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Feedback Real-Time Optimization Strategy Using a Novel Steady-state Gradient Estimate and Transient Measurements

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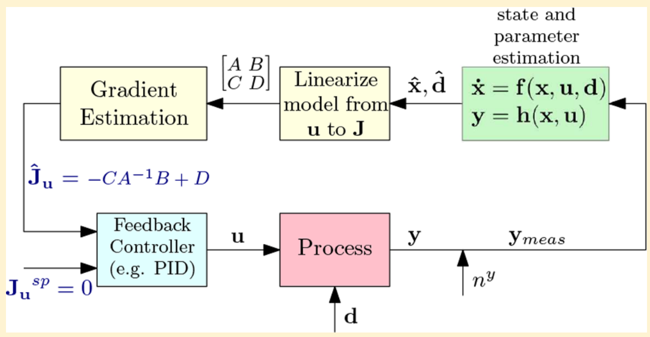
ABSTRACT: This paper presents a new feedback real-time optimization (RTO) strategy for steady-state optimization that directly uses transient measurements. The proposed RTO scheme is based on controlling the estimated steady-state gradient of the cost function using feedback. The steady-state gradient is estimated using a novel method based on linearizing a nonlinear dynamic model around the current operating point. The gradient is controlled to zero using standard feedback controllers, for example, a PI-controller. In the case of disturbances, the proposed method is able to adjust quickly to the new optimal operation. The advantage of the proposed feedback RTO strategy compared to standard steady-state real-time optimization is that it reaches the optimum much faster and without the need to wait for steady-state to update the model. The advantage, compared to dynamic RTO and the closely related economic NMPC, is that the computational cost is considerably reduced and the tuning is simpler. Finally, it is significantly faster than classical extremum-seeking control and does not require the measurement of the cost function and additional process excitation.



INTRODUCTION

Real-time optimization is traditionally based on rigorous steady-state process models that are used by a numerical optimization solver to compute the optimal inputs and set points. The optimization problem needs to be resolved every time a disturbance occurs. This step is also know as ”data reconciliation”. Since steady-state process models are used, it is necessary to wait so that the plant has settled to a new steady-state before updating the model parameters and estimating the disturbances. It was noted by Darby et al.[1] that this steady-state wait time is one of the fundamental limitations of the traditional RTO approach.

In the past two decades or so, there have been developments on several alternatives to the traditional RTO. A good classification and overview of the different RTO schemes is found in Chachuat et al.,[2] François et al.,[3] and the references therein. Recently, to address the problem of the steady-state wait time associated with the traditional steady-state RTO, a hybrid RTO (HRTO) approach was proposed by Krishnamoorthy et al.[4] Here, the model adaptation is done using a dynamic model and transient measurements, whereas the optimization is performed using a static model. The HRTO approach thus requires solving a numerical optimization problem in order to compute the optimal set points. It also requires regular maintenance of both the dynamic model and its static counterpart.

With the recent surge of developments in the so-called direct input adaptation methods, where the optimization problem is converted to a feedback control problem,[2,3] we here propose to convert the HRTO strategy proposed by Krishnamoorthy et al.[4] into a feedback steady-state RTO strategy. This is based on the principle that optimal operation can be achieved by controlling the estimated steady-state gradient from the inputs to the cost at a constant set point of zero. The proposed method involves a novel nonobvious method for estimating the steady-state gradient by linearizing a nonlinear dynamic model, which is updated using transient measurements. To be more specific, the nonlinear dynamic model is used to estimate the states and parameters by means of a dynamic estimation scheme in the same fashion as in the HRTO and dynamic RTO (DRTO) approaches. However, instead of using the updated model in an optimization problem, the state and the parameter estimates are used to linearize the updated dynamic model from the inputs to the cost. This linearized dynamic model is then used to obtain the mentioned nonobvious estimate of the steady-state gradient at the current operating point (Theorem 1). Optimal operation is achieved by controlling the estimated steady-state gradient to constant set point of zero by any feedback controller.

The concept of achieving optimal operation by keeping a particular variable at a constant set point is also the idea behind self-optimizing control, which is another direct input adaptation method; see Skogestad[5] and Jäschke et al.[6] It was also noted by Skogestad[5] that the ideal self-optimizing variable would be the steady-state gradient from the cost to the input, which when kept constant at a set point of zero, leads to optimal operation (thereby satisfying the necessary condition

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for optimality). This complements the idea behind our proposed method.

The concept of estimating and driving the steady-state cost gradients to zero is also the same as that used in methods such as extremum-seeking control,[7,8] necessary-conditions of optimality (NCO) tracking controllers,[9] and "hill-climbing" controllers.[10] However, these methods are model-free and hence require additional perturbations for accurate gradient estimation. The main disadvantages of such methods are that they require the cost to be measured directly and generally give prohibitively slow convergence to the optimum.[11,12]

The main contribution of this paper is a novel gradient estimation method (Theorem 1), which is used in a feedback-based RTO strategy using transient measurements. The proposed method is demonstrated using a CSTR case study. The proposed method is compared with the traditional SRTO (SRTO), DRTO, and the newer HRTO approach. It is also compared with two direct-input adaptation methods, namely, self-optimizing control and extremum-seeking control.

■ PROPOSED METHOD

In this section, we present the feedback steady-state RTO strategy. Consider a continuous-time nonlinear process:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{d}(t))$$
$$\mathbf{y}(t) = \mathbf{h}(\mathbf{x}(t), \mathbf{u}(t)) \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{u} \in \mathbb{R}^{n_u}$, and $\mathbf{y} \in \mathbb{R}^{n_y}$ are the states, process inputs, and process measurements, respectively. $\mathbf{d} \in \mathbb{R}^{n_d}$ is the set of process disturbances. $\mathbf{f}$: $\mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \rightarrow \mathbb{R}^{n_x}$ describes the differential equations, and the measurement model is given by $\mathbf{h}$: $\mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_y}$. Let the cost that has to be optimized J: $\mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}$ be given by

$$J(t) = \mathbf{g}(\mathbf{x}(t), \mathbf{u}(t)) \tag{2}$$

The measurement model and the cost function are not directly affected by the disturbances but are affected via the states. According to the plantwide control procedure,[5] we also assume that any active constraints are tightly regulated and that the n_u degrees of freedom considered here are the remaining unconstrained degrees of freedom available for optimization.

