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Use of Transient Measurements for Real-Time Optimization via Modifier Adaptation

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Abstract

Real-time optimization (RTO) methods use measurements to offset the effect of uncertainty and drive the *plant* to optimality. Explicit RTO schemes, which are characterized by solving a static optimization problem repeatedly, typically require multiple iterations to steady state. In contrast, implicit RTO methods, which do not solve an optimization problem explicitly, can use transient measurements and gradient control to bring the plant to steady-state optimality in a single iteration, provided the set of active constraints is known. This paper investigates the explicit RTO scheme "modifier adaptation" (RTO-MA) and proposes a framework that uses *transient measurements*. Convergence to the true plant optimum can be achieved in a single iteration provided the plant gradients can be estimated appropriately, for which we propose a linearization-based method. The approach is illustrated through the simulated example of a continuous stirred-tank reactor. It is shown that the time needed for convergence is of the order of the plant settling time, while more than five iterations to steady state are required when MA is applied in its classical form. In other words, the explicit RTO-MA scheme is able to compete in performance with the implicit RTO schemes based on gradient control, with the additional ability to handle process constraints.

Keywords: Real-time optimization, uncertainty, plant-model mismatch, modifier adaptation, experimental gradient.

1. Introduction

Driving a chemical process to (possibly drifting) optimal conditions is important for meeting productivity, quality, safety and environmental objectives. Many model-based and data-driven schemes are available to compute optimal operating conditions. However, most of the techniques suffer from their intrinsic inability to reject the effect of uncertainty, which is invariably present in the form of disturbances and plant-model mismatch. The reliability of model-based optimization techniques depends on the model accuracy, while it is widely recognized that accurate process models are difficult and costly to obtain. In contrast, data-driven optimization techniques rely on measurements to adjust the optimal inputs in real time. The field, which is labeled real-time optimization (RTO), has received growing attention in recent years. Note that the RTO schemes differ from other data-driven methods in that input adaptation is obtained in real time and does not require off-line computations. For example, with the well-known design of experiments (DoE) scheme, it is necessary to repeat the DoE procedure every time a new unexpected source of uncertainty appears.

Several RTO schemes have emerged since the development of the two-step approach in the seventies. The two-step approach uses measurements to adapt the model parameters, with the updated model being used to repeat the optimization (Marlin et al., 1997). Recently, it has been proposed to update the model differently. Instead of adjusting the model parameters, one updates correction terms that are added to the cost and constraint functions of the optimization problem. The technique, labeled modifier adaptation (RTO-MA), forces the modeled cost and constraints to match the plant values (Gao et al. 2005, Marchetti et al., 2009). The main advantage of RTO-MA compared to the two-step approach lies in its ability to converge to the true plant optimum, even in the presence of structural plant-model mismatch. Since RTO-MA is a static optimization method, its application to a continuous process requires waiting for steady state before taking measurements, updating the correction terms and repeating the numerical optimization. Hence, several iterations are generally required for convergence. In contrast, implicit methods, such as self-optimizing control (Skogestad, 2000) and NCO tracking (Francois et al., 2005), propose to adjust the inputs on-line in a control-inspired manner.

This paper proposes a framework for using RTO-MA during the transient phase toward steady state, thereby reaching optimality in a single operation to steady state. For this, two features are required: (i) the model-based optimization needs to be solved online, which is facilitated by the use of convex approximations (Francois et al., 2013), and (ii) transient measurements are needed to compute the modifiers. A method for estimating the modifiers, in particular a linearization-based method for estimating the plant gradients, is also proposed. The application of RTO-MA using transient measurements and the proposed gradient estimation technique is illustrated through a simulated 2-input 6-constraint continuous stirred-tank reactor (CSTR).

The paper is organized as follows. The problem formulation and the standard formulation of RTO-MA are presented in Section 2. Section 3 introduces the framework for using RTO-MA during transient operation and discusses the estimation of modifiers. Finally, the illustrative example is given in Section 5, and Section 6 concludes the paper.

