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Dual robust control of batch processes based on optimality-conditions parameterization

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Abstract: This paper presents a scheme for dual robust control of batch processes under parametric uncertainty. Some recently proposed approaches can be used to tackle this problem, however, this will be done at the price of conservativeness or significant computational burden. In order to increase computational efficiency, we propose a scheme that uses parametrized conditions of optimality in the adaptive predictive-control fashion. The dual features of the controller, i.e., balance between the control moves that excite the system to improve accuracy of the parameter estimation and between the moves that optimize process performance, is realized through scenario-based (multi-stage) approach, which allows for modeling of the adaptive robust decision problem and for projecting this decision into predictions of the controller. The proposed approach is illustrated on a case study from batch membrane filtration.

Keywords: Predictive control, Adaptive control, Robust control, Batch control, Pontryagin's minimum principle, Membrane separation, Parameter estimation.

1. INTRODUCTION

In this paper we consider a real-time implementation of a controller that solves the dynamic optimization problem of the form:

$$\min_{u(t),t_\mathrm{f}} \mathcal{J} := \min_{u(t),t_\mathrm{f}} \int_0^{t_\mathrm{f}} F_0(\boldsymbol{x}(t),\boldsymbol{p}) + F_u(\boldsymbol{x}(t),\boldsymbol{p})u(t)\,\mathrm{d}t \quad \text{(1a)}$$

$$\text{s.t. } \dot{\boldsymbol{x}}(t) = \boldsymbol{f}_0(\boldsymbol{x}(t),\boldsymbol{p}) + \boldsymbol{f}_u(\boldsymbol{x}(t),\boldsymbol{p})u(t), \quad \text{(1b)}$$

$$\boldsymbol{x}(0) = \boldsymbol{x}_0,\ \boldsymbol{x}(t_\mathrm{f}) = \boldsymbol{x}_\mathrm{f}, \quad \text{(1c)}$$

$$u(t) \in [u_L, u_U], \quad \text{(1d)}$$

where t is time with $t \in [0, t_\mathrm{f}]$, $\boldsymbol{x}(t)$ is an n-dimensional vector of state variables, $\boldsymbol{p}$ is an m-dimensional vector of time-invariant model parameters, $u(t)$ is a (scalar) manipulated variable, $F_0(\cdot)$, $F_u(\cdot)$, $\boldsymbol{f}_0(\cdot)$, and $\boldsymbol{f}_u(\cdot)$ are continuously differentiable functions, $\boldsymbol{x}_0$ represents a vector of initial conditions, and $\boldsymbol{x}_\mathrm{f}$ are specified final conditions. We note here that an inclusion of multi-input and/or state-constrained cases is a straightforward extension but it is not considered in this study for the sake of simplicity of the presentation. We also note that the specific class of input-affine systems is a suitable representation for a large variety of the controlled objects (Hangos et al., 2006).

The presented problem was studied in many previous works using on-line or batch-to-batch adaptation of the optimality conditions (Francois and Bonvin, 2013) or by design of robust controller for tracking the conditions of optimality (Nagy and Braatz, 2003). Recently, several advanced robust strategies were presented in the framework of model predictive control (Lucia et al., 2013; Houska et al., 2017). This paper proposes adaptation of the aforementioned approaches to the problem of robustly optimal control of batch processes.

We base our approach on parameterization of the optimal controller using the conditions of optimality given by Pontryagin's minimum principle. This step reduces computational burden when projecting the parametric uncertainty in controller performance and feasibility. In order to improve of the controller, we use on-line parameter estimation. Finally, we derive the dual controller that considers adaptation of the optimal control inputs based on projected uncertainty and on prediction of the future learning of the controller.

2. PRELIMINARIES

2.1 Conditions for Optimality

Pontryagin's minimum principle can be used (Srinivasan et al., 2003) to identify the optimal solution to (1) via enforcing the necessary conditions for minimization of a Hamilton function (Hamiltonian)

$$H(\boldsymbol{x}(t),\boldsymbol{\lambda}(t),\boldsymbol{p},u(t),\mu_L(t),\mu_U(t)) := \mu_L(u_L - u) + \mu_U(u - u_U) + \underbrace{F_0 + \boldsymbol{\lambda}^T\boldsymbol{f}_0}_{H_0(\boldsymbol{x}(t),\boldsymbol{\lambda}(t),\boldsymbol{p})} + \underbrace{(F_u + \boldsymbol{\lambda}^T\boldsymbol{f}_u)}_{H_u(\boldsymbol{x}(t),\boldsymbol{\lambda}(t),\boldsymbol{p})} u, \quad (2)$$

where $\boldsymbol{\lambda}(t)$ is a vector of adjoint variables, and $\mu_L(t)$ and $\mu_U(t)$ are Lagrange multipliers associated with bounds on control input. The minimization is carried out such that

