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# On the Implementation of Nonlinear Model Predictive Control for Simultaneous Design and Control Using a Back-Off Approach

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**Abstract:** In the present work, we investigate the challenges and limitations of the incorporation of nonlinear model predictive control (NMPC) for the integration of design and control of chemical processes. To tackle this problem, we implemented a simultaneous methodology based on a back-off approach, in which the process design moves away from the optimal steady-state to a new dynamically feasible operating condition under process disturbances. The procedure is formulated as a series of bounded optimization problems in a sequential manner to identify the optimal design of the process with optimal control performance. Power series expansion (PSE) is used to represent constraints and cost functions in the bounded optimization problems. The approach has been implemented on a wastewater treatment plant. Results indicate that the proposed methodology leads to considerable improvement in the process economics and performance compared to a decentralized PI control strategy.

*Keywords:* Interaction between design and control, Model predictive and optimization based control, Process optimization

## 1. INTRODUCTION

Classical approaches for process design focuses on the consideration of steady-state operation such that design and operating conditions are often decided in the absence of process uncertainty and disturbances. Subsequently, process dynamics are considered for the intended design. Traditionally, the connection of process dynamic behavior to design factors is considered in a sequential way. Instead, in modern approaches for process design, the controllability aspects are taken into account at the early stages of process design where the dynamic interactions between the design and control parameters are considered simultaneously. The integrated concept results in attractive alternatives to obtain optimal profitable process designs that remain dynamically feasible in the presence of disturbances and uncertainty.

Integration of design and control leads to more economically attractive process designs and plant performance. In further attempts to improve process performance, the application of advanced control strategies has been considered within the integrated design and control framework. Although the implementation of decentralized strategies based on PID controllers often results in acceptable control schemes, the application of modern control approaches, such as model predictive control (MPC), has shown significant improvements in terms of process performance and process economics (Francisco et al. (2009); Moon et al. (2011)). MPC strategy has some advantages over PID control in handling multivariable control problems and offers the possibility of including explicit constraints. Previously, simultaneous design and control techniques using MPC has been proposed in the literature (Brengel and Seider (1992)). Sanchez-Sanchez and Ricardez-Sandoval (2013) presented a methodology that incorporates structural decisions for the selection of optimal process flowsheet and control design by the evaluation of convex dynamic feasibility and asymptotic stability analysis. Implementation of a multi-parametric MPC approach for simultaneous design and control was presented by Diangelakis and Pistikopoulos (2017); that work suggested an improvement in operating cost compared to decentralized PI controllers. Furthermore, Bahakim and Ricardez-Sandoval (2014) reported economically attractive designs with high control performance for MPC-based simultaneous design and control in comparison to decentralized PI controllers under stochastic-based uncertainty descriptions. Simultaneous design and control is an area widely studied nowadays. A complete review and discussion about the state-of-the-art and future steps is discussed by Pistikopoulos and Diangelakis (2016). Nevertheless, the performance of NMPC within an integrated design and control framework has been identified as one of the open challenges in this field (Rafiei and Ricardez-Sandoval (2019)). To the authors' knowledge, previous studies addressing simultaneous design and control with an NMPC has not been reported.

NMPC relies on the nonlinear constraints and dynamics of the problem and has shown enhancements in control performance compared with linear MPC (Biegler and Thierry (2018)). Often, linear MPC may need to be avoided when processes exhibit nonlinear behavior; thus, the implementation of a controller with a nonlinear model to capture the actual behavior of the process is preferred. The back-off methodology for optimal simultaneous design and control using Power Series Expansions (PSE) has been proposed previously in our group (Rafiei and Ricardez-Sandoval (2018); Rafiei-Shishavan and Ricardez-Sandoval (2017); Mehta and Ricardez-Sandoval (2016)). In those studies, PID-based control approaches were considered. In the current work, we explore the implementation of an NMPC framework for simultaneous design and control using the back-off methodology previously developed in our group. To the authors' knowledge, this is the first study that explores the implementation of an NMPC scheme in the context of integration of design and control. The outline of this work is as follows: Section 2 presents the description of the proposed methodology for simultaneous design and control. Section 3 presents a wastewater treatment plant case study that is used to test the performance of the present approach. At the end, concluding remarks and directions for future works are provided.

