MODIFIER ADAPTATION APPROACH USING RELS TO COMPUTE PROCESS GRADIENTS

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Abstract

Real-Time Optimization (RTO) is not always able to achieve optimal process operation due to the presence of significant uncertainty about the plant models used to make decisions, and also due to the differences between control architecture layers which operate on different time-scales and use different kind of models. To overcome these issues, the economic optimization problem solved in the RTO layer can be changed following the Modifier Adaptation methodology (MA), which uses plant measurements to bring the process to the real optimum, despite the presence of uncertainty. Traditionally, modifiers are updated only at the steady state of the process using static information to compute the process gradients. It implies a slow convergence to the optimum operating point, especially in processes with a long settling time. This issue is considered in this paper, assuming that these gradients can be estimated from measured data during the transient using adaptive estimation techniques. The proposed approach is shown to avoid the necessity to wait for the steady state of the process being valid for parametric and structural uncertainty. A simulated example, the Otto-Williams reactor, is used to illustrate the effectiveness of the proposed technique.

Keywords

Real-Time Optimization, Modifier Adaptation, Uncertainty.

Introduction

The management of large scale systems, such as many in the petrochemical industry, consists of making decisions in order to satisfy process specifications and constraints on many variables. In addition, these decisions should be optimal with respect to efficiency, economy, environment, etc. This problem requires the use of large models and optimization methods. RTO consists of an optimization layer that operates above the control layer and makes decisions on a time scale of hours by explicitly considering economic objectives. The optimum operating point obtained by the RTO layer is passed to lower-level controllers that include basic control and model predictive control. However, optimal operation is not guaranteed since the process models are inaccurate, so the optimum computed from the model may not be the same as the optimum of the process. Usually, the RTO layer uses a steady-state model of the process to make decisions, where the RTO problem is formulated as follows:

$$\begin{aligned} &\min_{u} J(u,\beta) \\ &s.t \quad g(u,\beta) \le 0 \\ &\quad u^L \le u \le u^U \end{aligned} \tag{1}$$

where J is the cost function to be minimized, g represents the constraints, β the uncertain parameters, and u the decision variables which present lower and upper limits u^L and u^U.

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Several proposals have been developed to cope with the uncertainty already mentioned and to drive the process to its real optimum point. The first approach emerged in the late 1970s as an iterative two-stage algorithm involving a parameter estimation step (to update uncertain model parameters) followed by an economic optimization that is solved to obtain new decision variables (Chen and Joseph, 1987). This formulation works well only if there is little structural plant-model mismatch and the changing operating conditions provide sufficient excitation to estimate the uncertain parameters (Yip and Marlin, 2004).

A new approach was developed by Roberts who incorporated information regarding plant gradients, adding a modifier to the economic cost function that emerges from the equality of the necessary optimality conditions (NCO) for the real process and the static model used in the RTO layer (Roberts, 1979). This method was called "integrated system optimization and parameter estimation" (ISOPE). Tatjewski proved that the convergence to the optimum point does not depend on parameter estimation, but on the equality between the outputs of the process and the model at each RTO iteration (Tatjewski, 2002). For this reason, he introduced a new modifier that takes into account the difference between these outputs. New modifiers were also defined by Gao and Engell for process dependent constraints (Gao and Engell, 2005). The resultant modified RTO problem, Eq. (2), in which J_M and g_M are the modified cost function and constraints, u^*_{k-1} is the input applied in the previous steady state, that is, the optimal solution of the previous RTO, and the subscript "p" indicates that the variable is evaluated from the process measurements.

$$\begin{aligned} &\min_u J_M = J(u,\beta) + \lambda_k (u - u^*_{k-1}) \\ &s.t \quad g_M = g(u,\beta) + \gamma_k (u - u^*_{k-1}) + \varepsilon_k \le 0 \\ &\quad u^L \le u \le u^U \end{aligned} \tag{2}$$

The modifiers λ_k, γ_k and ε_k are given by Eq. (3):

$$\begin{aligned} &\lambda_k = \left.\frac{dJ_P}{du}\right|_{u^*_{k-1}} - \left.\frac{dJ}{du}\right|_{u^*_{k-1}} \qquad \gamma_k = \left.\frac{dg_P}{du}\right|_{u^*_{k-1}} - \left.\frac{dg}{du}\right|_{u^*_{k-1}} \\ &\varepsilon_k = g_P(u^*_{k-1}) - g(u^*_{k-1}) \end{aligned} \tag{3}$$

Figure 1 presents the general formulation of MA.