Assumption 1. *Equation 2 is sufficiently continuous and twice differentiable, such that for any* $\mathbf{d}$ *eq 2 has a minimum at* $\mathbf{u} = \mathbf{u}^*$. *According to the Karush–Kuhn–Tucker (KKT) conditions, the following then hold:*

$$\frac{\partial J}{\partial \boldsymbol{u}}(\mathbf{u}^*, \mathbf{d}) = \mathbf{J}_{\mathbf{u}}(\mathbf{u}^*, \mathbf{d}) = 0 \quad (3)$$
$$\frac{\partial^2 J}{\partial \mathbf{u}^2}(\mathbf{u}^*, \mathbf{d}) = \mathbf{J}_{\mathbf{uu}}(\mathbf{u}^*, \mathbf{d}) \geq 0 \quad (4) \tag{3}$$

Without loss of generality, we can assume that the optimization problem is a minimization problem.

The optimization problem can be converted to a feedback control problem by controlling the steady-state gradient $\mathbf{J}_{\mathbf{u}}$ to a constant set point of $\mathbf{J}_{\mathbf{u}}^{sp} = 0$. The main challenge is then to estimate the steady-state gradient efficiently. There are many different data-based gradient estimation algorithms that estimate the steady-state gradient using steady-state measurements; see Srinivasan et al.[13] In this paper, we propose to estimate the steady-state gradient using a nonlinear dynamic model and the process measurements y_{meas} by means of a combined state and parameter estimation framework. In this way, we can estimate the exact gradients around the current operating point.

Any state estimation scheme may be used to estimate the states $\hat{\mathbf{x}}$ and the unmeasured disturbances $\hat{\mathbf{d}}$ using the dynamic model of the plant and the measurements $\mathbf{y}_{meas}$. In this paper, for the sake of demonstration, we use an augmented extended Kalman filter (EKF) for combined state and parameter estimation; see Simon[14] for detailed description of the extended Kalman filter.

Once the states and unmeasured disturbances are estimated, eq 2 is linearized to obtain a local linear dynamic model from the inputs $\mathbf{u}$ to the objective function J. Let $\tilde{\mathbf{x}}(t)$, $\tilde{\mathbf{u}}(t)$, and $\tilde{\mathbf{d}}(t)$ denote the original dynamic trajectory that would result if we keep $\mathbf{u}$ unchanged (i.e., no control). Let $\Delta\mathbf{u}(t)$ represent the additional control input and $\Delta\mathbf{x}(t)$ the resulting change in the states:

$$\mathbf{x}(t) = \tilde{\mathbf{x}}(t) + \Delta\mathbf{x}(t)$$
$$\mathbf{u}(t) = \tilde{\mathbf{u}}(t) + \Delta\mathbf{u}(t)$$
$$\mathbf{d}(t) = \tilde{\mathbf{d}}(t) + \Delta\mathbf{d}(t) \tag{5}$$

where we assume $\tilde{\mathbf{u}}(t) = \hat{\mathbf{u}}(t_0)$ (constant) and $\tilde{\mathbf{d}}(t) = \hat{\mathbf{d}}(t_0)$ (constant), and t_0 denotes the current time. $\Delta\mathbf{d}(t) = 0$ because the control input does not affect the disturbances. For control purposes, the local linear dynamic model from the inputs to the cost in terms of the deviation variables is then be given by

$$\Delta\dot{\mathbf{x}} = A\Delta\mathbf{x}(t) + B\Delta\mathbf{u}(t)$$
$$\Delta J(t) = C\Delta\mathbf{x}(t) + D\Delta\mathbf{u}(t) \tag{6}$$

where $A \in \mathbb{R}^{n_x \times n_x}$, $B \in \mathbb{R}^{n_x \times n_u}$, $C \in \mathbb{R}^{1 \times n_x}$ and $D \in \mathbb{R}^{1 \times n_u}$. The system matrices are evaluated around the current estimates $\hat{\mathbf{x}}$ and $\hat{\mathbf{d}}$:

$$A = \left.\frac{\partial \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{d})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t_0), \mathbf{d}=\hat{\mathbf{d}}(t_0)}$$
$$B = \left.\frac{\partial \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{d})}{\partial \mathbf{u}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t_0), \mathbf{d}=\hat{\mathbf{d}}(t_0)}$$
$$C = \left.\frac{\partial \mathbf{g}(\mathbf{x}, \mathbf{u})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t_0), \mathbf{d}=\hat{\mathbf{d}}(t_0)}$$
$$D = \left.\frac{\partial \mathbf{g}(\mathbf{x}, \mathbf{u})}{\partial \mathbf{u}}\right|_{\mathbf{x}=\hat{\mathbf{x}}(t_0), \mathbf{d}=\hat{\mathbf{d}}(t_0)}$$

Since we do not assume full-state feedback, we need some nonlinear observer to estimate the states $\hat{\mathbf{x}}$ in order to evaluate the aforementioned Jacobians. Nonlinear observers may not be required if we have full state feedback information to compute the Jacobians, but this is seldom the case.

Theorem 1. *Given a nonlinear dynamic system, eqs 1 and 2, and that assumption 1 holds, the model from the decision variables* $\mathbf{u}$ *to the cost* J *can be linearized around the current operating point using any nonlinear observer to get eq 6, and the corresponding steady-state gradient is then*

$$\hat{\mathbf{J}}_{\mathbf{u}} = -CA^{-1}B + D \tag{7}$$

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The process can be driven to its optimum by controlling the estimated steady-state gradient to constant set point of zero using any feedback control law $\mathbf{u} = K(\hat{\mathbf{J}}_{\mathbf{u}})$.

Proof. *In eq 6, $\Delta\mathbf{x}(t)$, $\Delta\mathbf{u}(t)$, and $\Delta J(t)$ are deviation variables. Let $\Delta\mathbf{u}(t) = \delta\mathbf{u}$ be a small step change in the input occurring at t = 0, which will result in a steady-state change for the system as $t \to \infty$. This will occur when $\Delta\dot{\mathbf{x}} = 0$, and by eliminating $\Delta\mathbf{x}(t)$, it follows from eq 6 that the steady-state change in the cost is*

$$\delta J = \lim_{t\to\infty} \Delta J(t) = (-CA^{-1}B + D)\,\delta\mathbf{u} \tag{8}$$

Here, the steady-state gradient is defined as $\mathbf{J}_{\mathbf{u}} = \frac{\delta J}{\delta \mathbf{u}}$, and eq 7 follows. Driving the estimated steady-state gradients to a constant set point of zero ensures satisfying the necessary condition of optimality.