## 2. FORMULATION & METHODOLOGY

In this section, the NMPC formulation is introduced first. Then, we provide a detailed description of the method and challenges regarding to the implementation of NMPC for the integration of design and control.

### *2.1 Nonlinear Model Predictive Control*

NMPC is based on the solution of an optimization problem where the cost function penalizes the deviations of the controlled and manipulated variables with respect to a reference trajectory (i.e. a set-point). NMPC generates a prediction of the dynamic behavior of the process based on measurements obtained from the process at time $t$; the predictions are generated forward in time such that the controller can minimize the control actions required to reach the target. The optimization problem for an NMPC-based controller is as follows:

$$\min_{\Delta\widehat{u}(\cdot)} \quad \Psi(\widehat{\boldsymbol{x}}(\tau), \Delta\widehat{u}(\tau)) \tag{1a}$$

$$\text{s.t.} \qquad \dot{\widehat{\boldsymbol{x}}} = F(\widehat{\boldsymbol{x}}(\tau), \widehat{\boldsymbol{u}}(\tau), \boldsymbol{d}) \tag{1b}$$

$$H(\widehat{\boldsymbol{x}}(\tau), \widehat{\boldsymbol{u}}(\tau), \boldsymbol{d}) = 0 \tag{1c}$$

$$G(\widehat{\boldsymbol{x}}(\tau), \widehat{\boldsymbol{u}}(\tau), \boldsymbol{d}) \leq 0 \tag{1d}$$

$$\widehat{\boldsymbol{u}}(\tau) \in U, \ \ \forall \, \tau \in [t, t+t_C], \tag{1e}$$

$$\widehat{\boldsymbol{u}}(\tau) = \widehat{\boldsymbol{u}}(t+t_C), \ \ \forall \, \tau \in [t+t_C, t+t_P], \tag{1f}$$

$$\widehat{\boldsymbol{x}}(\tau) = \boldsymbol{x}(t), \ \ \forall \, \tau = t \tag{1g}$$

$$\widehat{\boldsymbol{x}}(\tau) \in X, \ \ \forall \, \tau \in [t, t+t_P] \tag{1h}$$

$$X := \left\{ x \in \mathbb{R}^n \middle| \ x^L \leq x \leq x^U \right\} \tag{1i}$$

$$U := \left\{ u \in \mathbb{R}^m \middle| \ u^L \leq u \leq u^U \right\} \tag{1j}$$

$$T := \left\{ \tau \in \mathbb{R}^l \middle| \ t \leq \tau \leq t+t_P \right\} \tag{1k}$$

where, $t_P$ and $t_C$ are the prediction and control horizon, respectively. $\boldsymbol{d}$ represents the set of measured disturbances affecting the process that remain constant during the prediction horizon. $\Delta\widehat{u}$ is the predicted change of the manipulated variables. Both $\Delta\widehat{u}$ and $\widehat{x}$ are bounded in the range of $u^L, u^U$ and $x^L, x^U$, respectively. $H$ represents the set of equality constraints. Moreover, $G$ represents the set of inequalities that define the feasibility region for the process. Likewise, $\Psi$ represents the controller cost function given by Equation (2).

$$\Psi = \int_t^{t+t_P} \|\widehat{\boldsymbol{x}}(\tau) - x^{sp}\|^2_{\boldsymbol{Q}} + \|\Delta\widehat{\boldsymbol{u}}(\tau)\|^2_{\boldsymbol{R}} \ \ d\tau \tag{2}$$

where $\mathbf{Q}$ and $\mathbf{R}$ are positive-defined weighting matrices. $\widehat{x}$ and $x^{sp}$ are the predicted value of states and their desired reference values, respectively. In the present NMPC problem we assume that we have access to the measurement for all states in the process, i.e. predicted variables ($\widehat{\boldsymbol{x}}$) are the same as measured states ($\boldsymbol{x}$) at time $\tau$ equal to $t$ (Equation (1g)).