$$\min_{u(t),\boldsymbol{\nu},t_\mathrm{f},\mu_L(t)\geq 0,\mu_U(t)\geq 0} H \quad \text{(3a)}$$

$$\text{s.t. } \dot{\boldsymbol{x}}(t) = \boldsymbol{f}_0 + \boldsymbol{f}_u u(t), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0, \quad \boldsymbol{x}(t_\mathrm{f}) = \boldsymbol{x}_\mathrm{f}, \quad \text{(3b)}$$

$$\dot{\boldsymbol{\lambda}} = -\frac{\partial H}{\partial \boldsymbol{x}}, \quad \boldsymbol{\lambda}(t_\mathrm{f}) = \boldsymbol{\nu}, \quad \text{(3c)}$$

$$\mu_L(u_L - u(t)) = 0, \quad \mu_U(u(t) - u_U) = 0, \quad \text{(3d)}$$

where $\boldsymbol{\nu}$ are Lagrange multipliers that correspond to end-point equality constraints.

The necessary conditions for optimality of (3) can be stated as (Srinivasan et al., 2003): $\forall t \in [0, t_\mathrm{f}]$

$$\frac{\partial H}{\partial u} := H_u(\boldsymbol{x}(t), \boldsymbol{\lambda}(t), \boldsymbol{p}) - \mu_L(t) + \mu_U(t) = 0, \quad (4)$$

$$H(\boldsymbol{x}(t), \boldsymbol{\lambda}(t), \boldsymbol{p}, u(t), \mu_L(t), \mu_U(t)) = 0, \quad (5)$$

$$H_0(\boldsymbol{x}(t), \boldsymbol{\lambda}(t), \boldsymbol{p}) = 0, \quad (6)$$

$$\boldsymbol{x}(t_\mathrm{f}) - \boldsymbol{x}_\mathrm{f} = 0. \quad (7)$$

The condition (5) arises from the transversality, since the final time is free (Pontryagin et al., 1962), and from the fact that the optimal Hamiltonian is constant over the whole time horizon, as it is not an explicit function of time. The condition (6) is the consequence of the former two. Since the Hamiltonian is affine in input variable (see (2)), the optimal trajectory of control variable is either determined by active input constraints or it evolves inside the feasible region. Let us first consider the latter case.

Assume that for some point t we have $H_u(\cdot) = 0$ and $u_L < u(t) < u_U$. It follows from (4) that the optimal control maintains $H_u(t) = 0$. Such control is traditionally denoted as singular. Further properties of the singular arc, such as switching conditions or state-feedback control trajectory can be obtained by differentiation of $H_u(\cdot)$ with respect to time (sufficiently many times) and by requiring the time derivatives of $H_u(\cdot)$ to be zero. The time derivatives of $H(\cdot)$ and $H_0(\cdot)$ are equal to zero as well. Earlier results on derivation of optimal control for input-affine dynamic systems (Jönsson and Trägårdh, 1990; Srinivasan et al., 2003) suggest that it is possible to eliminate adjoint variables from the optimality conditions and thus arrive at analytical characterization of switching conditions and optimal control for singular and saturated-control arcs.

As the optimality conditions obtained by the differentiation w.r.t. time are linear in the adjoint variables, the differentiation of H_u (or H_0) can be carried out until it is possible to transform the obtained conditions to a pure state-dependent switching function $S(\boldsymbol{x}, \boldsymbol{p})$. It is usually convenient to use a determinant of the coefficient matrix of the equation system $\boldsymbol{A}\boldsymbol{\lambda} = \boldsymbol{0}$ for this. The optimal control is then given as a step-wise strategy (Paulen et al., 2015)

$$u^*(t, \boldsymbol{\pi}) := \begin{cases} u_L, & t \in [0, t_1],\ S(\boldsymbol{x}(t), \boldsymbol{p}) > 0, \\ u_U, & t \in [0, t_1],\ S(\boldsymbol{x}(t), \boldsymbol{p}) < 0, \\ u_\mathrm{s}(\boldsymbol{x}(t), \boldsymbol{p}), & t \in [t_1, t_2],\ S(\boldsymbol{x}(t), \boldsymbol{p}) = 0, \\ u_L, & t \in [t_2, t_\mathrm{f}],\ S(\boldsymbol{x}_\mathrm{f}, \boldsymbol{p}) < 0, \\ u_U, & t \in [t_2, t_\mathrm{f}],\ S(\boldsymbol{x}_\mathrm{f}, \boldsymbol{p}) > 0, \end{cases} \quad (8)$$

$$\boldsymbol{x}_\mathrm{f} = \boldsymbol{x}(t_2) + \int_{t_2}^{t_\mathrm{f}} \boldsymbol{f}_0(\boldsymbol{x}(t), \boldsymbol{p}) + \boldsymbol{f}_u(\boldsymbol{x}(t), \boldsymbol{p}) u^*(t)\, \mathrm{d}t, \quad (9)$$

where $\boldsymbol{\pi} := (\boldsymbol{p}^T, t_1, t_2, t_\mathrm{f})^T$ is the vector that parameterizes the optimal control strategy. The singular control $u_\mathrm{s}(\boldsymbol{x}(t), \boldsymbol{p})$ is found from

