined as in Eq. (58) with the appropriate dimensions according to δu_{j1}^*. Similar to the fixed terminal time case, the expression for the optimal inputs δu_{i1}^* can be rearranged dependent on the past back offs and parameter estimates:

$$\begin{aligned} \delta u_{i1}^* &= \sum_{j=0}^{i} K_{ij}\beta_j + \sum_{j=1}^{i} L_{ij}\delta\hat{p}_j \\ &= \sum_{j=0}^{i} K_{ij}\beta_j + \sum_{j=1}^{i} L_{ij}D_j W\eta + \sum_{j=1}^{i} L_{ij}E_j Q_j \varepsilon_j. \end{aligned} \quad (79)$$

The matrices K_{ij} and L_{ij} are defined as in Eqs. (60)–(63) dependent on A_i and B_i, respectively. Thus, the optimal input variables, that are determined during on-line optimization with n EOTs, are a function of the set of back offs, β, and the set of parameter estimates, $\delta\hat{p}$:

$$\begin{aligned} \delta u_1^* &= \begin{bmatrix} q_0\delta u_{01}^* \\ q_1\delta u_{11}^* \\ \vdots \\ q_n\delta u_{n1}^* \end{bmatrix} = \delta u_1^*(\beta_0, \ldots, \beta_n, \delta\hat{p}_0, \ldots, \delta\hat{p}_n) \\ &= \delta u_1^*(\beta, \delta\hat{p}) \end{aligned} \quad (80)$$

A.2.3. Average deviation from optimum

The deviation of the achieved final batch time from the true minimum final time is integrated with respect to the distribution functions of the parametric uncertainty and the measurement error. This gives the following expression for the average deviation from optimum for the on-line optimization with n EOTs:

$$\Theta = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\Big[\delta t_f^*(\delta u_1^*(\delta p), \delta p) - \delta t_f^*\big(\delta u_1^*(\beta, \delta\hat{p}), \delta p, \beta_n\big)\Big] f(\eta) f(\varepsilon)\mathrm{d}\varepsilon\mathrm{d}\eta \quad (81)$$

$$
\begin{aligned}
&= \mathrm{tr}\left(W^{-T}C_2BW^{-1}\right)+\frac{1}{2}\mathrm{tr}\left(W^{-T}B^TC_3BW^{-1}\right)\\
&-\sum_{i=0}^{n}\left[C_1P_iR_i+\frac{1}{2}R_i^TP_i^TC_3P_iR_i+\mathrm{tr}\left(W^{-T}C_2P_iN_i\right)\right.\\
&+\frac{1}{2}\mathrm{tr}\left(N_i^TP_i^TC_3P_iN_i\right)+\sum_{j=1}^{i}\frac{1}{2}\mathrm{tr}\left(M_{ij}^TP_i^TC_3P_iM_{ij}\right)\\
&\left.+\sum_{j=1}^{i}\sum_{k=j+1}^{i}\mathrm{tr}\left(M_{ij}^TP_i^TC_3P_iM_{ik}\right)+\beta_n^TC_7P_iR_i\right]\\
&-\sum_{i=0}^{n}\sum_{j=i+1}^{n}\left[R_i^TP_i^TC_3P_jR_j+\mathrm{tr}\left(N_i^TP_i^TC_3P_jN_j\right)\right.\\
&\left.+\sum_{k=1}^{i}\sum_{l=1}^{j}\mathrm{tr}\left(M_{ik}^TP_i^TC_3P_jM_{jl}\right)\right]-C_6\beta_n-\frac{1}{2}\beta_n^TC_9\beta_n
\end{aligned}
\tag{82}
$$

with

$$R_i=\sum_{j=0}^{i}K_{ij}\beta_j$$

$$N_i=\sum_{j=0}^{i}L_{ij}D_j$$

$$M_{ij}=L_{ij}E_j, j\le i$$

The summations start at $i=0$ to allow for the back off in the first time interval before the first EOT is carried out. The permutation matrices P_i are introduced to account for the fact that only the first element of the calculated input vector at EOT $i, \delta u_{i1}^*(\beta_i,\delta\hat{p}_i,\delta\bar{u}_i)$, is applied to the process.

The average deviation from optimum for off-line optimization is given by the following expression:

$$
\begin{aligned}
\Theta_{\text{off-line}} &= \mathrm{tr}\left(W^{-T}C_2BW^{-1}\right)+\frac{1}{2}\mathrm{tr}\left(W^{-T}B^TC_3BW^{-1}\right)\\
&-C_1A_0\beta_0-\frac{1}{2}\beta_0^TA_0^TC_3A_0\beta_0-C_6\beta_0\\
&-\beta_0^TC_7A_0\beta_0-\frac{1}{2}\beta_0^TC_9\beta_0.
\end{aligned}
\tag{83}
$$

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