The tuning parameters for NMPC are the weighting matrices and the control and prediction time horizons. A primary approximation for the weighting matrices ($\mathbf{Q}$ and $\mathbf{R}$), and prediction and control horizons ($t_P$ and $t_C$, respectively) is carried out through closed-loop simulations. The closed-loop system is tested with a set of disturbances such that $\mathbf{Q}$, $\mathbf{R}$, $t_P$, and $t_C$ are adjusted based on the observed performance of the controller to reject the pre-specified disturbances. However, increasing or decreasing the magnitude of weighting matrices, $\mathbf{Q}$ and $\mathbf{R}$, can reduce the sensitivity of the controller to changes in the controlled variables or inhibit the controller actions. On the other hand, increasing $t_P$ and $t_C$ may require a higher computational cost, thus making their implementation challenging for online control. The selection of the tuning parameters is directly related to the speed of the controller response to dynamic changes in the process (i.e. $\mathbf{R}$, $t_P$, and $t_C$) and the precision of the controller in maintaining the control variables at their corresponding desired set-points (i.e. $\mathbf{Q}$). Therefore, these parameters can be considered as part of the optimization variables, i.e. control decision variables, in the simultaneous design and control optimization problem, which is described next.

### *2.2 Simultaneous Design & Control with NMPC*

The integration of design and control considers the solution of an optimization problem where economic profits (design aspects) and control performance (operating aspects) are simultaneously considered. Then the conceptual mathematical formulation for the simultaneous design and control with NMPC is as follows:

$$\min_{\boldsymbol{\eta}=[\boldsymbol{\gamma},\boldsymbol{\varsigma}],\boldsymbol{x},\overline{\boldsymbol{u}},\boldsymbol{y}} \quad \Phi(\boldsymbol{\varsigma}, \boldsymbol{x}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{y}(t), \boldsymbol{d}(t)) \tag{3a}$$

$$\text{s.t.} \qquad \dot{\boldsymbol{x}} = f(\boldsymbol{\gamma}, \boldsymbol{\varsigma}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) \tag{3b}$$

$$h(\boldsymbol{\gamma}, \boldsymbol{\varsigma}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) = 0 \tag{3c}$$

$$g(\boldsymbol{\gamma}, \boldsymbol{\varsigma}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) \leq 0 \tag{3d}$$

$$\overline{\boldsymbol{u}}(\tau) = \arg\left\{ \min_{\widehat{\boldsymbol{u}}} \ \Psi(\cdot) \ \text{ s.t. } \dot{\widehat{\boldsymbol{x}}}, H(\cdot), G(\cdot), \ \widehat{\boldsymbol{u}} \in U \right\} \tag{3e}$$

where $h$ denotes the equality constraints of the process and $g$ represents the process feasibility constraints. The states of the system are given by $\boldsymbol{x}$ with time derivatives indicated as $\dot{\boldsymbol{x}}$; $\overline{\boldsymbol{u}}$ represents the control actions obtained from the NMPC formulation as shown in Equation (3e); whereas $\boldsymbol{y}$ are the measured states of the system. Decision variables, $\boldsymbol{\eta} = [\boldsymbol{\gamma}, \boldsymbol{\varsigma}]$, contain the process design variables ($\boldsymbol{\gamma}$) such as equipment sizing parameters, e.g. area and volume; and the controller tuning parameters ($\boldsymbol{\varsigma}$) such as weighting matrices, $\mathbf{Q}$ and $\mathbf{R}$. Note that control actions $\overline{\boldsymbol{u}}$ stated in Equation (3e) are given by the solution the NMPC optimization problem described in the Equation (1). The cost function $\Psi$ is given by Equation (1a) and is subject to the dynamic model for system states $\dot{\boldsymbol{x}}$, and constraints $H$ and $G$ (i.e. Equations (1b), (1c), and (1d), respectively). In the NMPC formulation, the inclusion of nonlinear differential equations $\dot{\boldsymbol{x}}$ is carried out by the discretization of these equations using orthogonal collocation on finite elements. For design and control purposes a set of disturbances ($\boldsymbol{d}(t)$) is considered to ensure robustness of the solution to perturbations that can take place during the process' operation. Note that $\boldsymbol{d}(t)$ is not available *a priori* for the controller as part of the input information to predict control actions; however, it is assumed that measurement for states and disturbances are available for the NMPC at any time interval, where the disturbances are kept constant to their current values along the prediction and control horizons in the NMPC formulation.