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\partial S}{\partial \boldsymbol{x}^T} \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \frac{\partial S}{\partial \boldsymbol{x}^T} (\boldsymbol{f}_0 + \boldsymbol{f}_u u_\mathrm{s}) = 0, \quad (10)$$

as

$$u_\mathrm{s}(\boldsymbol{x}(t), \boldsymbol{p}) = -\frac{\partial S}{\partial \boldsymbol{x}^T} \boldsymbol{f}_0 \Big/ \frac{\partial S}{\partial \boldsymbol{x}^T} \boldsymbol{f}_u, \quad (11)$$

Note that the presented optimal strategy determines implicitly the switching times t_1 from saturated to singular control and t_2 from singular to saturated control terminal time as well as the terminal time t_f.

In case the switching function $S(\boldsymbol{x}, \boldsymbol{p})$ is unidentifiable by the aforementioned procedure, the differentiation of H_u (or H_0) is carried out until the manipulated variable appears explicitly in one of the optimality conditions. It is then possible to devise an expression for singular control that is independent of adjoint variables. This is done by reducing the adjoint-affine system to triangular form from which the unknown adjoint variables can be expressed as functions of state variables.

3. IMPLEMENTATION OF OPTIMAL CONTROL

As the optimal control structure is a function of uncertain parameters of the process model, the uncertainty should be taken into account when devising a real-time implementation of the optimal control on the process. We will assume that the uncertainty is bounded as $\boldsymbol{p} \in \boldsymbol{P} := [\boldsymbol{p}^L, \boldsymbol{p}^U]$ and has a nominal realization $\boldsymbol{p}_0$.

3.1 Implementation via robust control

Given the optimal control sequence (8), it is possible to enclose all the reachable states $x(t, \boldsymbol{P}) \ni x(t, \boldsymbol{p}), \forall \boldsymbol{p} \supset \boldsymbol{P}$ of (1b) (Villanueva et al., 2015) such that one can identify realization of optimal control inputs sequence (e.g., $u^* = \{u^L, u_\mathrm{s}(\boldsymbol{x}(t), \boldsymbol{p}), u^U\}$) and switching times of the control structure as functions of uncertain parameters $t_1(\boldsymbol{p})$, $t_2(\boldsymbol{p})$, and $t_\mathrm{f}(\boldsymbol{p}), \forall \boldsymbol{p} \in P$. One can then formulate a semi-infinite program similar to Stuber and Barton (2011) or some related problem (e.g., using polynomial expansion (Houska et al., 2017)), to determine the parameters of the optimal control structure that lead to the best performance in the worst case. For the parameterized optimal control sequence, we can solve

$$\min_{t_1, t_2, t_\mathrm{f}} \ \|\mathcal{J}(\boldsymbol{P}) - \mathcal{J}(\boldsymbol{p}_0)\|_2^2 \quad (12)$$

$$\text{s.t. } \dot{\boldsymbol{x}}(t) = \boldsymbol{f}_0(\boldsymbol{x}(t), \boldsymbol{p}) + \boldsymbol{f}_u(\boldsymbol{x}(t), \boldsymbol{p}) u^*,\ \forall \boldsymbol{p} \in P, \quad (13)$$

$$\boldsymbol{x}(t_\mathrm{f}, \boldsymbol{P}) \ni \boldsymbol{x}_\mathrm{f}, \quad (14)$$

for a given $\boldsymbol{x}(0) = \boldsymbol{x}_0$ and $\boldsymbol{P}$, where we propose to minimize variance of the objective under all the possible realizations of the measurement noise, but we note that other formulations are possible, e.g., to optimize for mean or worst-case realization. Note that this approach represents an open-loop strategy, i.e., it does not consider feedback. As a consequence, it will result in infeasibility w.r.t. terminal conditions, as the terminal state constraints can only be enforced if there exists a full-state measurement. A possible remedy to this issue lies in receding horizon approach with shrinking horizon. This can be also implemented using multi-stage optimization approach (Lucia et al., 2013), which takes explicitly into account the presence of feedback via full-state measurement and thus avoids conservatism to some extent.