The proposed method is schematically represented in Figure 1. It can be seen that steady-state gradient is obtained from the

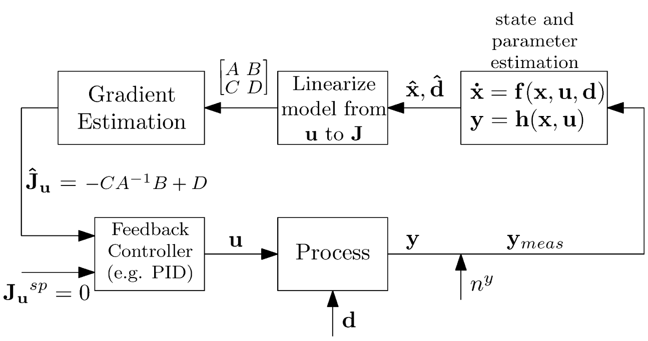

Figure 1. Block diagram of the proposed method.

dynamic model and not from the steady-state model, as would be the conventional approach. With a dynamic model we are able to use the transient measurements to estimate the steady-state gradient.

We have used the dynamic model from $\mathbf{u}$ to J. To tune the controller, another dynamic model from the inputs $\mathbf{u}$ to the gradient $\hat{\mathbf{J}}_{\mathbf{u}}$ is required. The steady-state gain of this model is the Hessian $\mathbf{J}_{\mathbf{uu}}$ which is constant if the optimal surface is quadratic, and according to Assumption 1, the Hessian does not change sign. In any case, this model is not the focus of this article. More discussions on controller tuning are provided in the Discussion. The combined state and parameter estimation framework using extended Kalman filter is discussed in detail by Simon.[14]

Although we use an extended Kalman filter to demonstrate the proposed method in the example, any observer may be used to estimate the states and the parameters. Using the estimated states, the dynamic model may be linearized and the steady state gradient estimated using eqs 6 and 7, which is the key point in the proposed method.

■ ILLUSTRATIVE EXAMPLE

In this section, we test the proposed method using a continuous stirred tank reactor (CSTR) process from Economou et al.[15] (Figure 2). This case study has been widely used in academic research.[16−18] The proposed method is compared to traditional steady-state RTO, HRTO, and DRTO. It also benchmark against two existing direct-

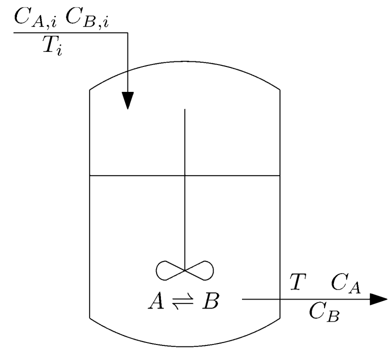

Figure 2. Case 1: Exothermic reactor process.

adaptation-based method, namely, self-optimizing control and extremum-seeking control.

Exothermic Reactor. The CSTR case study consists of a reversible exothermic reaction where component A is converted to component B ($A \rightleftharpoons B$), and the reaction rate is given as $r = k_1C_A - k_2C_B$ where $k_1 = C_1\,e^{-E_1/RT}$ and $k_2 = C_2\,e^{-E_2/RT}$. The dynamic model consists of two mass balances and an energy balance:

$$\frac{dC_A}{dt} = \frac{1}{\tau}(C_{A,i} - C_A) - r \quad \text{where } \tau = \frac{M}{F} \tag{9a}$$

$$\frac{dC_B}{dt} = \frac{1}{\tau}(C_{B,i} - C_B) + r \tag{9b}$$

$$\frac{dT}{dt} = \frac{1}{\tau}(T_i - T) + \frac{-\Delta H_{rx}}{\rho C_p} r \tag{9c}$$

Here, C_A and C_B are concentrations of the two components in the reactor, whereas $C_{A,i}$ and $C_{B,i}$ are in the inflow. T_i is the inlet temperature and T is the reaction temperature. Other model parameters for the process are given in Table 1.

Table 1. Nominal Values for CSTR Process

	description	value	unit
F^*	feed rate	1	mol min^{-1}
C_1	constant	5000	s^{-1}
C_2	constant	10^6	s^{-1}
C_p	heat capacity	1000	cal kg^{-1} K^{-1}
E_1	activation energy	10^4	cal mol^{-1}
E_2	activation energy	15000	cal mol^{-1}
$C^*_{A,i}$	inlet A concentration	1	mol L^{-1}
$C^*_{B,i}$	inlet B concentration	0	mol L^{-1}
R	universal gas constant	1.987	cal mol^{-1} K^{-1}
ΔH_{rx}	heat of reaction	−5000	cal mol^{-1}
ρ	density	1	kg L^{-1}
τ	time constant	1	min

The cost function to be minimize is defined as[16]

$$J = -[2.009C_B - (1.657 \times 10^{-3}T_i)^2] \tag{10}$$

The manipulated variable is $\mathbf{u} = T_i$, the temperature in the inlet stream. The state variables are the concentrations and reactor temperature $\mathbf{x}^T = [C_A\ C_B\ T]$; the disturbances are assumed to be the feed concentrations $\mathbf{d}^T = [C_{A,i}\ C_{B,i}]$. The available measurements are $\mathbf{y}^T = [C_A\ C_B\ T\ T_i]$.

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Feedback Steady-State RTO. The proposed feedback RTO strategy described above (Proposed Method) is now implemented for the CSTR case study. For the state estimation, we use an extended Kalman filter as described by Simon.[14] The disturbances $\mathbf{d}^T = [C_{A,i}\ C_{B,i}]$ are assumed to be unmeasured and are estimated together with the states in the extended Kalman filter. A simple PI controller is used to control the estimated steady-state gradient to a constant set point of $\mathbf{J}_u^{sp} = 0$. The PI controller gains are tuned using SIMC tuning rules with the proportional gain $K_p = 4317.6$ and integral time $T_I = 60$ s. The process is simulated with a total simulation time of 2400 s with disturbances in $C_{A,i}$ from 1 to 2 mol L^{-1} at time $t = 400$ s and $C_{B,i}$ from 0 to 2 mol L^{-1} at time $t = 1409$ s. The measurements are assumed to be available with a sampling rate of 1 s.