Implementation of NMPC for simultaneous design and control represents a challenging task since it implies the solution of a sub-level optimization problem to calculate the control actions required to maintain at the dynamic operation of the process on target and feasible. Then, the optimization model becomes a bi-level optimization problem that consists of two levels. The outer level represents the design problem whereas the inner level is the optimal (NMPC) control problem. The solution of the NMPC sub-level (inner) aims to calculate the control actions. Accordingly, NMPC has a different dimension of time $\tau \in [t, t+t_P]$ as shown in Equation (1h), while the primary (outer) problem takes place between the initial simulation time $t_0$ and the final time $t_f$ (i.e. $t \in [t_0, t_f]$). Interactions between the inner and outer optimizations problems are given by the design variables ($\boldsymbol{\gamma}$) and the set of controller tuning parameters ($\boldsymbol{\varsigma}$). As described above, solving the conceptual problem presented in Equation (3) may become challenging even for medium-size applications. Thus, a reformulation of the original problem is required to reduce the complexity burden. Typically, the problem is decomposed and solved using sequential algorithms. Although a direct solution can be addressed using mathematical programs with complementarity constraints, it increases the complexity of the model and the computational demands (Migdalas et al. (2013)). In the present work, we use a back-off approach previously developed in our group to examine the behavior of the model using piecewise PSE models in an iterative manner. The back-off is an attractive alternative since it reduces the complexity of the problem and thus requires lower computational demands. The methodology seeks for the optimal design and control parameters that maintain the process in a dynamically feasible state, given a set of process disturbances. The description of the methodology is provided next.

### *2.3 Back-off Approach*

A back-off methodology is employed to integrate design and a NMPC-based control scheme. An extended description of the back-off methodology can be found elsewhere (Rafiei and Ricardez-Sandoval (2018)). In this section, we present a brief description of the NMPC-based implementation proposed in the current work to address simultaneous design and control. This methodology is illustrated in Figure 1.

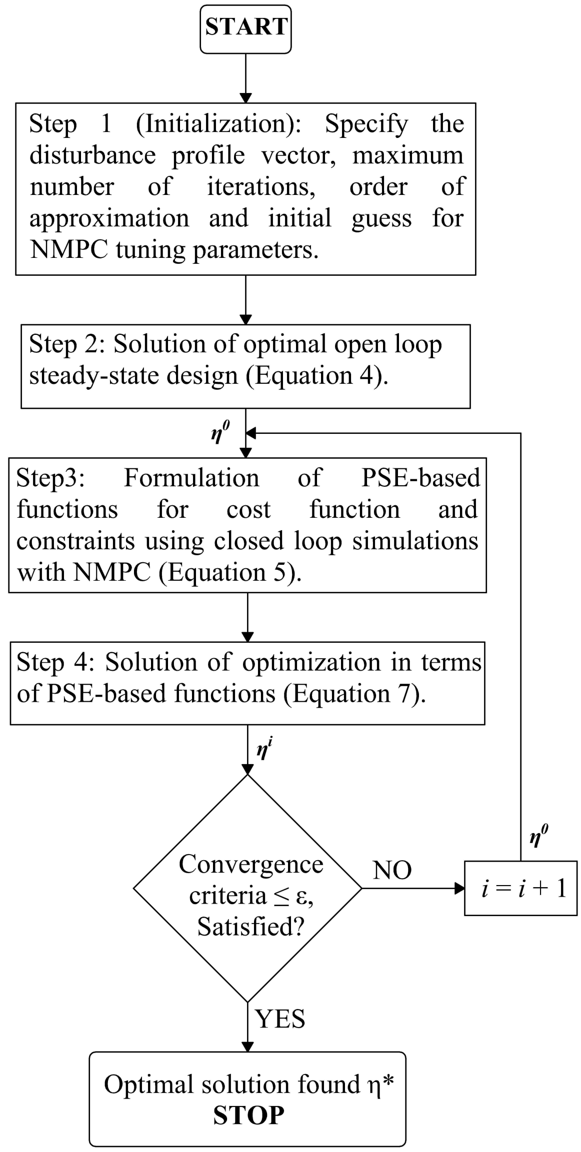


Fig. 1. Algorithm for NMPC-based simultaneous design and control approach.