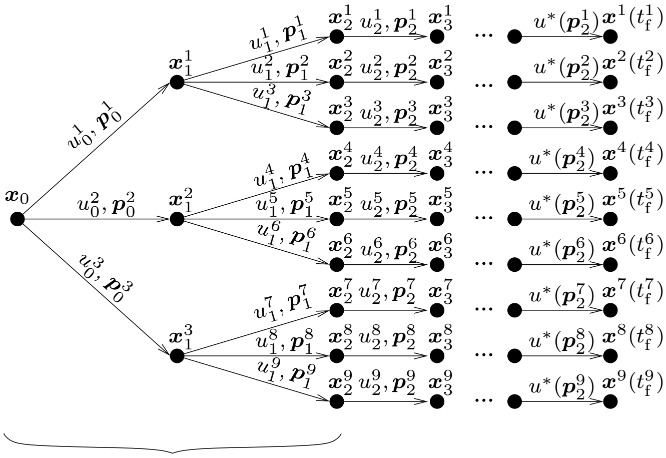

Fig. 1. Scenario tree representation of the uncertainty evolution for a multi-stage controller.

3.2 Implementation via adaptive robust control

As shown in Adetola et al. (2009) and in Lucia and Paulen (2014), in order to further reduce conservatism of the multi-stage (robust) scheme, parameter estimation can be used for exploitation of data gathered along the process run. The employed parameter estimation scheme should take into account noise in measurements and, if applied recursively for each newly gathered measurements set, it should result in a sequence of the confidence intervals

$$\boldsymbol{P}_k \subseteq \boldsymbol{P}_{k-1} \subseteq \cdots \subseteq \boldsymbol{P}_1 \subseteq \boldsymbol{P}_0 \subseteq \boldsymbol{P}. \tag{15}$$

A possible estimation procedure is outlined in Appendix A. The problem (12) can then be resolved with the initial state conditions $\boldsymbol{x}(k) = \boldsymbol{x}_k$ and with updated parameter bounds $\boldsymbol{P}_k$ in shrinking-horizon fashion. Once the optimal value of the objective function of (12) reaches $\|\mathcal{J}(\boldsymbol{P}) - \mathcal{J}(\boldsymbol{p}_0)\|_2^2 < \varepsilon$, the calculated control actions can be implemented, possibly with a feedback scheme (Francois and Bonvin, 2013), until the terminal conditions are met.

3.3 Implementation via dual robust control

Several recent works (Thangavel et al., 2015; Hanssen and Foss, 2015; La et al., 2017) presented novel implicit and explicit schemes to dual control based on receding-horizon control. We adapt the implicit dual-control methodology presented in Thangavel et al. (2015) in this study as, despite being computationally more demanding, it requires no a priori tuning of the objective regarding the importance of experiment-design objective. It models the evolution of the uncertainty in the states and parameters as a tree of discrete realizations of the uncertainty

$$\min_{\substack{t_1^j, t_2^j, t_\mathrm{f}^j, \forall j \in I \\ u_k^j, \forall k \leq N_r, \forall j \in I}} \quad \|\boldsymbol{\mathcal{J}}(\boldsymbol{p}) - \mathcal{J}(\boldsymbol{p}_0)\|_2^2 \tag{16a}$$

s.t. $\forall j \in I:$

$$\dot{\boldsymbol{x}}^j = \boldsymbol{f}_0(\boldsymbol{x}^{p(j)}, p_k^{r(j)}) + \boldsymbol{f}_u(\cdot)u_k^j, \ \forall k < N_r, \tag{16b}$$

$$\dot{\boldsymbol{x}}^j = \boldsymbol{f}_0(\boldsymbol{x}^{p(j)}, p_k^{r(j)}) + \boldsymbol{f}_u(\cdot)u^{j,*}, \ \forall k \geq N_r, \tag{16c}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)}, \ \forall l \in I, \tag{16d}$$

$$\boldsymbol{p}_{k+1}^{r(j)} = h(\boldsymbol{x}_k^{p(j)}, u_k^j, \boldsymbol{p}_k^{r(j)}), \ \forall k < N_r, \tag{16e}$$