2. Static Real-Time Optimization

2.1 Problem Formulation

We consider the problem of optimizing the steady-state performance of a chemical process:

$$\begin{aligned} \min_{\mathbf{u}} \quad & \phi_{\mathrm{p}}\left(\mathbf{u}\right) \\ \text{s.t.} \quad & \mathbf{G}_{\mathrm{p}}\left(\mathbf{u}\right) \leq \mathbf{0} \end{aligned}, \tag{1}$$

where ϕ_p is the plant cost, $\mathbf{G}_p$ the n_g-dimensional vector of plant constraints and $\mathbf{u}$ the m-dimensional vector of constant inputs. The necessary conditions of optimality (NCO) for the plant read (Bazarra et al. 1993):

$$\begin{aligned} \mathbf{G}_{\mathrm{p}}(\mathbf{u}^*) \leq \mathbf{0}, \quad \boldsymbol{\nu}_{\mathrm{p}}^* \geq \mathbf{0}, \quad \boldsymbol{\nu}_{\mathrm{p}}^{*T}\mathbf{G}_{\mathrm{p}}(\mathbf{u}^*) = 0 \\ \nabla\phi_{\mathrm{p}}(\mathbf{u}^*) + \boldsymbol{\nu}_{\mathrm{p}}^{*T}\nabla\mathbf{G}_{\mathrm{p}}(\mathbf{u}^*) = \mathbf{0} \end{aligned}, \tag{2}$$

where $\boldsymbol{\nu}_p$ is a vector of Lagrange multipliers. Problem (1) can be solved using model-based optimization techniques provided a steady-state model of the process is available:

$$\begin{aligned} \min_{\mathbf{u}} \quad & \varphi\left(\mathbf{u}, \bar{\mathbf{y}}, \boldsymbol{\theta}\right) \\ \text{s.t.} \quad & \dot{\bar{\mathbf{x}}} = \mathbf{F}\left(\mathbf{u}, \bar{\mathbf{x}}, \boldsymbol{\theta}\right) = \mathbf{0} \\ & \bar{\mathbf{y}} = \mathbf{h}\left(\mathbf{u}, \bar{\mathbf{x}}, \boldsymbol{\theta}\right) \\ & \mathbf{g}\left(\mathbf{u}, \bar{\mathbf{y}}, \boldsymbol{\theta}\right) \leq \mathbf{0} \end{aligned}, \tag{3}$$

where φ is the model cost function, $\mathbf{F}$ the n-dimensional vector representing the nonlinear dynamic model, $\mathbf{g}$ the n_g-dimensional vector of constraint functions, $\bar{\mathbf{x}}$ the n-dimensional state vector at steady state, $\bar{\mathbf{y}}$ the p-dimensional output vector at steady state, $\boldsymbol{\theta}$ the n_θ-dimensional vector of model parameters. For the sake of simplicity, we will assume that there exists an explicit function such that $\bar{\mathbf{y}} = \mathbf{H}(\mathbf{u}, \boldsymbol{\theta})$, which allows reformulating the optimization problem (3) as follows:

$$\begin{aligned} \min_{\mathbf{u}} \quad & \phi\left(\mathbf{u}, \boldsymbol{\theta}\right) \\ \text{s.t.} \quad & \mathbf{G}\left(\mathbf{u}, \boldsymbol{\theta}\right) \leq \mathbf{0} \end{aligned}, \tag{4}$$

where ϕ is the model cost and $\mathbf{G}$ the n_g-dimensional vector of model constraints. The model NCO read (Bazarra et al. 1993):

$$\begin{aligned} \mathbf{G}\left(\mathbf{u}^*,\boldsymbol{\theta}\right) \le \mathbf{0}, \quad \boldsymbol{\nu}^* \ge \mathbf{0}, \quad \boldsymbol{\nu}^{*T}\mathbf{G}\left(\mathbf{u}^*,\boldsymbol{\theta}\right) = 0 \\ \nabla\phi\left(\mathbf{u}^*,\boldsymbol{\theta}\right) + \boldsymbol{\nu}^{*T}\nabla\mathbf{G}\left(\mathbf{u}^*,\boldsymbol{\theta}\right) = \mathbf{0} \end{aligned}, \tag{5}$$

where $\boldsymbol{\nu}$ is the vector of Lagrange multipliers for the model. To be optimal for the plant, the optimal inputs $\mathbf{u}^*$ must satisfy the NCO (2). However, due to plant-model mismatch and disturbances, the solution of Problems (1) and (3) will typically differ, with the solution of (5) not satisfying (2).