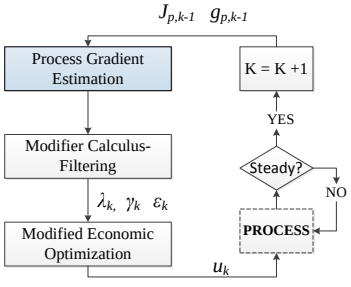

Figure 1. General formulation of MA

From these ideas, several methods have emerged; most of them requiring the computation of experimental gradients, which is a difficult task. In particular, Dual Modifier Adaptation (DMA) (Marchetti et al., 2010) estimates experimental gradients from past operating points generated by the previous RTO iterations by using the definition of directional derivative. To ensure that gradients are obtained accurately, a new constraint ($\delta \ge a$) is added to the optimization problem, where δ represents the condition number of the gradient estimation. This constraint represents the dual characteristic of the method: while the rest of the optimization aims to converge to the optimum of the modified model (primal objective), the dual constraint ensures that, in the next RTO iteration, the system will have enough excitation to estimate the process gradient adequately (dual objective).

The calculation of experimental gradients can be avoided by using a different formulation called Nested-Modifier Adaptation (NMA) (Navia et al., 2015). This method uses a nested optimization architecture with a gradient-free optimization algorithm, for example, the Nelder-Mead algorithm, to directly update the modifiers, iterating with them over the modified optimization until the optimum of the process is found. In this way, the process gradient estimation is replaced by another method that takes into account the minimization of the cost function measured directly from the process.

One of the main disadvantages of MA is the necessity to wait for the steady state of the process before updating the modifiers. In many real applications, the transients can last for several hours, so the convergence of MA can be very slow and the real optimum may only be achieved after several days of operation. During this period of time, the operating conditions or the plant-model mismatch may change and the method will not converge to the real optimum. This issue makes the application of this methodology impractical in these cases.

In order to speed up the convergence of MA methodology for slow dynamic processes, several researchers have suggested the use of transient measurements to estimate the variables required by the steady-state optimization. This idea was pursued by Zhang and Roberts in 1990 (Zhang and Roberts, 1990), who combined the ISOPE scheme with a linear dynamic model identification to compute process gradients for the steady state optimization of nonlinear constrained processes with slow dynamics, but this work did not address the problem of shortening the gradient estimation time. In contrast, François and Bonvin (François and Bonvin, 2014) proposed an approach that uses transient measurements to compute process gradients by the neighbouring extremal method which relies on the accuracy of the linearization resulting from a variational analysis of the nominal model. However, none of these techniques work well in the presence of strong structural plant-model mismatch.

This paper tries to extend the idea of using transient measurements to speed up the convergence to the optimum of MA, since waiting for the steady state at each RTO iteration is no longer necessary, estimating the process cost and constraint gradients directly by means of a recursive identification method, dealing with both parametric and structural uncertainties. The performance of the proposed method is illustrated through a case study corresponding to the Otto- Williams reactor.

The paper is organized as follows. The section MA using transient information describes the problem to deal with showing how the process gradients are estimated and applied in this kind of method. Later on, the application of this technique to a simulated process will be presented, showing, in the next section, the obtained results, followed by brief conclusions.

Modifier Adaptation Using Transient Information

MA is normally applied based on static information. However, the implementation of these methods is sometimes impractical, especially in processes with a long settling time, as the process needs to reach the steady-state at each RTO execution to estimate the process gradients. Over these long periods of time, the operating conditions or differences between process and model may change and the method may not converge to the real optimum.