*Step 1: Initialization.* The procedure is initialized by establishing trajectory profiles for disturbances $\boldsymbol{d}(t)$, maximum number of iterations ($N_{iter}$), order of the PSE function, search space region for the decision variables ($\delta$), and initial guesses for the controller tuning parameters $\boldsymbol{\varsigma}$.

*Step 2: Optimal open-loop steady-state design.* As discussed in section 2.2, a direct implementation of NMPC to solve a closed-loop design optimization problem leads to a challenging task since the resulting model is a bi-level optimization problem (Baker and Swartz (2008)). Therefore, to obtain a first nominal starting point for the development of PSE-based functions, an optimal steady-state problem is solved. The solution obtained from the steady-state problem (4) determines the nominal values for process design variables ($\boldsymbol{\gamma}$).

$$\min_{\gamma} \; \Gamma_{SS}(\boldsymbol{\gamma}, \boldsymbol{x}, \boldsymbol{y}) \tag{4a}$$

$$\text{s.t.} \quad \dot{\boldsymbol{x}} = f(\boldsymbol{\gamma}, \boldsymbol{x}, \boldsymbol{y}) \tag{4b}$$

$$h(\boldsymbol{\gamma}, \boldsymbol{x}, \boldsymbol{y}) = 0 \tag{4c}$$

$$g(\boldsymbol{\gamma}, \boldsymbol{x}, \boldsymbol{y}) \leq 0 \tag{4d}$$

where $\Gamma_{SS}$ represents the cost function for steady-state design.

*Step 3: Development of PSE-based functions.* PSEs are mathematical expressions that can be used to state the functions in our optimization model in explicit terms of design variables and the system's uncertain parameters around specific operating points. This low-order model representation enables fast calculation of optimal values for the decision variables. Thereby, to reduce the nonlinearity burden of our optimization problem, the cost and constraint functions are replaced with their PSE functions around a nominal condition. In this work, the calculation of PSE-based functions is carried out around the worst-case variability point obtained from the closed-loop simulation of the process under disturbances $\boldsymbol{d}$. The worst-case variability conditions correspond to the largest violations in the constraints as shown in Figure 2. The closed-loop process that needs to be solved at each sampling instant is presented in Equation 5.

$$\dot{\boldsymbol{x}} = f(\boldsymbol{\eta}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) \tag{5a}$$

$$h(\boldsymbol{\eta}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) = 0 \tag{5b}$$

$$g(\boldsymbol{\eta}, \boldsymbol{x}(t), \boldsymbol{y}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{d}(t)) \leq 0 \tag{5c}$$

$$\Phi(\boldsymbol{\eta}, \boldsymbol{x}(t), \overline{\boldsymbol{u}}(\tau), \boldsymbol{y}(t), \boldsymbol{d}(t)) = 0 \tag{5d}$$

$$\overline{\boldsymbol{u}}(\tau) = \arg\left\{ \min_{\widehat{\boldsymbol{u}}} \; \Psi(\cdot) \text{ s.t. } \dot{\widehat{\boldsymbol{x}}}, H(\cdot), G(\cdot), \; \widehat{\boldsymbol{u}} \in U \right\} \tag{5e}$$

For example, the worst-case variability of the $s^{th}$ constraint function ($g_s$) can be expanded in terms of decision variables ($\boldsymbol{\eta}$) as follows:

$$g_{s,PSE}(\boldsymbol{\eta})|_{d(t),t_{wc}} = g_s(\boldsymbol{\eta_{nom}}) + \nabla g_s(\boldsymbol{\eta})\,(\boldsymbol{\eta} - \boldsymbol{\eta_{nom}}) + \frac{1}{2}\,(\boldsymbol{\eta} - \boldsymbol{\eta_{nom}})^T\,\nabla^2 g_s(\boldsymbol{\eta})\,(\boldsymbol{\eta} - \boldsymbol{\eta_{nom}}) \tag{6}$$

where $\nabla g_s(\boldsymbol{\eta})$ and $\nabla^2 g_s(\boldsymbol{\eta})$ are the first and second order sensitivities of the function with respect to the decision variables ($\boldsymbol{\eta}$) evaluated at the worst-case variability point represented by $t_{wc}$ in Figure 2. Gradients are required at the nominal condition ($\boldsymbol{\eta_{nom}}$) for the PSE expansions (Equation 6). Therefore, to compute PSE for cost and constraint functions, it is necessary to enforce small forward and backward variations in every decision variable ($\boldsymbol{\eta}$) and complete a closed-loop simulation for every variation in $\boldsymbol{\eta}$ to determine gradients. The finite difference method has been used to calculate the gradients.