2.2 Implicit RTO with Gradient Control

Implicit RTO schemes recast Optimization problem (1) as a control problem whose controlled variables are the NCO (2). Gradient control works well in the absence of constraints, as the NCO reduce to $\nabla\phi_{\mathrm{p}}(\mathbf{u}^*) = \mathbf{0}$, so that the controller's task is to drive the plant gradient to zero. Typically, the following control law is implemented in real time:

$$\dot{\mathbf{u}}(t) = -\kappa\,\mathbf{P}^{-1}\mathbf{g}(t) \quad \mathbf{u}(0) = \mathbf{u}_0 \quad , \tag{6}$$

where κ is the controller gain, $\mathbf{P}$ an estimate of the Hessian of the plant cost, and $\mathbf{g}(\mathrm{t})$ a time-dependent signal that estimates (and thus should converge to) the gradient of the plant cost. Indeed, the control problem is such that, at steady state, $\dot{\mathbf{u}}(\infty) = \mathbf{0}$ and $\mathbf{g}(\infty) = \nabla\phi_{\mathrm{p}}\left(\mathbf{u}(\infty)\right) = \mathbf{0}$. Several methods exist for implementing (6), which mainly differ in the way $\mathbf{g}(\mathrm{t})$ is obtained (Francois et al., 2012). However, in the presence of constraints, assumptions have to be made regarding the constraints that are active at the plant optimum, which allows implementing (6) for the control of a reduced gradient. Also, direct use of the dual feasibility condition (the 2nd row of (2)) as a control law has been considered (Arrow et al., 1958, Dürr et al., 2012). However, these approaches have only been investigated for the case of perfect modeling or for the numerical optimization of analytical functions, i.e., with no model error. In the presence of uncertainty and constraints, one can also rely on extremum-seeking control techniques for driving a dynamic plant to steady-state optimum by using transient measurements (DeHaan et al. 2005; Guay et al. 2005). But, as shown in (Francois et al. 2012), these techniques require multiple time-scale separations that strongly penalize the convergence time. Hence, to the best of the authors' knowledge, there are no implicit RTO techniques that are capable of driving a process to optimal performances in the presence of uncertainty and constraints, with a convergence time of the order of the plant settling time.

2.3 Explicit RTO with Modifier Adaptation

As discussed above, the model-based optimization problem (4) is not able to compute the solution to Problem (1) in the presence of plant-model mismatch. With RTO-MA, a modified version of Problem (4) is solved repeatedly at steady state, until convergence to the plant optimum is reached. For example, at the *k*th iteration, the following problem is solved:

$$\begin{aligned} \mathbf{u}_{k+1}^* = \arg\min_{\mathbf{u}} \quad & \phi_m\left(\mathbf{u},\boldsymbol{\theta}\right) := \phi\left(\mathbf{u},\boldsymbol{\theta}\right) + \boldsymbol{\Lambda}_k^{\phi^T}\left(\mathbf{u}-\mathbf{u}_k^*\right) \\ \text{s.t.} \quad & \mathbf{G}_m\left(\mathbf{u},\boldsymbol{\theta}\right) := \mathbf{G}\left(\mathbf{u},\boldsymbol{\theta}\right) + \boldsymbol{\varepsilon}_k + \boldsymbol{\Lambda}_k^{G^T}\left(\mathbf{u}-\mathbf{u}_k^*\right) \le \mathbf{0} \end{aligned}, \tag{7}$$

where $\mathbf{u}_{\mathrm{k+1}}^*$ denotes the solution at iteration *k* that will be used at the next iteration. Optimization problem (4) is modified by the addition of a linear correction term to the cost and an affine correction term to the constraints, with the modifiers defined as follows $\boldsymbol{\varepsilon}_k := \mathbf{G}_p(\mathbf{u}_k^*) - \mathbf{G}(\mathbf{u}_k^*,\boldsymbol{\theta})$, $\boldsymbol{\Lambda}_k^{\phi} := \nabla\phi_p(\mathbf{u}_k^*) - \nabla\phi(\mathbf{u}_k^*,\boldsymbol{\theta})$ and $\boldsymbol{\Lambda}_k^{G} := \nabla\mathbf{G}_p(\mathbf{u}_k^*) - \nabla\mathbf{G}(\mathbf{u}_k^*,\boldsymbol{\theta})$. The nicest feature of RTO-MA lies in that, upon convergence, (7) and (1) share the same NCO, that is, convergence to the plant optimum is possible despite the presence of uncertainty (Marchetti et al. 2009). The corresponding converged modifiers are $\boldsymbol{\varepsilon}_\infty$, $\boldsymbol{\Lambda}_\infty^\phi$ and $\boldsymbol{\Lambda}_\infty^G$.