Optimization-Based Approaches. In this subsection, the simulation results of the proposed method are compared with other optimization-based approaches, namely, SRTO, DRTO, and HRTO, for the same disturbances as mentioned above. The SRTO, DRTO, and HRTO structures were used to compute the optimal input temperature. In practice, this could correspond to a set point under the assumption of tight control at the lower regulatory control level.

Traditional Static RTO (SRTO). In this approach, before we can estimate the disturbances and update the model, we need to ensure that the system is operating in steady state. This is done using a steady-state detection (SSD) algorithm that is commonly used in industrial RTO system.[19] The resulting steady-state wait time is a fundamental limitation in many processes and the plant may be operated suboptimally for significant periods of time before the model can be updated and the new optimal operation recomputed.

Hybrid RTO (HRTO). As mentioned earlier, in order to address the steady-state wait time issue of traditional RTO approach, a HRTO approach was proposed,[4] where a dynamic nonlinear model is used online to estimate the parameters and disturbances. The updated static model is then used by a static optimizer to compute the optimal inlet temperature as shown in Figure 3. In this case study, we use the same extended Kalman filter as the one used in the proposed feedback RTO method for the dynamic model adaptation. We then compare the performance of the proposed feedback RTO to the HRTO approach. These two approaches only differ in the fact that in HRTO, a static optimization problem is solved to compute the optimal inlet temperature, whereas in the proposed method optimization is done via feedback.

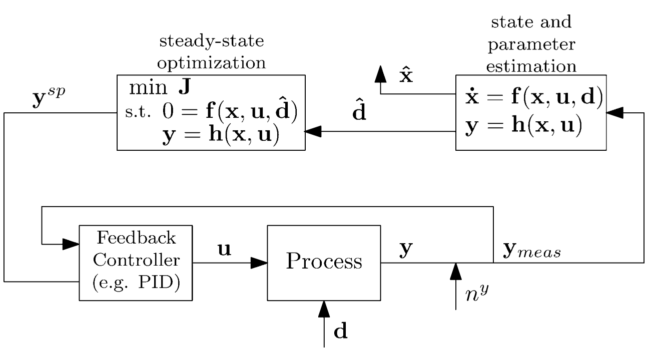

Figure 3. Block diagram of the Hybrid RTO scheme proposed by Krishnamoorthy et al.[4]

Dynamic RTO (DRTO). Recently there has been a surge of research activity toward dynamic optimization and centralized integrated optimization and control such as economic nonlinear model predictive control (EMPC), which is also closely related to DRTO. Since the proposed method uses a nonlinear dynamic model online, a natural question that may arise is why not use the same dynamic models also for optimization. For the sake of completeness, we therefore compare the performance of the proposed method with DRTO.

For the DRTO, the same extended Kalman filter as that in the proposed feedback RTO method and HRTO was used to update the dynamic model online. The updated nonlinear dynamic model was then used in the dynamic optimization problem with a prediction horizon of 20 min and a sampling time of 10 s.

Comparison of RTO Methods. The cost J and the optimal control input $\mathbf{u}$ provided by the proposed feedback RTO method, SRTO, HRTO, and DRTO, are shown in Figure 4a,b, respectively.

It can be clearly seen that for the SRTO (black dashed and dotted lines), the steady-state wait time delays the model adaptation and hence the system operates suboptimally for significant time periods. Once the process reaches steady-state and the model is updated, we see that the steady-state RTO brings the system to the ideal optimal operation. For example, in this simulation case, it takes around 400 s after each disturbances for the SRTO to update the optimal operating point. The change in the cost observed during the transients, before the new optimum point is recomputed, is due to the natural drift in the system. This is more clearly seen after the second disturbance at time $t = 1400$ s.

HRTO (cyan solid lines) and DRTO (green solid lines) provide performance similar to that of the new proposed feedback RTO strategy (red solid lines), due to the fact that all these three approaches use transient measurements and a nonlinear dynamic model online. These three methods however differ in the way the optimization is performed. As mentioned earlier, DRTO solves a dynamic optimization problem using the updated nonlinear dynamic model, and HRTO solves a static optimization problem using the updated static counterpart of the model. Feedback RTO estimates the steady state gradient by linearizing the nonlinear dynamic model and controls the estimated steady-state gradients to a constant set point of zero. The integrated loss is given by

$$L_{\text{int}}(t) = \int_0^t (J_{\text{opt,SS}}(t) - J(t))\, dt \tag{11}$$

To compare the different approaches further, the integrated loss for the different RTO approaches are shown in Figure 4c and noted in Table 2 for $t = 1400$ s and 2400 s.

We note here that until time $t = 1400$ s, the new feedback RTO method has the lowest loss of \$73.73 closely followed by DRTO and HRTO with losses of \$73.81 and \$74.77, respectively. Following the second disturbance, the integrated loss for the interval $t = 1400-2400$ s is the lowest for DRTO with \$247.69. The new feedback RTO has a very similar loss of \$248.07 followed by HRTO with an integrated loss of \$257.97. SRTO is much worse with a loss of \$355.78. This is mainly because of the fact that in the new feedback RTO approach optimization is done via feedback and hence can be implemented at higher sampling rate. The SRTO, DRTO, and HRTO approaches requires additional computation time