To overcome this problem, a MA technique based on the use of transient measurements is presented, speeding up the convergence to the plant and being valid for parametric and structural uncertainty.

This approach considers that process gradients can be estimated from input-output data during the transient using adaptive estimation techniques (Goodwin and Sin, 1984). In this case, the recursive extended least squares algorithm (RELS) has been used for this task.

Process Gradient Estimation

As it was mentioned before an adaptive estimation technique will be used to estimate the process gradients and therefore the modifiers of the modified RTO problem. The essential ingredient of a parameter estimation problem is to choose the class of model. In this case, the dynamics of the cost function has been parametrized as Eq. (4) considering a quadratic Taylor polynomial that relates the variation of the process cost function ΔJ_k to the variation of the input variables Δu_k (decision variables of the RTO problem). Other simpler functions can be supposed, for example, a first order approximation. However, this approximation would be realistic only for linear systems which are rarely met in practice.

$$\Delta\hat{J}_k = \varphi_k^T\hat{\theta}_k = \frac{\partial J}{\partial u_k}\Delta u_k + \frac{\partial J}{\partial u_{k-1}}\Delta u_{k-1} + \frac{\partial^2 J}{\partial u_k^{\,2}}1/2\Delta u_k^{\,2} + \frac{\partial^2 J}{\partial u_k u_{k-1}}\Delta u_k\Delta u_{k-1} + \frac{\partial^2 J}{\partial u_{k-1}^{\,2}}1/2\Delta u_{k-1}^{\,2} \quad (4)$$

$$\varphi_k^T = \left[\Delta u_k \quad \Delta u_{k-1} \quad 1/2\Delta u_k^{\,2} \quad \Delta u_k\Delta u_{k-1} \quad 1/2\Delta u_{k-1}^{\,2}\right] \quad (5)$$

$$\hat{\theta}_k^T = \left[\frac{\partial J}{\partial u_k} \quad \frac{\partial J}{\partial u_{k-1}} \quad \frac{\partial^2 J}{\partial u_k^{\,2}} \quad \frac{\partial^2 J}{\partial u_k u_{k-1}} \quad \frac{\partial^2 J}{\partial u_{k-1}^{\,2}}\right] \quad (6)$$

where $\Delta\hat{J}_k$ is the estimator for the variation of the cost function, and $\hat{\theta}_k$ is the vector of estimated parameters which contains the required process gradients to compute the modifiers, i.e., the gradients of the process cost function with respect to the decision variables u_k .

The gradients contained in $\hat{\theta}_k$ are estimated by employing RELS with forgetting factor α. This algorithm has been applied because is simple, easy to implement and generally has much faster convergence than other methods such as the projection algorithm. It is based on the difference between the current input u_k and the previous ones, and the difference between the measured ΔJ_k and the predicted $\Delta\hat{J}_k$ change in the cost function (Guay, 2014). Then, the parameter estimation update approach is given as follows:

$$\Sigma_0 = \frac{1}{\alpha}I \quad (7)$$

$$\Delta u_k = u_{k-1} - u_{k-2} \quad (8)$$

$$\Delta u_{k-1} = u_{k-2} - u_{k-3} \quad (9)$$

$$\Delta\hat{J}_k = \varphi_k^T\hat{\theta}_k \quad (10)$$

$$e_k = \Delta J_k - \Delta\hat{J}_k \quad (11)$$

$$(\Sigma_k)^{-1} = \frac{1}{\alpha}(\Sigma_{k-1})^{-1} - \frac{1}{\alpha^2}(\Sigma_{k-1})^{-1}\varphi_k\left(1+\frac{1}{\alpha}\phi_k^T(\Sigma_{k-1})^{-1}\varphi_k\right)^{-1}\varphi_k^T(\Sigma_{k-1})^{-1} \quad (12)$$

$$\hat{\theta}_k = \hat{\theta}_{k-1} + \frac{1}{\alpha}(\Sigma_{k-1})^{-1}\varphi_k\left(1+\frac{1}{\alpha}\varphi_k^T(\Sigma_{k-1})^{-1}\varphi_k\right)^{-1}(e_k) \quad (13)$$

where Σ is the covariance matrix of the estimate error whose initial value is Σ_0, e_k the output prediction error, u_{k-1} is the input applied to the process until the current sample time k, u_{k-2} and u_{k-3}, are the inputs applied two and three sample instants before. In addition, $\Delta J_k = J_k - J_{k-1}$ is the difference between the current process cost function and the cost function measured one sampling time before. Figure 2 presents an overview of the described method:

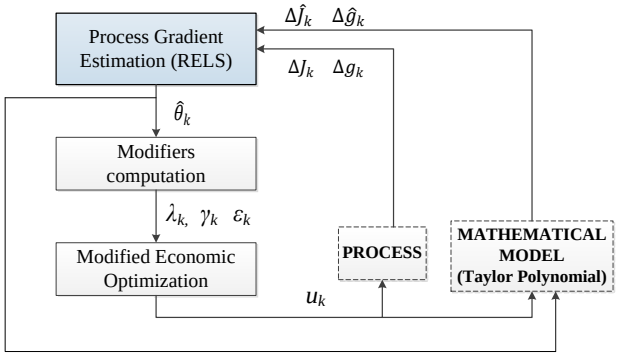

Figure 2. Schematic of MA based on the direct estimation of process gradients over the transient

One advantage of this technique is that does not require any assumption about the type of uncertainty of the model, parametric or structural, or the knowledge of the parameter responsible for the plant- model mismatch. Consequently, the proposed method can be applied to both parametric and structural uncertainty without modifying the RTO model or identifying what the uncertain parameters are. Another advantage is that this method works well even with a high number of decision variables since the experimental gradients are estimated from an adaptive estimation technique without requiring an extra excitation for each input.

Simulation Study

A sampled- data reactor system has been considered to show the performance of the described approach comparing to the traditional static MA.

This example is the Otto Williams reactor, illustrated in the Figure 3. It is a CSTR that has been used widely in the literature to study the performance of different RTO approaches with modelling mismatch (Roberts, 1979), (Forbes and Marlin, 1994) and (Marchetti et al., 2010).

The system consists of a continuous reactor that is fed with two sources of raw material *A* and *B*, by means of the streams F_A and F_B respectively. Inside the vessel, three parallels reactions take place forming 4 new compounds: *C*, *G*, *E* and *P*, as Eq. (14) shows. These compounds, along with the unused reactive, leave the reactor from the bottom of the vessel in a single stream F_R. X_i represents the mass fraction of the *i* compound inside the reactor and T_R is the reactor temperature.

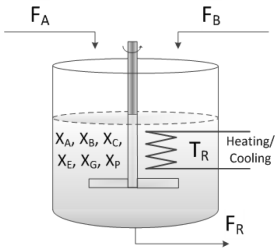

Figure 3. Diagram of the Otto-Williams reactor. Real Process

The system can be described using a first principles model, where the mass balance for each compound in the reactor is defined as follows:

$$A + B \xrightarrow{k_1} C, \quad B + C \xrightarrow{k_2} P + E, \quad C + P \xrightarrow{k_3} G \tag{14}$$

$$V_R \frac{dX_A}{dt} = F_A - F_R X_A - V_R r_1 \tag{15}$$

$$V_R \frac{dX_B}{dt} = F_B - F_R X_B - V_R r_1 \frac{M_B}{M_A} - V_R r_2 \tag{16}$$

$$V_R \frac{dX_C}{dt} = -F_R X_C + V_R r_1 \frac{M_C}{M_A} - V_R r_2 \frac{M_C}{M_B} - V_R r_3 \tag{17}$$

$$V_R \frac{dX_E}{dt} = -F_R X_E + V_R r_2 \frac{M_E}{M_B} \tag{18}$$

$$V_R \frac{dX_G}{dt} = -F_R X_G + V_R r_3 \frac{M_G}{M_C} \tag{19}$$

$$V_R \frac{dX_P}{dt} = -F_R X_P + V_R r_2 \frac{M_P}{M_B} - V_R r_3 \frac{M_P}{M_C} \tag{20}$$