3. Modifier Adaptation using Transient Measurements

3.1 Idea of Using Transient Measurements

Modifier adaptation has two main features, namely, convergence to the plant optimum even in the presence of structural plant-model mismatch and possibility to handle constraints explicitly. In this subsection, we propose a RTO-MA framework that uses transient measurements to estimate "modifiers at steady state", thus allowing convergence to the plant optimum within a single iteration to steady state. At each re-optimization instant during transient operation, denoted here by the index *j*, the scheme determines the constant inputs $\mathbf{u}_{j+1}^*$ that are applied until the next re-optimization instant. The optimization problem for computing $\mathbf{u}_{j+1}^*$ at instant *j* reads:

$$\begin{aligned} \mathbf{u}_{j+1}^* = \arg\min_{\mathbf{u}} \quad & \phi_m(\mathbf{u},\boldsymbol{\theta}) := \phi(\mathbf{u},\boldsymbol{\theta}) + \hat{\boldsymbol{\Lambda}}_j^{\phi^T}(\mathbf{u}-\mathbf{u}_j^*) \\ \text{s.t.} \quad & \mathbf{G}_m(\mathbf{u},\boldsymbol{\theta}) := \mathbf{G}(\mathbf{u},\boldsymbol{\theta}) + \hat{\boldsymbol{\varepsilon}}_j + \hat{\boldsymbol{\Lambda}}_j^{G^T}(\mathbf{u}-\mathbf{u}_j^*) \leq \mathbf{0} \\ \text{with} \quad & \begin{cases} \hat{\boldsymbol{\varepsilon}}_j := \widehat{\mathbf{G}_p}(\mathbf{u}_j^*) - \mathbf{G}(\mathbf{u}_j^*,\boldsymbol{\theta}) \\ \hat{\boldsymbol{\Lambda}}_j^{\phi} := \widehat{\nabla\phi_p}(\mathbf{u}_j^*) - \nabla\phi(\mathbf{u}_j^*,\boldsymbol{\theta}) \\ \hat{\boldsymbol{\Lambda}}_j^{G} := \widehat{\nabla\mathbf{G}_p}(\mathbf{u}_j^*) - \nabla\mathbf{G}(\mathbf{u}_j^*,\boldsymbol{\theta}) \end{cases}, \end{aligned} \tag{8}$$

where the notation $\widehat{(.)}$ indicates the estimate of a value that the plant would have at the *steady state* corresponding to the inputs $\mathbf{u}_j^*$. Since strictly speaking the modifiers are only defined at steady state, it is necessary to estimate them this way. The conditions ensuring convergence to the plant optimum are given in the following theorem.

Theorem 1.
Consider the control problem with the inputs computed iteratively as the solution to the optimization problem (8). If the controlled plant reaches steady state and the estimates $\widehat{\mathbf{G}_p}$, $\widehat{\nabla\phi_p}$ *and* $\widehat{\nabla\mathbf{G}_p}$ *converge to the corresponding true values, then the plant will satisfy the NCO (2) and be optimal.*

Proof:
Let start by making the obvious remark that the plant reaching steady state implies convergence of the iterative scheme (8), since otherwise the inputs $\mathbf{u}_j^*$ will change, thereby preventing the system to reach steady state. The conditions $\widehat{\mathbf{G}_p}(\mathbf{u}_\infty^*) = \mathbf{G}_p(\mathbf{u}_\infty^*)$, $\widehat{\nabla\phi_p}(\mathbf{u}_\infty^*) = \nabla\phi_p(\mathbf{u}_\infty^*)$ and $\widehat{\nabla\mathbf{G}_p}(\mathbf{u}_\infty^*) = \nabla\mathbf{G}_p(\mathbf{u}_\infty^*)$ upon convergence imply $\hat{\boldsymbol{\varepsilon}}_\infty = \boldsymbol{\varepsilon}_\infty$, $\hat{\boldsymbol{\Lambda}}_\infty^\phi = \boldsymbol{\Lambda}_\infty^\phi$ and $\hat{\boldsymbol{\Lambda}}_\infty^G = \boldsymbol{\Lambda}_\infty^G$, and thus the plant satisfies the NCO (2).