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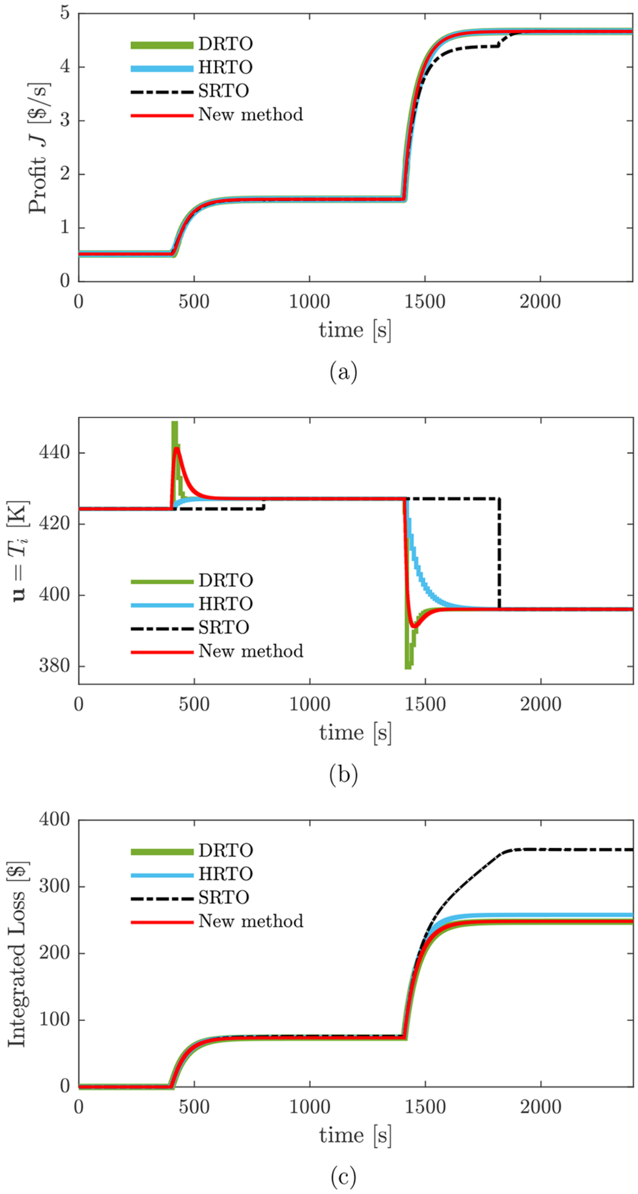

Figure 4. Simulation results of the proposed feedback RTO method (red solid lines) compared to traditional SRTO (black dashed and dotted lines), HRTO (cyan solid lines) and DRTO (green solid lines) for disturbance in $C_{A,i}$ at time t = 400 s and $C_{B,i}$ at time t = 1400 s. (a) Plot comparing the cost function. (b) Plot comparing the input usage. (c) Plot comparing the integrated loss.

Table 2. Average Computation Time and Integrated Loss at the End of Simulation Time for the Proposed Method Compared with Traditional SRTO, HRTO, and Economic MPC

	computation time [s]	integrated loss t = 1400 s [\$]	integrated loss t = 2400 s [\$]
new method	0.004	73.73	248.07
SRTO	0.007	75.75	355.78
HRTO	0.01	74.77	257.97
DRTO	0.14	73.81	247.69

to solve the optimization problem online, and hence may be implemented at slower sampling rates. As mentioned earlier, in our case study, the feedback RTO approach is implemented every 1 s as opposed to SRTO, DRTO, and HRTO approaches, which are solved every 10 s. This is clearly shown in Figure 5a, where the control input from Figure 4b is magnified between time 350−550 s. Following the disturbance at t = 400 s, the SRTO, DRTO, and HRTO updates the set point at time step t = 410 s unlike the feedback RTO, which updates the new control input already at time t = 401 s giving it an advantage over other RTO methods. As a result, the new feedback RTO method has the lowest integrated loss up to time t = 1400 s. The control input between time 1300−1500 s is shown in Figure 5b, where following the disturbance at t = 1409 s, new proposed feedback RTO, SRTO, DRTO, and HRTO all update the optimal control input at time step t = 1410 s simultaneously. Therefore, the DRTO has the best integrated loss as expected. This example clearly shows the importance of being able to implement a controller at higher sampling rates.

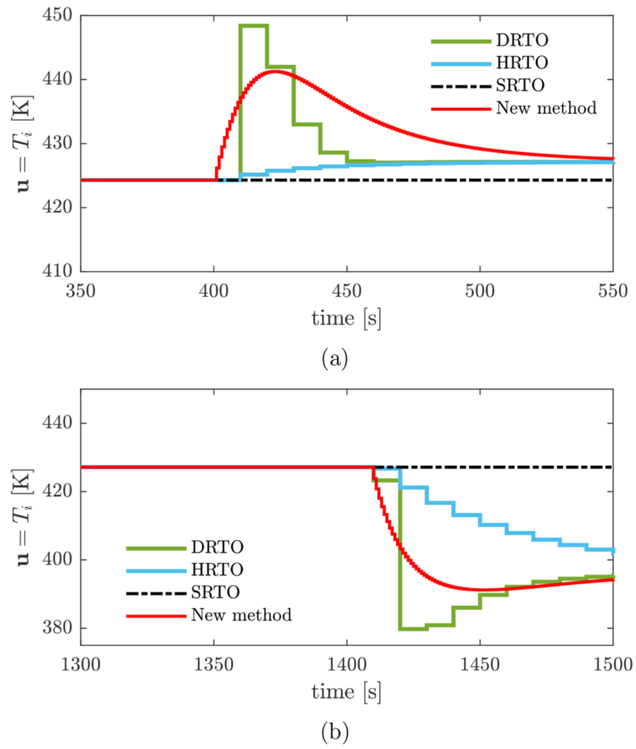

Figure 5. Magnified plot of the control input from Figure 4b between time (a) 350−550 s and (b) 1300−1500 s.

The simulations are performed on a workstation with the Intel Core i7−6600U CPU (dual-core with the base clock of 2.60 GHz and turbo-boost of 3.40 GHz), and 16GB memory. The average computation times for the different RTO approaches are also compared in Table 2. The proposed feedback RTO method is the least computationally intensive method due to the fact the optimization is done via feedback, and as expected, DRTO is the most computationally intensive.

Comparison with Direct-Input Adaptation Methods. In this subsection, we compare the proposed method with two direct input adaptation based methods, namely, self-optimizing control and extremum-seeking control.

Self-Optimizing Control (SOC). Since we have 3 measurements, 2 disturbances and 1 control input, the nullspace

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method can be used to identify the self-optimizing variable. For the case-study considered here, the optimal selection matrix computed using nullspace method (around the nominal optimal point when $\mathbf{d}^T = [C_{A,i}\ C_{B,i}]=[1.0\ 0.0]$) is given by $\mathbf{H} = [-0.76880\ 63940\ 0046]$, see Alstad Ch.4.[16]. The resulting self-optimizing variable $\mathbf{c} = -0.7688C_A + 0.6394C_B + 0.0046T$ is controlled to a constant set point of $\mathbf{c}_s = 1.9012$. The PI controller tunings used in the self-optimizing control structure were tuned using SIMC rules with proportional gain $K_p = 188.65$ and integral time $T_I = 75$ s.