$$\boldsymbol{x}^j(t_\mathrm{f}) = \boldsymbol{x}_\mathrm{f}, \tag{16f}$$

where $\boldsymbol{\mathcal{J}}(\boldsymbol{p}) := (\mathcal{J}(\boldsymbol{p}_{N_r}^{r(1)}), \mathcal{J}(\boldsymbol{p}_{N_r}^{r(2)}), \ldots, \mathcal{J}(\boldsymbol{p}_{N_r}^{r(n_s)}))^T$. We adopt the notation from Lucia and Paulen (2014); Jang et al. (2016) where index k denotes the sample-and-hold value of a variable on the interval $[t_k, t_{k+1}]$, j represents a particular realization of uncertainty and $p(j)$ is the realization at parent node of the scenario tree 1. The tree contains n_s scenarios that correspond to index set I of the uncertainty propagation through dynamics of the system. The function $h(\cdot)$ denotes the estimation and bounding equations (A.4) and (A.7). The value of N_r represents the length of the so-called robust horizon, which marks the stage, until which the tree is considered to branch. Note that this models a possible variability in the parametric uncertainty and, in proposed methodology, it models the estimation of the bounds of uncertain parameters. Note also that the control inputs are free until the stage N_r—they only need to fulfill the non-anticipativity constraints (16d)—so the proposed scheme shows a significant reduction of the number of degrees of freedom of the optimization as opposed to the situation, where only the multi-stage approach (equivalent under some assumptions to robust dynamic programming) would be used without the parameterized solution to nominal optimal control problem. The value of N_r should be set as big as possible, ideally until the stage when the earliest possible switching of the optimal control input occurs. A similar approach is utilized for uncertainty propagation in set-membership context by Yousfi et al. (2017). However, as the simulation experiments have showed for standard multi-stage predictive control Lucia et al. (2013), $N_r = 1$ or $N_r = 2$ is a practical and sufficient choice w.r.t. to the performance of the scheme in most cases.

A possible interpretation of the presented dual-control scheme is that:

- the optimal excitation of the system, which results in improved precision of parameter bounds, is obtained as a consequence of minimization of the variance of the objective function under uncertainty and by freeing the (initial) control moves on the robust horizon from the optimality conditions of (1);
- the optimality of each scenario is guaranteed by control parametrization using optimality conditions and from principle of dynamic programming, which means that, despite initial control moves are not fixed, the control moves until the end of the horizon are optimal w.r.t. state values of each scenarios.

Note that because of the switching nature of the optimal control strategy, the proposed problem might show discontinuity as a consequence of activation of the input constraints based on uncertain parameters $(S(\boldsymbol{x}(t), \boldsymbol{p}))$. Simply speaking, it may happen that for a subset of $\boldsymbol{P}$ the resulting optimal sequence commences with $u(t) = u_L$ and vice versa for other subset of $\boldsymbol{P}$. This can be remedied by an adaptation of the continuous-formulation technique for scheduling presented in de Prada et al. (2011).

4. CASE STUDY

We consider a case study of time-optimal control of a batch diafiltration process from Paulen et al. (2012). The scheme of the plant is shown in Fig. 2. The goal is to process

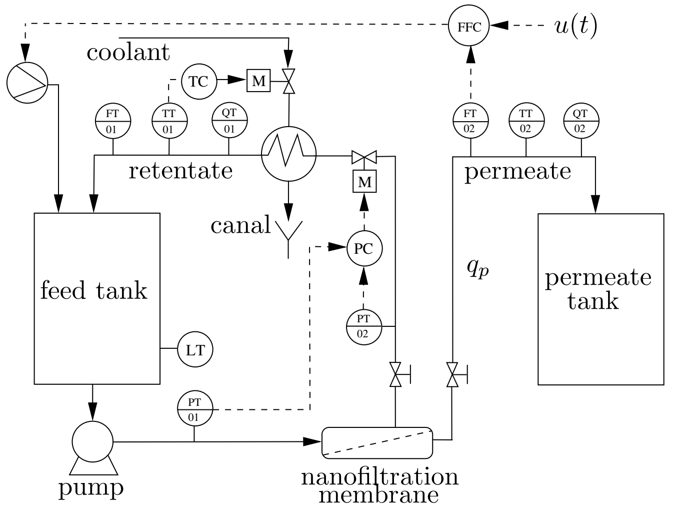

Fig. 2. Nanodiafiltration process scheme.

a solution with initial volume (V_0) that is fed into the feed tank at the start of the batch and that comprises two solutes of initial concentrations $c_{1,0}$ and $c_{2,0}$. At the end of the batch, the prescribed final concentrations $c_{1,\mathrm{f}}$ and $c_{2,\mathrm{f}}$ must be met. The transmembrane pressure is controlled at a constant value. The temperature of the solution is maintained around a constant value using a heat exchanger. The manipulated variable $u(t)$ is the ratio between fresh water inflow into the tank and the permeate outflow q_p that is given by

$$q_p = \gamma_1 \ln\left(\frac{\gamma_2}{c_1 c_2^{\gamma_3}}\right) = \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2)\right). \tag{17}$$