■

3.2. Estimation of Static Modifiers using Transient Measurements

Let us assume that the outputs and the constraints of the plant can be measured online as $\mathbf{y}_p(t)$ and $\mathbf{G}_p(t)$, respectively. The 0th-order modifiers $\boldsymbol{\varepsilon}_j$ are estimated online as the difference between the measured constraints $\mathbf{G}_p(t_j)$ and the constraints predicted by the model at steady state for the inputs $\mathbf{u}_j^*$:

$$\hat{\boldsymbol{\varepsilon}}_{\mathbf{j}} = \mathbf{G}_{\mathrm{p}}(\mathrm{t}_j) - \mathbf{G}\left(\mathbf{u}_{\mathbf{j}}^*, \boldsymbol{\theta}\right). \tag{9}$$

When the plant reaches steady state, the signals $\mathbf{G}_{\mathrm{p}}(\mathrm{t}_\infty)$ will be the plant constraints $\mathbf{G}_{\mathrm{p}}\left(\mathbf{u}_\infty^*\right)$ associated with the converged inputs $\mathbf{u}_\infty^*$. Hence, the assumptions of Theorem 1 hold for the 0^{th}-order modifiers.
For estimating the gradients, let us assume that the uncertainty is of parametric nature with q inaccurate parameters among the n_θ parameters $\boldsymbol{\theta}$. A variational analysis of the outputs and of the cost and constraint gradients can be performed around the nominal steady-state operating point $\left(\mathbf{u}_{nom}^*, \bar{\mathbf{y}}_{nom}^*\right)$ (Gros et al., 2009). For $p \geq q$, this analysis gives:

$$\begin{aligned} \nabla\phi(\mathbf{u}) - \nabla\phi(\mathbf{u}_{\mathrm{nom}}^*) &= \left(\nabla_{\mathrm{u}}^2\phi - \left(\nabla_\theta\mathbf{H}\right)^\dagger \nabla_{\mathrm{u}}\mathbf{H}\right)\delta\mathbf{u} + \nabla_{\mathrm{u}\theta}^2\phi\left(\nabla_\theta\mathbf{H}\right)^\dagger \delta\mathbf{y} \\ \nabla\mathbf{G}(\mathbf{u}) - \nabla\mathbf{G}(\mathbf{u}_{\mathrm{nom}}^*) &= \left(\nabla_{\mathrm{u}}^2\mathbf{G} - \left(\nabla_\theta\mathbf{H}\right)^\dagger \nabla_{\mathrm{u}}\mathbf{H}\right)\delta\mathbf{u} + \nabla_{\mathrm{u}\theta}^2\mathbf{G}\left(\nabla_\theta\mathbf{H}\right)^\dagger \delta\mathbf{y} \end{aligned}, \tag{10}$$

with $\delta\mathbf{y} = \mathbf{y} - \bar{\mathbf{y}}_{nom}^*$, $\delta\mathbf{u} = \mathbf{u} - \mathbf{u}_{nom}^*$, and the dagger superscript denoting the pseudo-inverse of a matrix. The plant gradients can be estimated as follows:

$$\begin{aligned} \widehat{\nabla\phi_p}(\mathbf{u}_j^*) &= \nabla\phi(u_{\mathrm{nom}}^*) + \left(\nabla_u^2\phi - \left(\nabla_\theta\mathbf{H}\right)^\dagger \nabla_u\mathbf{H}\right)\left(\mathbf{u}_j^* - \mathbf{u}_{nom}^*\right) + \nabla_{u\theta}^2\phi\left(\nabla_\theta\mathbf{H}\right)^\dagger\left(\mathbf{y}_p(t_j) - \bar{\mathbf{y}}_{nom}^*\right) \\ \widehat{\nabla\mathbf{G}_p}(\mathbf{u}_j^*) &= \nabla G(u_{\mathrm{nom}}^*) + \left(\nabla_u^2\mathbf{G} - \left(\nabla_\theta\mathbf{H}\right)^\dagger \nabla_u\mathbf{H}\right)\left(\mathbf{u}_j^* - \mathbf{u}_{nom}^*\right) + \nabla_{u\theta}^2\mathbf{G}\left(\nabla_\theta\mathbf{H}\right)^\dagger\left(\mathbf{y}_p(t_j) - \bar{\mathbf{y}}_{nom}^*\right) \end{aligned}, \tag{11}$$

where $\nabla_u\mathbf{G}$, $\nabla_u^2\phi$, $\nabla_{u\theta}^2\phi$, $\nabla_u^2\mathbf{G}$, $\nabla_{u\theta}^2\mathbf{G}$, $\nabla_\theta\mathbf{H}$, and $\nabla_u\mathbf{H}$ are evaluated using the model at the nominal steady-state operating point $\left(\mathbf{u}_{nom}^*, \bar{\mathbf{y}}_{nom}^*\right)$. Note that the estimation of the plant gradients (i) requires the identity of the uncertain parameters but does not need their values, and (ii) uses the output signals $\mathbf{y}_{\mathrm{p}}(\mathrm{t})$ to offset the effect of uncertainty. Injecting (11) to into (8) allows estimating the first-order modifiers.