The simulations were performed with the same disturbances as in the previous case. The objective function for the two methods are shown in Figure 6a, and the corresponding control input usage is shown in Figure 6b. When compared to self-optimizing control, we can see that there is an optimality gap when the disturbances occur. This is because self-optimizing control is based on linearization around the nominal optimal point, as opposed to linearization around the current operating point in the proposed feedback RTO approach. Because of the nonlinear nature of the processes, the economic performance degrades for operating points far from the nominal optimal point, hence leading to steady-state losses.

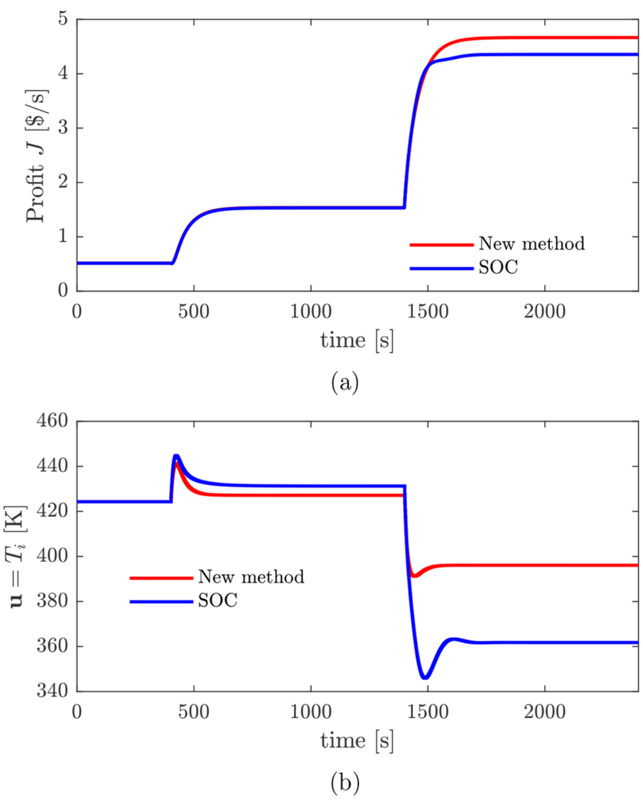

Figure 6. Simulation results of the proposed feedback RTO method (red solid lines) compared to self-optimizing control (blue solid lines) for disturbance in $C_{A,i}$ at time $t = 400$ s and $C_{B,i}$ at time $t = 1400$ s. (a) Plot comparing the cost function. (b) Plot comparing the input usage.

Extremum Seeking Control (ESC). The concept of estimating and driving the steady-state gradient to zero in the proposed feedback RTO strategy is also used in data-driven methods such as extremum-seeking control and NCO-tracking. However, the methods are fundamentally different and complementary rather than competing.

For the sake of brevity, we restrict our comparison to extremum-seeking control. We consider the least-squares based extremum-seeking control proposed by Hunnekens et al.[20] because it has been shown to provide better performance than classical extremum-seeking control.[20,21] The least-squares based extremum-seeking controller also estimates the gradient rather than just the sign of the gradient.[22] The least-squares based extremum-seeking controller estimates the steady-state gradient using the measured cost and input data with the moving window of fixed length in the past. The gradient estimated by the least-square method is then driven to zero using a simple integral action. The integral gain was chosen to be $K_{ESC} = 2$.

Due to the slow convergence of the extremum-seeking controller, the process with simulated with a total simulation time of 600 min with disturbances in $C_{A,i}$ from 1 to 2 mol L^{-1} at time $t = 10\,800$ s and $C_{B,i}$ from 0 to 2 mol L^{-1} at time $t = 21\,600$ s. The results using extremum-seeking control are compared with that the of the proposed method in Figure 7a. It can be seen that the extremum-seeking controller reaches the optimal point, however, the convergence to the optimum point is very slow compared to the proposed method. The proposed method has a fast reaction to the disturbances and hence reaches the optimum significantly faster than the extremum-seeking controller. The integrated loss compared to the ideal steady-state optimum (eq 11) shown in Figure 7c reflects this.

It should be added this is a simulation example because strictly speaking it may not be possible to directly measure an economic cost J with several terms. The simple cost in eq 10 may be computed by measuring individually the composition C_B and the inlet temperature T_i, but more generally for process systems, direct measurement of all the terms and adding them together is not accurate. This is discussed further in the Discussion.

Other Multivariable Case Studies. In addition to the CSTR case study, the new proposed feedback RTO method has been successfully applied to a 3-bed ammonia reactor case study by Bonnowitz et al.[23] and to an oil and gas production optimization problem by Krishnamoorthy et al.[24] In all these case studies, the new feedback RTO method was compared with other optimization methods and was shown to provide consistent results as in the CSTR case study shown in this paper. Both these cases studies are multivariable processes, where the steady-state gradients must be estimated and controlled to zero.

For example, let us consider the ammonia reactor process studied by Bonnowitz et al.,[23] which consists of 3 ammonia reactor beds. The optimization problem is concerned with computing the three optimal feeds in order to maximize the reaction extent. The proposed method was applied to this system, where the steady-state gradients of the cost with respect to the three inputs were estimated using eq 7. The reader is referred to Bonnowitz et al.[23] for more detailed information about the process and the simulation results, which shows that the proposed method works also for multi-input processes that are coupled together.