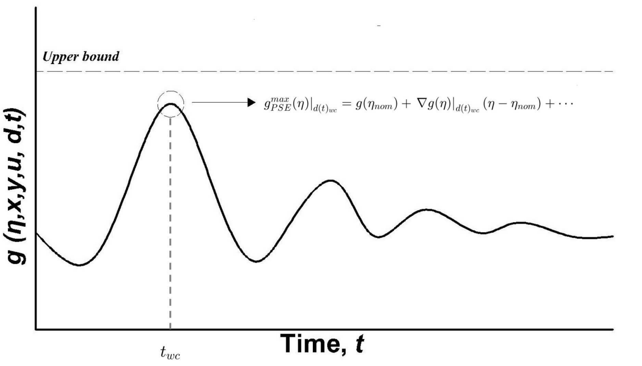


Fig. 2. Identification of the worst-case scenario required for the PSE expansions.

*Step 4: Optimization of the PSE-based functions.* The PSE-based optimization problem (Equation 7) is formulated using the PSE-based functions developed in Step 3. The optimization variables ($\boldsymbol{\eta}$) in the model are restricted to upper and lower bounds determined with respect to their nominal values ($\boldsymbol{\eta_{nom}}$). $\delta$ is a parameter that represents the region where the approximation made by the PSE-based model is valid (Rafiei and Ricardez-Sandoval (2018)).

$$\min_{\boldsymbol{\eta}, \boldsymbol{\lambda}} \; \Gamma_{PSE}(\boldsymbol{\eta}) + \sum_{s=1}^{S} M\lambda_s \tag{7a}$$

$$\text{s.t.} \quad h_{PSE}(\boldsymbol{\eta}) \leq \lambda_s \;\; \forall \; s = 1, \cdots, S \tag{7b}$$

$$\boldsymbol{\eta_{nom}}(1-\delta) \leq \boldsymbol{\eta} \leq \boldsymbol{\eta_{nom}}(1+\delta) \tag{7c}$$

$$\lambda_s \geq 0 \;\; \forall \; s = 1, \cdots, S \tag{7d}$$

In this PSE-based optimization problem, $\Gamma_{PSE}(\boldsymbol{\eta})$ and $h_{PSE}(\boldsymbol{\eta})$ are the PSE-based functions for the cost and the inequality constraint functions, respectively. The optimization problem shown in Equation (7a) contains the parameter $\lambda_s$ that is used to avoid infeasibility of $s^{th}$ constraint. The optimization is formulated to drive infeasibility variables ($\lambda$) to zero. Parameter $M$ represents a penalty term that requires to be at least three orders of magnitude higher than the actual cost function value. Note that the PSE-based optimization formulation presented in Equation (7) represents the simultaneous design and control optimization model stated in the Equation (5) around a nominal condition.

As shown in Figure 1, the values obtained as a result of the solution of the PSE-based optimization problem ($\boldsymbol{\eta}^*$) are taken as new nominal values ($\boldsymbol{\eta_{nom}}$) and returned to step 3 to generate a new nominal closed-loop simulation of the process and identify a new worst-case variability point (see Figure 1).