$$F_R = F_A + F_B \tag{21}$$

where Mi represents the molecular weight of the compound *i*, and r_j is the molecular reaction rate of the chemical reaction *j* defined with respect to its limiting reactive. Since we are dealing with pseudo-compounds it is necessary to define the relation among their molecular weight. This can be obtained assuming that $M_A = M_B = M_C$. Under this consideration the ratios from Eq. (15-20) are:

$$\frac{M_P}{M_B} = 1 \quad \frac{M_C}{M_A} = \frac{M_C}{M_B} = \frac{M_E}{M_B} = 2 \quad \frac{M_G}{M_C} = 1.5 \quad \frac{M_P}{M_C} = 0.5 \tag{22}$$

Regarding the reaction rate, it can be calculated as follows:

$$r_1 = k_1 X_A X_B \tag{23}$$

$$r_2 = k_2 X_B X_C \tag{24}$$

$$r_3 = k_3 X_C X_P \tag{25}$$

where k_j is the kinetic constant of the reaction *j* that can be obtained using an Arrhenius expression, and E_{A_j} is the activation energy from reaction *j*.

$$k_j = k_j^0 e^{\left(\frac{E_{A,j}}{T_R}\right)}, \qquad j = 1,2,3 \tag{26}$$

Cost Function

The objective is to maximize the operating profit, which is expressed as the cost difference between the product and reactant flowrates:

$$J = F_R(X_P P_P + X_E P_E) - F_A X_A C_A - F_B X_B C_B \tag{27}$$

The flowrate of reactant A (F_A) is fixed at 1.8275 kg/s. The flowrate of reactant B (F_B) and the reactor temperature (T_R) are the decision variables, thus u = (F_B, T_R).

Process Optimum

The optimal solution for the plant (simulated reality) is presented in Table 1. The mass fractions obtained at the optimal solution are given in Table 2.

Table 1. Process optimum

F_B^* (Kg/s)	T_R^* (ºC)	J^* ($/s)
4.78	89.70	191.22

Table 2. Mass fractions at the optimum

X_A^*	X_B^*	X_C^*	X_E^*	X_G^*
0.0874	0.3896	0.0153	0.2906	0.1075

Steady State Model

The mass fraction of the product C is one order of magnitude below the rest of the compounds. Therefore, a common choice in a gross representation of the process is considering only the other five species, with the corresponding modelling mismatch. Then, only two parallel reactions inside the reactor are considered:

$$A + 2B \xrightarrow{\tilde{k}_1} P + E, \quad A + B + P \xrightarrow{\tilde{k}_2} G + E \tag{28}$$

with this given source of modeling mismatch, the steady state model to be used in the RTO layer is the following:

$$F_A - F_R X_A - V_R \tilde{r}_1 - V_R \tilde{r}_2 = 0 \tag{29}$$

$$F_B - F_R X_B - 2V_R \tilde{r}_1 - V_R \tilde{r}_2 = 0 \tag{30}$$

$$-F_R X_E + 2V_R \tilde{r}_1 = 0 \tag{31}$$

$$-F_R X_G + 3V_R \tilde{r}_2 = 0 \tag{32}$$

$$-F_R X_P + V_R \tilde{r}_1 - V_R \tilde{r}_2 = 0 \quad (33)$$

$$F_R = F_A + F_B \quad (34)$$

$$\tilde{r}_1 = \tilde{k}_1 X_A (X_B)^2 \quad (35)$$

$$\tilde{r}_2 = \tilde{k}_2 X_A X_B X_P \quad (36)$$

$$\tilde{k}_j = \tilde{k}_j^0 e^{\left(\frac{\tilde{E}_{A,j}}{T_R}\right)}, \qquad j = 1,2 \quad (37)$$

where the tilde represents the parameters used in the model which includes mismatch.