DISCUSSION

Comparison with Optimization-Based Approaches. With the traditional steady-state RTO approach, it was seen clearly that the steady-state wait time resulted in suboptimal operation, clearly motivating the need for alternative RTO

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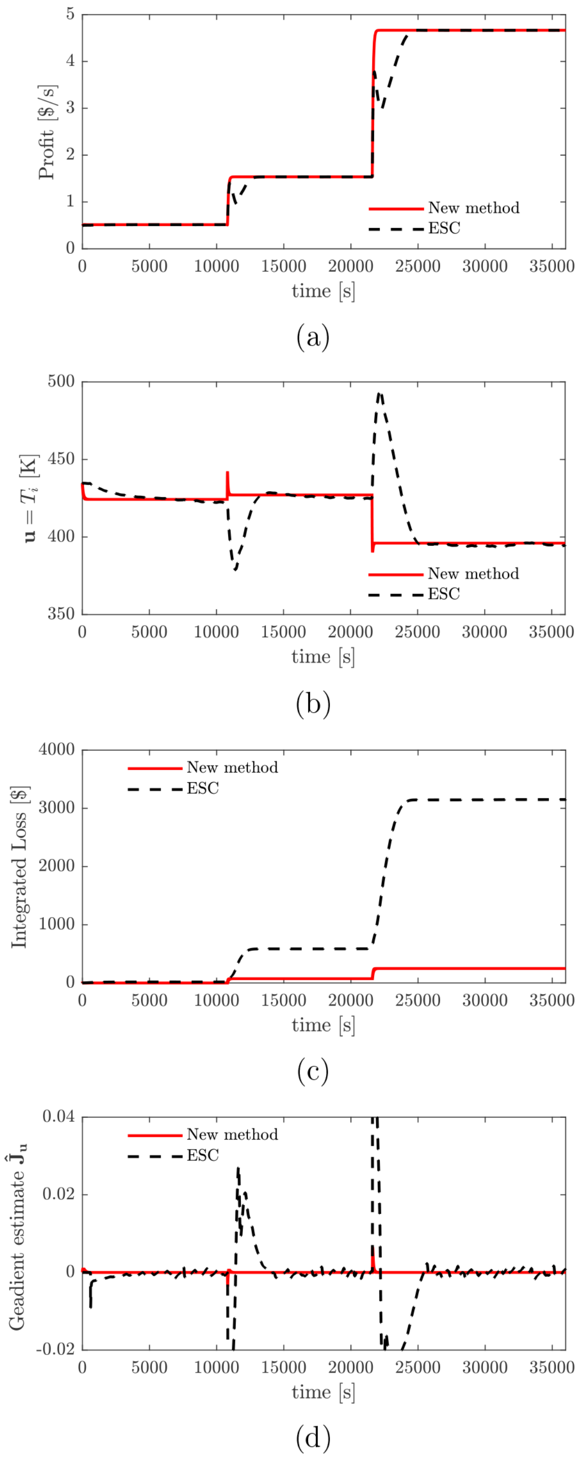

Figure 7. Comparison of the proposed feedback RTO method (red solid lines) with extremum-seeking control (black dashed lines) for disturbance in $C_{A,i}$ at time t = 10 800 s and $C_{B,i}$ at time t = 21 600 s. (a) Plot comparing the cost function. (b) Plot comparing the input usage. (c) Plot comparing the integrated loss. (d) Plot comparing the estimated gradients.

strategies that can use transient measurements. Dynamic optimization frameworks, such as DRTO and economic MPC that use transient measurements, provide the optimal solution, but it comes at the cost of solving computationally intensive optimization problems as noted in Table.2. This is even worse for large-scale systems where the sample time will be restricted by the computational time. Indeed, the computational delay has also been shown to result in performance degradation or even instability.[25]

The feedback RTO strategy proposed in this paper is closely related to the recently proposed HRTO scheme[4] and has similar performance (see Figure 4a). The main difference is that in the new strategy, the steady-state gradient is obtained as part of the solution to the estimation problem and the optimization is then solved by feedback control rather than numerically solving a steady-state optimization problem. Thus, we avoid maintaining the steady-state models in addition to the dynamic model (i.e., avoids duplication of models and it avoids the numerical optimization).

However, a drawback of the proposed method is that it cannot handle changes in the active constraint set as easily as optimization-based methods. Changes in the active constraint set would require redesign and retuning of the feedback controllers.

Comparison with Self-Optimizing Control. Self-optimizing control is based on linearization around the nominal optimal point. The economic performance degrades for operating points far from the nominal optimal point due to the nonlinear nature of the process. This is the reason for the sustained steady-state loss of self-optimizing control seen in the simulation results. The proposed method, however, is based on linearization around the current operating point and hence does not lead to steady-state losses. The price for this performance improvement is the use of the model online instead of offline. In other words, the proposed method requires computational power for the nonlinear observers which are not required in the standard self-optimizing control. However, nonlinear observers such as extended Kalman filters can be used, as demonstrated in the simulations, which are known to be simple to implement and computationally fast.[26] The EKF used in the simulations had an average computation time of 0.0036 s.

Comparison with Extremum-Seeking Control. As mentioned earlier, extremum-seeking control estimates the steady-state gradient by fitting a local linear static model using the cost measurements. Therefore, transient measurements cannot be used for the gradient estimation. However, since our proposed method linearizes the nonlinear dynamic system to get a local linear dynamic model, it does not require a time scale separation for the gradient estimation. Hence the convergence to the optimum is significantly faster compared to the extremum-seeking control, as demonstrated in our simulation results.

In order to address the issue of time-scale separation in extremum-seeking control, McFarlane and Bacon[27] also considered using a local linear dynamic model to estimate the steady-state gradient. They proposed to identify a linear dynamic model directly from the measurements, as opposed to estimating the states using a nonlinear dynamic model as in our proposed method. Therefore, the method by McFarlane and Bacon[27] is a data-based approach that requires persistent and sufficient excitation to identify the local linear dynamic system. However, our proposed approach of estimating the states using a nonlinear dynamic model and linearizing around the state estimates does not require any additional perturbation (but at the cost of modeling effort).

It is also important to note that extremum-seeking (and NCO-tracking) approaches can handle structural uncertainty. The proposed method, like any other model-based method,

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works well only when the model is structurally correct. In the presence of plant−model mismatch, the proposed method may lead to an optimality gap, leading to some steady-state loss, unlike the model-free approaches, which would perform better. Therefore, extremum-seeking or NCO-tracking methods (including modifier adaptation) methods should be considered to handle structural mismatch.