and is measured at intervals of one minute with the assumed measurement noise that is bounded by $\sigma = 1 \times 10^{-6}\mathrm{m}^3/\mathrm{h}$. The model of the permeate flux can be reduced to another widely used *limiting flux model* if $\gamma_3 = 0$, so this case study offers to study both parametric and non-parametric plant-model mismatch. The measurement of q_p is used for inferring the values of the parameters $\gamma_1, \gamma_2, \gamma_3$. Note that this leads to linear parameter estimation problem with the regressor $\boldsymbol{c} = (1, \ln(c_1), \ln(c_2))^T$ and parameters $\hat{\boldsymbol{p}} = (\gamma_1 \ln(\gamma_2), \gamma_1, \gamma_1\gamma_3)^T$, from which the values of $\gamma_1, \gamma_2, \gamma_3$ follow directly. Concentrations of both components $c_1(t)$ and $c_2(t)$, where the first component is retained by the membrane and the second one can freely pass through, are measured as well and will be assumed to be perfectly known. This is only assumed for simplicity. Should an uncertainty be considered in measured values of $c_1(t)$ and $c_2(t)$, an error-in-variables approach (Söderström, 2007) can be adopted for parameter estimation.

The objective is to find a time-dependent input function $u(t)$, which guarantees the transition from the given initial $c_{1,0}, c_{2,0}$ to final $c_{1,\mathrm{f}}, c_{2,\mathrm{f}}$ concentrations in minimum time. This problem can be formulated as:

$$\mathcal{J}^* = \min_{u(t)\in[0,\infty)} \int_0^{t_\mathrm{f}} 1\,\mathrm{d}t, \tag{18a}$$

$$\text{s.t. } \dot{c}_1 = \frac{c_1^2 q_p}{c_{1,0} V_0}(1-u),\ c_1(0) = c_{1,0},\ c_1(t_\mathrm{f}) = c_{1,\mathrm{f}} \tag{18b}$$

$$\dot{c}_2 = -\frac{c_1 c_2 q_\mathrm{p}}{c_{1,0} V_0} u,\ c_2(0) = c_{2,0},\ c_2(t_\mathrm{f}) = c_{2,\mathrm{f}} \tag{18c}$$

$$q_p = \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2)\right). \tag{18d}$$

The parameters of the problem are $c_{1,0} = 10\,\mathrm{mol/m^3}$, $c_{1,\mathrm{f}} = 200\,\mathrm{mol/m^3}$, $c_{2,0} = 100\,\mathrm{mol/m^3}$, $c_{2,\mathrm{f}} = 0.01\,\mathrm{mol/m^3}$, $V_0 = 0.1\,\mathrm{m^3}$, $\gamma_1 = 3600 \times 4.79 \times 10^{-6}\,\mathrm{m/h}$ $\gamma_2 = 319\,\mathrm{mol/m^3}$, $\gamma_3 = 0.2$. The extremal values of $u(t)$ stand for a mode with no water addition, i.e., pure filtration, when $u(t) = 0$ and pure dilution, i.e., a certain amount of water is added at a single time instant, $u(t) = \infty$.

The nominal (parametrized) optimal control of this process can be identified using Pontryagin's minimum principle (Pontryagin et al., 1962) as:

$$u^*(t, \boldsymbol{\pi}) = \begin{cases} 0, & t \in [0, t_1],\ S(\boldsymbol{x}(t), \boldsymbol{p}) > 0, \\ \infty, & t \in [0, t_1],\ S(\boldsymbol{x}(t), \boldsymbol{p}) < 0, \\ u_s, & t \in [t_1, t_2],\ S(\boldsymbol{x}(t), \boldsymbol{p}) = 0, \\ 0, & t \in [t_2, t_\mathrm{f}],\ S(\boldsymbol{x}_\mathrm{f}, \boldsymbol{p}) < 0, \\ \infty, & t \in [t_2, t_\mathrm{f}],\ S(\boldsymbol{x}_\mathrm{f}, \boldsymbol{p}) > 0, \end{cases} \tag{19}$$

where the singular control and the respective switching function can be found explicitly (Paulen et al., 2012) as

$$u_s(\boldsymbol{x}(t), \boldsymbol{p}) := \frac{1}{1+\gamma_3}, \tag{20}$$

$$S(\boldsymbol{x}(t), \boldsymbol{p}) := \gamma_1 \left(\ln(\gamma_2) - \ln(c_1) - \gamma_3 \ln(c_2) - \gamma_3 - 1\right). \tag{21}$$

For the given parameters of the problem, the optimal control sequence is $u^* = \{0, 0.8333, \infty\}$ with switching times $t_1 = 2.2087\,\mathrm{h}$ and $t_2 = t_\mathrm{f} = 3.17\,\mathrm{h}$.