4. Illustrative Example

The isothermal CSTR considers the competing reactions $A + B \rightarrow C$ and $2B \rightarrow D$ that can be steered by the flowrates u_{A} and u_{B} of the species *A* and *B*. The objective -- maximize the productivity of *C* while penalizing the control action -- can be reached by solving the following steady-state optimization problem:

$$\begin{aligned} &\max_{u_A,\, u_B} \quad J := \left(\frac{\left(u_A + u_B\right)^2 \bar{c}_C^2}{u_A c_{A,\, in}} - w\left(u_A^2 + u_B^2\right)\right) \\ &\text{s.t.} \quad \dot{\bar{c}}_A = -k_1\bar{c}_A\bar{c}_B + \left(\frac{u_A}{V}\right)c_{A,\, in} - \left(\frac{u_A + u_B}{V}\right)\bar{c}_A = 0 \qquad \dot{\bar{c}}_C = k_1\bar{c}_A\bar{c}_B - \left(\frac{u_A + u_B}{V}\right)\bar{c}_C = 0 \\ &\qquad \dot{\bar{c}}_B = -k_1\bar{c}_A\bar{c}_B - 2k_2\bar{c}_B^2 + \left(\frac{u_B}{V}\right)c_{B,\, in} - \left(\frac{u_A + u_B}{V}\right)\bar{c}_B = 0 \qquad \dot{\bar{c}}_D = k_2\bar{c}_B^2 - \left(\frac{u_A + u_B}{V}\right)\bar{c}_D = 0 \\ &\qquad Q = -V\left(k_1\bar{c}_A\bar{c}_B\Delta H_{r,\, 1} + k_2\bar{c}_B^2\Delta H_{r,\, 2}\right) \qquad D = \frac{\bar{c}_D}{\bar{c}_A + \bar{c}_B + \bar{c}_B + \bar{c}_D} \\ &\qquad G_1 := \frac{Q}{Q_{max}} - 1 \leq 0 \qquad G_2 := \frac{D}{D_{max}} - 1 \leq 0 \\ &\qquad 0 \leq u_A \leq u_{max} \qquad 0 \leq u_B \leq u_{max} \end{aligned}. \tag{12}$$

Note that this simulated example corresponds to the tendency model used to describe the diketene chemistry in an industrial reactor at the Lonza Company in Switzerland. The same CSTR example has also been used to compare the performance of RTO schemes, in particular the convergence time of implicit and explicit schemes (see Francois et al., 2012 and Francois et al., 2013). It was shown that implicit schemes converge within the settling time of the process, whereas 5 iterations (or settling times) are required with the standard modifier-adaptation scheme.

There are constraints on the heat generation and the molar fraction of *D*. Table 1 summarizes the parameters of the model, the plant and the optimization problem. Uncertainty affects the values of the two kinetic constants and the inlet concentration of *A*. Note that, although it is assumed that the identity of the unknown parameters is known, their real values are neither known nor estimated. The plant performance corresponding to the model and plant optimal inputs is given in Table 2.

Table 1. Parameters of the model, the plant and the optimization problem

	Model and Plant Parameters		Optimization Parameters	
	Model	Plant	Parameter	Value
k_1	0.75 $l.mol^{-1}.min^{-1}$	**1.4** $l.mol^{-1}.min^{-1}$	w	0.004 $mol.min.l^{-2}$
k_2	1.5 $l.mol^{-1}.min^{-1}$	**0.4** $l.mol^{-1}.min^{-1}$	Q_{max}	110 kcal
$c_{A,in}$	2 $mol.l^{-1}$	**2.5** $mol.l^{-1}$	D_{max}	0.1
$c_{B,in}$	1.5 $mol.l^{-1}$	1.5 $mol.l^{-1}$	u_{max}	50 $l.mol^{-1}$
V	500 l	500 l		
$\Delta H_{r,1}$	-3.5 $kcal.mol^{-1}$	-3.5 $kcal.mol^{-1}$		
$\Delta H_{r,2}$	-1.5 $kcal.mol^{-1}$	-1.5 $kcal.mol^{-1}$		