*Step 5: Convergence criterion.* We evaluate the convergence of this methodology by the evaluation of a floating average. Accordingly, mean values for the cost function obtained from Equation (7) of two different sampling periods $N$ are compared. If the difference in means is

Table 1. Cost function and constraints.

| Cost Function |
|---|
| $\Theta = 0.16(3500V + 2300A_d) + 870(q_p + f_k) + 10^5(100 - s_w)^2$ |
| Constraints |
| $0.01 \leq \frac{q_p}{q_r+q_p} \leq 0.2$ |
| $0.8 \leq \frac{V x_w(t) + A\, l_r\, x_r(t)}{24\, q_p\, x_r(t)} \leq 15$ |
| $s_w(t) \leq 100$ |

Table 2. Disturbance trajectory profiles

| $t$ hr | $q_i$ $m^3$/hr | $s_i$ mg/L | $x_i$ mg/L |
|---|---|---|---|
| 0 | 500 | 366 | 80 |
| 50 | 480 | 371 | 75 |
| 100 | 510 | 361 | 85 |
| 150 | 480 | 371 | 75 |
| 200 | 500 | 366 | 80 |
| 250 | 505 | 363 | 83 |
| 300 | 500 | 366 | 80 |

less or equal to a threshold value ($\epsilon$), then the method has converged. More details about this methodology are omitted for brevity and can be found in our previous work (Rafiei and Ricardez-Sandoval (2018)).

## 3. CASE STUDY

An existent wastewater treatment plant was used as a case study to test the performance of the NMPC framework (Rafiei and Ricardez-Sandoval (2018)). This plant includes a biological reactor and a secondary settler to control the substrate concentration ($s_w$) in the biodegradable waste stream. Purge flow rate ($q_p$) and turbine speed ($f_k$) are selected as manipulated variables to control the substrate concentration ($s_w$) and dissolved oxygen concentration ($c_w$). The model equations, parameters and their corresponding nominal values can be found elsewhere (Rafiei and Ricardez-Sandoval (2018)).

Table 1 provides the annualized cost function and constraints of the current model. The cost function consists of annualized capital cost ($CC$), annual operating cost ($OC$), and a variability cost ($VC$). Variability cost is specified to drive the system to restrain the substrate ($s_w$) close to saturation ($s_w \leq 100$). Likewise, the constraints listed in Table 1 identifies the feasible operating region for this process. The set of decision variables $\boldsymbol{\eta}$ is given by the volume of the reactor ($V$) and the area of the settler ($A_d$) as the design parameters ($\boldsymbol{\gamma}$); the NMPC tuning parameters ($\boldsymbol{\varsigma}$) are given by the weighting matrix $\mathbf{Q}$, and the controller set points for $s_w$ and $c_w$ (i.e. $s_w^{sp}$ and $c_w^{sp}$, respectively). To simplify the analysis, the control and prediction horizons were set to 5 hours for each. Moreover, second order PSE functions are considered for both the cost functions and process constraints. A constant search space ($\delta$) was employed for the current case study, i.e. at every iteration of the back-off procedure, the decision variables in the PSE-based optimization problem are set to be explored up to 1% of their nominal value. More details regarding the search space is provided in Rafiei and Ricardez-Sandoval (2018).

Table 3. Comparison of NMPC-based approach and PI-based methodology.

| Decision Variable | NMPC | PI |
|---|---|---|
| $A_d$ [$m^2$] | 991.0 | 2386.15 |
| $V$ [$m^3$] | 2133.8 | 1541.9 |
| $s_w^{sp}$ [mg/L] | 97.0 | 86.25 |
| $c_w^{sp}$ | 0.001 | 0.037 |
| $\mathbf{Q}_s$ | 42.25 | - |
| $\mathbf{Q}_c$ | 0.001 | - |
| $K_{cs}$ | - | 1.160 |
| $K_{cc}$ | - | 0.205 |
| $\tau_{cs}$ | - | 16.23 |
| $\tau_{cc}$ | - | 7.99 |
| Total Cost [$/yr] | $5.389\times10^6$ | $2.022\times10^7$ |
| Iterations | 74 | 102 |
| Amount of back-off | $4.039\times10^6$ | $1.887\times10^7$ |