Original Optimization Problem

Hence, the model based optimization can be summarized as: finding the decision variables F_B and T_R which maximize the profit, subject to a model that takes into account only five compounds and two chemical reactions, corresponding to the simulated modeling mismatch:

$$\begin{aligned} &\min_{\{F_B, T_R\}} -J \\ &s.t \\ &steady-state \quad model \quad with \quad mismatch \\ &F_B \in \left[F_B^L, F_B^U\right] \quad T_R \in \left[T_R^L, T_R^U\right] \end{aligned} \quad (38)$$

The values of the parameters used from Eq. (15) to Eq. (37) are summarized in Table 3.

Table 3. Value of the model parameters

Parameter	Value	Parameter	Value
F_A	1.8725	$\tilde{E}_{A1}$	-8077.6
V_R	2105	$\tilde{E}_{A2}$	-12438.5
k_1^0	1.6599×10^{6}	F_B^L	3
k_2^0	7.2177×10^{8}	F_B^U	6
k_3^0	2.6745×10^{13}	T_R^L	70
E_{A1}	-6666.7	T_R^U	100
E_{A2}	-8333.3	P_P	1143.38
E_{A3}	-11111	P_E	25.92
$\tilde{k}_1^0$	2.611×10^{12}	C_A	76.23
$\tilde{k}_2^0$	1.655×10^{8}	C_B	114.34

Modified Optimization Problem

The modified optimization problem solved at each RTO iteration is defined as follows:

$$\begin{aligned} &\min_{\{F_B, T_R\}} -J + \lambda_1 (F_B - F_{B,k-1}) + \lambda_2 (T_R - T_{R,k-1}) \\ &s.t \\ &steady-state \quad model \quad with \quad mismatch \\ &F_B \in \left[F_B^L, F_B^U\right] \quad T_R \in \left[T_R^L, T_R^U\right] \end{aligned} \quad (39)$$

where the modifiers λ_1, λ_2 are computed as the difference between experimental gradients (obtained from past operating points using DMA and estimated by RELS using the MA approach based on transient information), and the model gradients. J_P is the value of the cost function directly measured from the process.

$$\lambda_1 = \frac{\partial J_P}{\partial F_B} - \frac{\partial J}{\partial F_B}, \qquad \lambda_2 = \frac{\partial J_P}{\partial T_R} - \frac{\partial J}{\partial T_R} \quad (40)$$

Results

Results applying Dual Modifier Adaptation

DMA has been implemented over the Otto- Williams reactor with a value of *a* equal to 0.01 ($\delta \geq a$, dual constraint that ensures that in the next RTO iteration the system will have enough excitation to estimate the process gradient accurately). The RTO is executed every hour, the time required for the process to achieve a new steady-state. Figure 4 shows the evolution of the process cost function whereas Figures 5 and 6 show the evolution of the RTO decision variables:

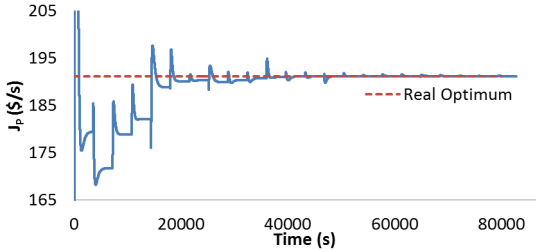

Figure 4. Evolution of the process cost function J_P

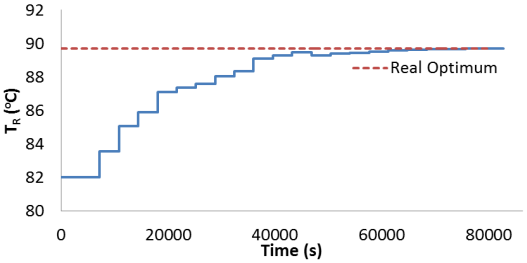

Figure 5. Evolution of the decision variable T_R

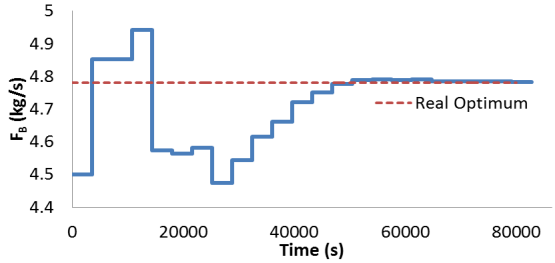

Figure 6. Evolution of the decision variable F_B

Fixing a tolerance band of 0.5% with respect to the optimal value of the cost function, the graphs (in particular, Figure 4) show that the optimum of the process is achieved after approximately 46800 seconds using static MA (13 hours). It involves 13 steady states, 11 RTO executions plus n_u initial steady states required to estimate the gradients, where n_u is the number of decision variables. For this long period of time operating conditions and the plant-model mismatch could change resulting in a loss of optimality since the MA method would not converge to the process optimum.

Results applying MA using transient measurements to estimate process gradients.

The described MA approach based on transient measurements has been implemented with a RTO sample time of 600 seconds that is one sixth of the process

stabilization time. The forgetting factor α considered for the estimation of the process gradient has been 0.90. Figure 7 shows the evolution of the process cost function whereas Figures 8 and 9 show the evolution of the RTO decision variables:

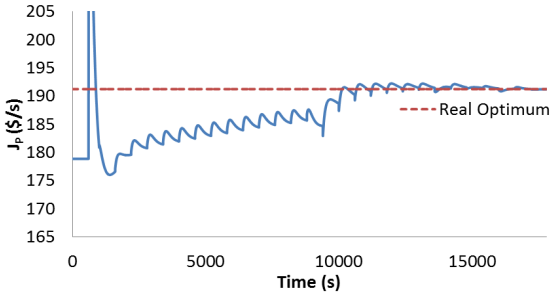

Figure 7. Evolution of the process cost function J_P

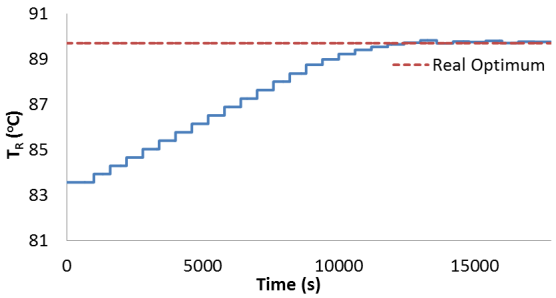

Figure 8. Evolution of the decision variable T_R

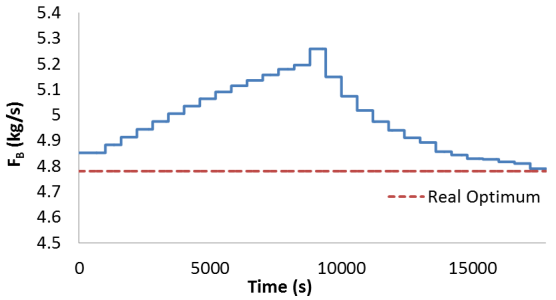

Figure 9. Evolution of the decision variable F_B

By applying the new approach, updating the modifiers during the transient, and fixing a tolerance band of 0.5%, the optimum operating point is achieved after 12000 seconds, approximately 3.5 hours, which means a considerable time reduction compared to 46800 of the static MA approach. It involves 20 RTO solutions executed during the transient.

A comparison of the performance of the two implemented approaches is shown in Table 4.

Table 4. Summary results

	DMA	Transient MA
Convergence time (s)	46800	12000
RTO sampling time (s)	3600	600
RTOs executed (#)	11	20

Conclusions

In this paper, a new method to speed up the convergence of RTO-MA to the real plant optimum has been proposed. It is based on transient information, obtaining process gradients directly from truncated Taylor expansions of the process cost and gradients combined with adaptive filtering estimation techniques.

The method has been tested in the Otto Williams reactor and the results obtained show that it is possible to effectively perform the optimization of this reactor in the presence of structural plant-model mismatch reducing by a factor of 4 the time required to achieve the process optimum as compared with standard static MA techniques, such as DMA.

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