The plant is initially at the steady state corresponding to the model optimal inputs given in the LHS of Table 2. The goal is to drive the plant to its *unknown* optimum corresponding to the RHS of Table 2 by applying RTO-MA using transient measurements. Concretely, the inputs are computed every 30 seconds using (8), with the modifiers estimated as indicated in Section 3. Since the optimization problem (8) needs to be solved quickly and efficiently online, the solution method does not use the process model (12) but rather a convex response-surface approximation that can be solved much faster and enforce the adequacy condition (Francois et al., 2013), which is a prerequisite for the application of RTO-MA (Marchetti et al., 2009). 2% white noise is added to the online measurements of the 4 species, which calls for exponential filtering in the adaptation of the modifiers, e.g., $\hat{\boldsymbol{\varepsilon}}_{\mathrm{j}} = \left(1-\mathrm{K_f}\right)\hat{\boldsymbol{\varepsilon}}_{\mathrm{j-1}} + \mathrm{K_f}\left(\mathbf{G}_{\mathrm{p}}(\mathrm{t_f}) - \mathbf{G}\left(\mathbf{u}_{\mathrm{j}}^*, \boldsymbol{\theta}\right)\right)$ for 0^{th}-order modifiers.

Table 2. Plant performance using the model and plant optimal inputs

Model optimal inputs	Plant optimal inputs
$u_A^* = 14.52\ \mathrm{l.min^{-1}}$	$u_{A,p}^* = 17.20\ \mathrm{l.min^{-1}}$
$u_B^* = 14.90\ \mathrm{l.min^{-1}}$	$u_{B,p}^* = 30.30\ \mathrm{l.min^{-1}}$
$J_p\left(\mathbf{u}^*\right) = 9.11\ \mathrm{mol.min^{-1}}$	$J_p\left(\mathbf{u}_p^*\right) = 15.42\ \mathrm{mol.min^{-1}}$
$G_{1,p}\left(\mathbf{u}^*\right) = -0.36$	$G_{1,p}\left(\mathbf{u}_p^*\right) = 0$
$G_{2,p}(\mathbf{u}^*) = -0.87$	$G_{2,p}\left(\mathbf{u}_p^*\right) = -0.19$

The same adaptation scheme with the gain $K_f = 0.3$ is used for all modifiers. Figure 1 shows the inputs, the constraints and the cost as functions of time. The inputs converge toward the plant optimum in about 40 min, which is about the reactor settling time. Note that the plant cost can exceed its optimal steady-state value during transient. As observed in the bottom plot of Figure 1, the correct set of active constraints is determined (in this example, the set of active constraints differs for the model and the plant optimal solutions). The small offsets observed with respect to $u_{A,p}^*$, $u_{B,p}^*$, $G_{1,p}(\mathbf{u}_p^*)$ and $G_{2,p}(\mathbf{u}_p^*)$ are due to the inaccuracy of the linearization-based estimation scheme (11) for large variations, but these offsets are marginal and do not penalize the converged value of the plant cost function. Simulations have also been also carried out for the case of perfect gradient estimation and no measurement noise, which leads to perfect convergence to the plant optimum (not included here due to space limitation).