We consider the parametric uncertainty to be given by:

$$\boldsymbol{P} := \begin{pmatrix} [\gamma_1^L, \gamma_1^U] \\ [\gamma_2^L, \gamma_2^U] \\ [\gamma_3^L, \gamma_3^U] \end{pmatrix} = \begin{pmatrix} [4.65, 4.85] \times 10^{-6} 3600\,\mathrm{m/h} \\ [300, 700]\,\mathrm{mol/m^3} \\ [0.15, 0.3] \end{pmatrix}. \tag{22}$$

The nominal values of parameters are taken as mid($\boldsymbol{P}$). With respect to the nominal values the uncertainties in parameters are 2.11% for γ_1, for 40% γ_2, 33.33% for γ_3. This is assumed to mimic practical considerations, where γ_1 represents a mass-transfer coefficient, whose value is usually known with relatively high accuracy. It is clear that the real-time optimality of the operation is strongly influenced by accuracy of the estimation of the parameters γ_2 and γ_3. Preliminary numerical tests with optimal experiment design (OED) methodology (Gottu Mukkula and Paulen, 2017) showed that for the most accurate estimation of γ_2 the manipulated variable $u(t) = 0$ and, on the other hand, the best estimation accuracy of γ_3 is reached when $u(t) = 1$. This shows mutual benefit of the optimal control strategy $u^* = \{0, 0.8333, \infty\}$ and estimation of γ_2, and a potential conflict of accurate estimation of γ_3 and the optimal control policy. This can also be seen from (17) and (18c), where it is clear that when the (nominally) optimal controller applies $u(t) = 0$, the parameter γ_3 is unidentifiable as the concentration $c_2(t)$ remains constant. The OED studies also showed that the best time to excite

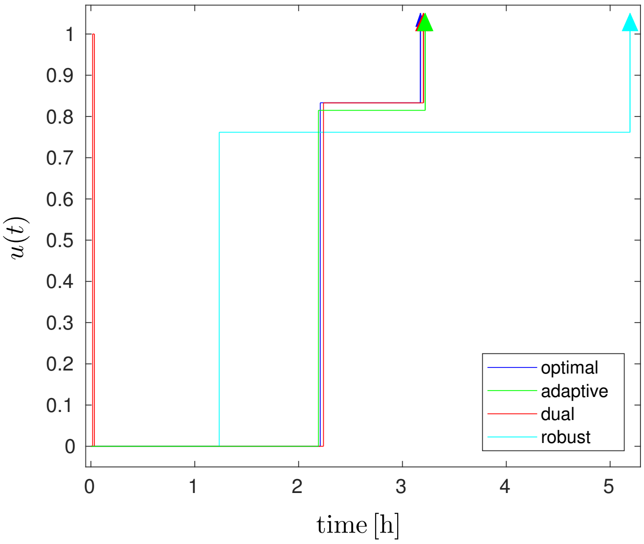

Fig. 3. Comparison of control profiles of different controllers.

the plant is in the beginning of the operation. This stems from the absolute error of the measurement (see (A.2)) and from the fact that the measured permeate flux is highest in the beginning of the operation and drops dramatically with the increase of concentration $c_1(t)$. For the estimation procedure described in Appendix A we have used $\beta = 0.25$.

Application of the proposed controllers results in the control profiles that are shown in Fig. 3. Both adaptive and dual controller reach almost the same performance as the (hypothetic) optimal controller, which has a perfect knowledge of the true values of parameters, which comes as a consequence of the constant singular control, the nature of the singular control in general ($\partial H/\partial u = 0$, see the discussion in Srinivasan et al. (2003)) and the ability of the controllers to guess the value of t_1 relatively well despite the imprecise estimates. The importance of this guess can be documented by the performance of the min-max robust controller (cyan curve in Fig. 3), where even though the controller finds a value of singular control that is close to the optimal one, the early switch to the singular arc results in poor performance. Performance of the dual controller ($t_\mathrm{f} = 3.20\,\mathrm{h}$) is slightly better than the performance of the adaptive controller ($t_\mathrm{f} = 3.22\,\mathrm{h}$). This arises from the probing action that is performed by the dual controller at the beginning of the batch, where the control-moves sequence of the dual controller is $\{u_1, u_2, u_3, \dots\} := \{0, 1, 0, \dots\}$.

Figure 4 shows the mean and the variance in the performance of the studied controllers in 1,000 simulations with different true values of parameters $\boldsymbol{p}$ taken from uniform grid of $\boldsymbol{P}$. It is clear that adaptive and dual controller reach performance very close to the optimal one. They also greatly reduce the variance of the min-max or nominal controller (not shown for brevity). It is also clear for this case study that for the actual realization of the control of this plant, a dual controller would not be essential. So in this case, the presented methodology would serve in the design phase to assess the need of advanced robust adaptive controller.