### *3.1 Results*

The implementation of the NMPC-based simultaneous design and control framework was performed in GAMS V28.2.0. using CONOPT4 as the NLP solver, for the NMPC model, the orthogonal collocation discretization was made with 20 finite elements and 3 collocation points, then the model has 1,061 nonlinear algebraic equations with 961 variables. Likewise, the plant model was discretized with 1 finite element and 3 collocation points, then the model has 56 equations with 56 variables. The solution obtained from the NMPC-based back-off approach is presented in Table 3. The performance of the proposed NMPC-based framework has been compared with a decentralized PI-based approach previously reported in the literature involving two PI controllers paired as follows $s_w$-$q_p$ and $c_w$-$f_k$ (Rafiei-Shishavan et al. (2017)). As indicated in Table 3, a 73% improvement has been achieved with the present NMPC-based methodology in terms of cost function compared to the decentralized PI-based approach. The two methods converged to different design configurations, i.e. area ($A_d$) and volume ($V$). Although, the volume is 38% larger than that obtained by the PI-based approach, it allowed the system to operate at higher set-points thus allowing the reduction of 73% in the overall cost. The NMPC-based approach enables the system to operate at higher substrate set-points, i.e. a closer set-point to the saturation limit ($s_w \leq 100$), without any violations of constraints. Figure 3 shows the convergence of the methodology in terms of the objective function. As expected, the amount of back-off required from the steady-state in the NMPC-based approach is lower than the PI-based approach, i.e. the process is more economical. On the other hand, the CPU time for the current approach is five orders of magnitude higher than the decentralized PI-based approach. The CPU cost are mostly due to the identification of the PSE functions needed to replace the nonlinear constraints and cost functions. In particular, the NMPC framework requires the solution of an NLP at each time step in Step 3 of the algorithm and for all the iterations. The design and control strategy obtained from the NMPC framework was validated. As shown in Figure 4, the NMPC is able to maintain dynamic feasibility for the substrate in the presence of disturbances. The rest of the constraints also remained dynamically feasible and are not shown here for brevity.

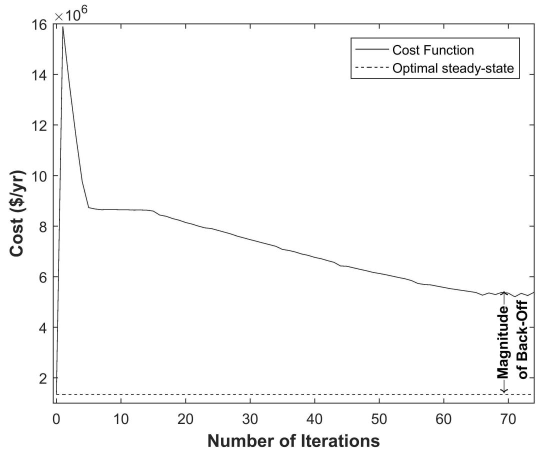


Fig. 3. Cost function convergence profile.

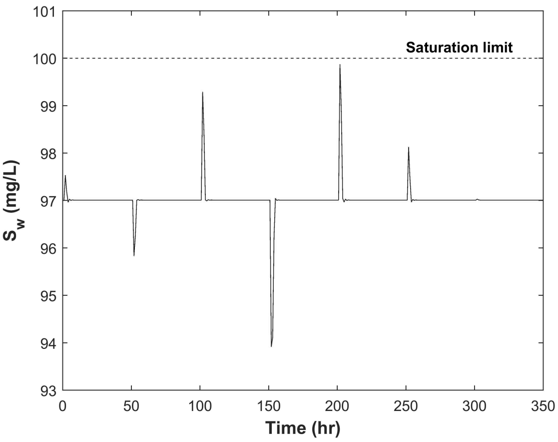


Fig. 4. Closed-loop simulation using results obtained from Back-off methodology: substrate ($s_w$) dynamic profile.

## 4. CONCLUSION

We presented an NMPC-based simultaneous design and control methodology based on a back-off approach. The key idea is to initiate the search for the optimal design and control from the optimal steady-state design using bounded optimization problems that are constructed based on PSE functions. The current methodology leads to considerable improvement in annualized cost and performance. Consequently, the integration of a sophisticated control scheme such as NMPC into the design process results in significant advantages in process economics and performance compared to classical decentralized PID control strategies. The complexity of the problem and high computational costs act as the main barriers to implement the present NMPC-based framework, particularly for large-scale systems. For future work, uncertainty in parameters will be considered with the aim to explore the robustness in the solution. Moreover, the direct solution of the simultaneous design and NMPC control will be tackled using mathematical programs with complementarity constraints. Furthermore, we will consider the proposed simultaneous design and NMPC-based control for large-scale applications.

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