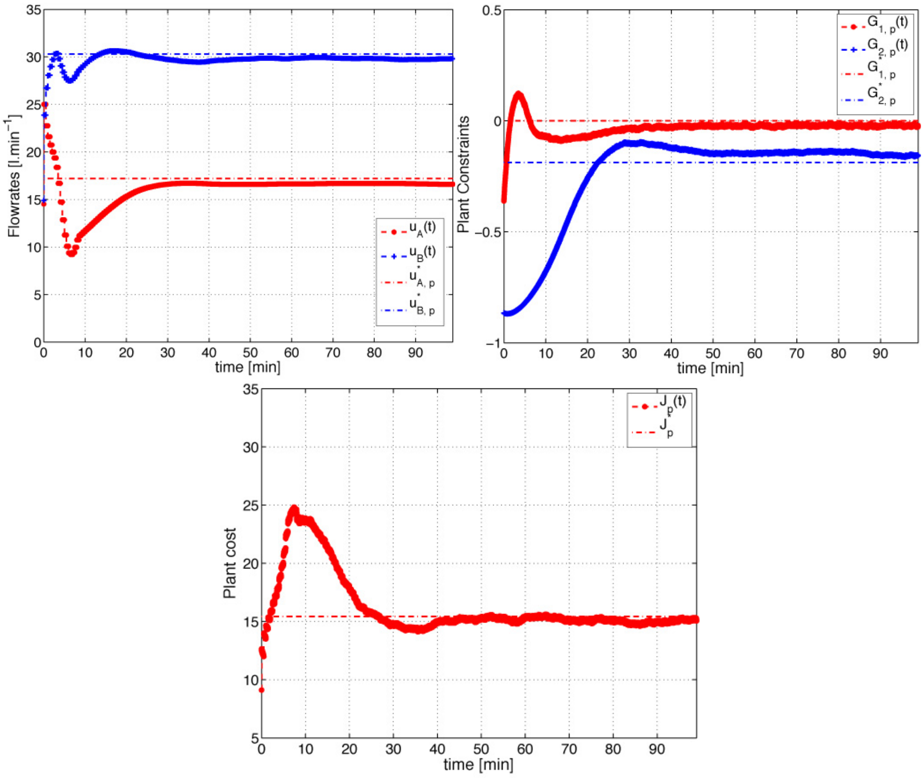

Figure 1. Input flowrates, plant constraints and plant cost vs. time

5. Conclusions

This article has proposed a framework for using RTO-MA with transient measurements. Despite plant-model mismatch, convergence to the true plant optimum is possible with a single operation to steady state. In addition, a linearization-based scheme for estimating the cost and constraint gradients in the presence of parametric uncertainty has been proposed. The scheme appears to be quite powerful, whereby the advantages of model-based explicit RTO methods (handling of process constraints) can be combined with the advantages of implicit control-inspired methods (fast convergence). The proposed methodology has been applied to a simulated CSTR in the presence of noise, constraints and parametric uncertainty. The time needed for convergence is of the order of the settling time, that is, a factor 5 reduction compared to its standard form under the same uncertain scenario (Francois et al., 2013). Although a workable scheme has been proposed in this paper, more work is needed to address the estimation of plant gradients. For example, a regularization-based method for estimating gradients at steady state has recently been proposed (Bunin et al., 2013), which seems well suited to fit this framework. A stability analysis is also needed to ensure that the use of static optimization to control a dynamic system does not preclude its stabilization. In this context, very promising results have been obtained with a simulated CSTR involving unstable internal dynamics (not included here due to space limitation).

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Utilisation de Mesures Transitoires pour l'Optimisation en Temps Réel par Adaptation de Modificateurs

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Résumé

Les méthodes d'optimisation en temps réel (RTO) utilisent les mesures disponibles pour compenser l'effet de l'incertitude et conduire un procédé à l'optimalité. Les méthodes explicites, qui s'appuient sur la résolution itérative d'un problème d'optimisation statique, nécessitent typiquement plusieurs itérations de régime établi à régime établi. En revanche, les méthodes implicites, i.e. sans résolution explicite du problème d'optimisation en ligne, peuvent utiliser les mesures transitoires pour conduire le procédé à un régime établi optimal en une seule itération, pour autant que les contraintes actives soient connues. Dans cet article, le schéma explicite « modifier adaptation » (RTO-MA) est étudié. Un canevas est proposé qui permet l'utilisation des mesures transitoires. Il est démontré que la convergence à l'optimum du procédé réel peut être obtenue en une seule itération, pour autant que les gradients du procédé réel puissent être estimés, tâche pour laquelle une méthode basée sur la linéarisation est proposée. L'approche est illustrée au moyen d'un réacteur parfaitement agité, simulé, à marche continue. Il apparaît que le temps nécessaire pour converger est du même ordre de grandeur que le temps de stabilisation du procédé, là où plus de cinq itérations sont nécessaires si l'on applique RTO-MA dans sa formulation originelle. En d'autres termes, RTO-MA, ainsi modifié, a des performances équivalentes à celles des schémas implicites basés sur le contrôle du gradient, avec la capacité supplémentaire de traiter la présence de contraintes.

Mots-clés : Optimisation en temps réel, incertitude, erreurs de modélisation, adaptation de modificateurs, estimation du gradient expérimental.