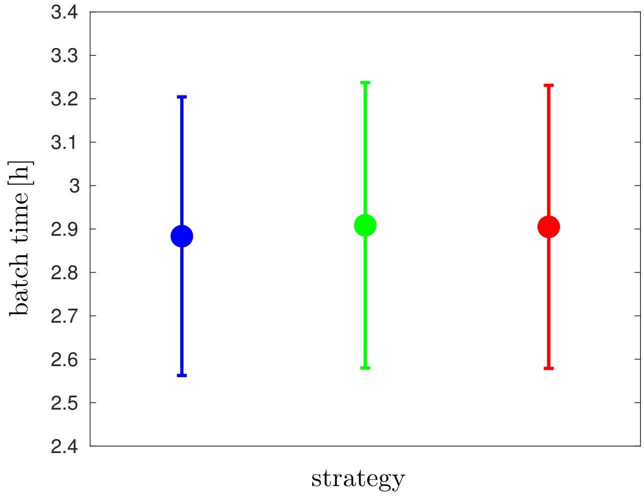

Fig. 4. Mean and variance of performance of the different controllers. The same color coding as in Fig. 3 is used.

5. CONCLUSION

We have presented a novel methodology for dual robust controller design for the (real-time) optimal control of batch processes. The controller achieves the dual action by explicit consideration of the effects of the future exciting control signal on the performance of the plant. The crucial step is the parameterization of the (open-loop) optimal controller. This allows for adaptation and implementation of the dual robust control strategies devised earlier in the literature. The benefits of the approach were shown in the case study on batch membrane filtration. Set-membership estimation was used for the parameter estimation, as a technique that can provide guaranteed bounds on the parametric uncertainty. The future work will concentrate on the experimental validation of the presented methodology at the laboratory membrane plant.

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Appendix A. SET-MEMBERSHIP ESTIMATION

We will focus on the case when the model is linear in parameters such that

$$\hat{y}(\boldsymbol{p}) = \boldsymbol{c}^T \boldsymbol{p}, \tag{A.1}$$

where $\hat{y}$ is the prediction of the plant output y and $\boldsymbol{c}$ is a so-called regressor vector. The linearity of the model in parameters is not restrictive, the presented methodology applies to systems that are non-linear in parameters too, and is considered for simplicity. We will further assume that the measurement noise is bounded so that

$$|y - \hat{y}(\boldsymbol{p})| \leq \sigma. \tag{A.2}$$

Under these assumptions a recursive set-membership parameter estimation scheme was presented in Fogel and Huang (1982); Chabane et al. (2014), which over-bounds the set of all parameter values that satisfy (A.2) as an ellipsoid

$$(\boldsymbol{p} - \hat{\boldsymbol{p}})^T \boldsymbol{V}^{-1} (\boldsymbol{p} - \hat{\boldsymbol{p}}) \leq 1, \tag{A.3}$$

where $\hat{p}$ is the expected true value of the parameters and $\boldsymbol{V}$ is parameter covariance matrix. Upon receiving a new measurement, $\hat{p}$ and $\boldsymbol{V}$ are updated by

$$\hat{\boldsymbol{p}}_+ = \hat{\boldsymbol{p}} + \frac{\beta d}{1 + \beta g} \boldsymbol{V} \tilde{c}, \tag{A.4}$$

$$\boldsymbol{V}_+ = \left(1 + \beta - \frac{\beta d^2}{1 + \beta g}\right) \left(\boldsymbol{V} - \frac{\beta}{1 + \beta g} \boldsymbol{V} \tilde{\boldsymbol{c}} \tilde{\boldsymbol{c}}^T \boldsymbol{V}\right), \tag{A.5}$$

where

$$\tilde{\boldsymbol{c}} := \boldsymbol{c}/\sigma, \quad g := \tilde{\boldsymbol{c}}^T \boldsymbol{V} \tilde{\boldsymbol{c}}, \quad d := y/\sigma - \tilde{\boldsymbol{c}}^T \hat{\boldsymbol{p}}. \tag{A.6}$$

The parameter $\beta \in (0, 1)$ can be selected in order to minimize trace or determinant of the covariance matrix $\boldsymbol{V}$ (Fogel and Huang, 1982). The updated bounds of parameters can be found via

$$\boldsymbol{P}_+ := \left[\hat{\boldsymbol{p}}_+ - \operatorname{diag}\left(\boldsymbol{V}_+^{\frac{1}{2}}\right), \hat{\boldsymbol{p}}_+ + \operatorname{diag}\left(\boldsymbol{V}_+^{\frac{1}{2}}\right)\right]. \tag{A.7}$$

We note that it is also equally possible to form a series of linear programs that would bound the parameter values that are consistent with the measurements. This might improve accuracy of the estimates. For the implementation of the dual controller, optimality conditions of the linear program would be embedded into the problem (16).