However, in practice, extremum-seeking methods may not be completely model-free and may then suffer from structural errors, although it will be different from when using model-based optimization. The reason is that a direct measurement of the cost J is often not possible, especially if J is an economic cost with many terms, and it may then be necessary to use model-based methods to estimate one or more terms in the cost J. Typically the cost function for a process plant is of the form

$$J = c_q Q + c_f F - c_{p1} P_1 - c_{p2} P_2 \tag{12}$$

where Q, F, P_1, and P_2 are flows in [kg/s] of utility, feed, and products 1 and 2, respectively, and c_q, c_f, c_{p1}, and c_{p2} are the corresponding prices in [\$/kg]. In many cases, for example in refineries, the operating profit is made by shifting smaller amounts of the feed to the most valuable product (1 or 2), and very accurate measurements would be needed for the flows (F, P_1, P_2) to capture this. In practice, the best way to get accurate flows is to estimate them using a nonlinear process model (e.g., using data reconciliation). This means that for optimization of larger process systems an extremum-seeking or NCO-tracking controller will not be truly model-free, because a model is needed to get an acceptable measurement (estimate) of the cost.

In addition, one main advantage of the proposed method is that it acts on a fast time scale, thus reaching the optimal point (or near-optimal point in the case of model mismatch) significantly faster than model-free approaches which are known to have very slow convergence. In such cases, model-free methods like ESC or NCO tracking that act in the slow time scale can be placed on top of the proposed method to account for the plant−model mismatch (e.g., Jäschke and Skogestad,[17] Straus et al.).[28]

Table 3. Gain and Phase Margins at the Different Steady-States for the Three PI Controllers with Varying τ_c

		gain margin	phase margin
steady-state 1	τ_c = 10 s	17.3	84.8°
	τ_c = 60 s	95.8	89.1°
	τ_c = 240 s	379	89.8°
steady-state 2	τ_c = 10 s	9.99	81.0°
	τ_c = 60 s	55.4	88.4°
	τ_c = 240 s	219	89.6°
steady-state 3	τ_c = 10 s	6.14	75.3°
	τ_c = 60 s	34.1	87.4°
	τ_c = 240 s	135	89.3°

Table 4 summarizes the advantages and disadvantages of the proposed method compared to other tools commonly used for real-time optimization. With this comparison, we want to stress that our new proposed method is not a replacement of any other method but rather adds to the toolbox of available methods for economic optimization.

Tuning. As mentioned earlier, the steady-state gradient is controlled to a constant set point of zero using feedback controllers. The controller tuning is briefly discussed in this section. For the CSTR case study, PI controllers were used. The PI controllers were tuned using the SIMC PID tuning rules.[29] For each input, let the process model from the corresponding gradient $\mathbf{y} = \mathbf{J_u}$ to the input $\mathbf{u}$ be approximated by a first order process. For a scalar case

$$\mathbf{J_u} = \frac{\mathbf{k}}{(\tau_1 s + 1)} e^{-\theta s} \mathbf{u} \tag{13}$$

where τ_1 is the dominant time constant, θ is the effective time delay, and $\mathbf{k}$ is the steady-state gain. These three parameters can be found experimentally or from the dynamic model.[29] Note that the process dynamics include both the effect of the process itself and the estimator; see Figure 1. In our case, we found experimentally by simulations that $\mathbf{k} = 2.25 \times 10^{-4}$, τ_1 = 60 s, and θ = 1 s. The time delay for the process is very small and mainly caused by the sampling time of 1 s.

In general, the steady-state gain is equal to the Hessian, $\mathbf{K} = \mathbf{J_{uu}}$, which according to Assumption 1 should not change sign. The Hessian $\mathbf{J_{uu}}$ was computed for the CSTR case study and it was verified that this assumptions holds. In particular, the value of $\mathbf{K} = \mathbf{J_{uu}}$ for the three steady-states shown in Figure 4 were $\mathbf{J_{uu}} = 2.25 \times 10^{-4}$ (nominal), $\mathbf{J_{uu}} = 3.89 \times 10^{-4}$, and $\mathbf{J_{uu}} = 6.33 \times 10^{-4}$, respectively. The gain increases by a factor of 3, which may lead to instability, but if robust PID tunings are used, then tuning the controller at the nominal point should be sufficient. For a PI-controller

$$c(s) = K_C + \frac{K_I}{s} \tag{14}$$

the SIMC-rules give the proportional and integral gain.[29]

$$K_C = \frac{1}{\mathbf{k}} \frac{\tau_1}{\tau_c + \theta} \qquad K_I = \frac{K_C}{T_I} \tag{15}$$

where the integral time is $T_I = \min(\tau_1, 4(\tau_c + \theta))$, and τ_c is the desired closed-loop time response time constant, which is the sole tuning parameter.[29]

It is generally recommended to select $\tau_c \geq \theta$[29] to avoid instability, and a larger τ_c gives less aggressive control and more robustness. In our case, the controlled variable is $\mathbf{J_u}$ (the gradient), but there is little need to control $\mathbf{J_u}$ tightly because it is not an important variable in itself. Therefore, to get better robustness we recommend selecting a larger value for τ_c (assuming that $\tau_1 > \theta$, which is usually the case):

$$\tau_c \geq \tau_1 \tag{16}$$

Selecting $\tau_c > \tau_1$ means that the closed-loop response is slower than the open-loop response. This avoids excessive use of the input $\mathbf{u}$ and the system is more robust with respect to gain variations. This is confirmed by the simulations in Figure 8b for three different choices of τ_c. With τ_c = 10 s $\ll \tau_1$ = 60 s, we get aggressive input changes with large overshoots in $\mathbf{u} = T_{in}$ for both disturbances. The control of gradient is good (Figure 8c), but this in itself is not important. The improvement in profit J is fairly small compared to the choice $\tau_c = \tau_1$ = 60 s, which is the nominal value used previously. The integrated loss when τ_c = 10 s was \$245.99 as opposed to \$248.07 when $\tau_c = \tau_1$ = 60 s. With $\tau_c = 4\tau_1$ the input change is even smoother, but the performance in terms of the profit (J) is almost the same (with an integrated loss of \$259.07).

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Table 4. Advantages and Disadvantages of the Proposed Method Compared to Other RTO Approaches

	self-optimizing control[a]	extremum-seeking control[b]	new proposed method (feedback RTO)	SRTO	HRTO	economic MPC/DRTO[c]
cost measured	no	yes	no	no	no	no
model	static model used offline	model-free	dynamic model used online	static model used online	static and dynamic model used online	dynamic model used online
perturbation	no	yes	no	no	no	no
transient measurements	yes	no	yes	no	yes	yes
long-term performance	near-optimal	optimal[e]	optimal[d]	optimal[d]	optimal[d]	optimal[d]
convergence time	very fast	very slow	fast	slow[f]	fast	fast[g]
handle change in active constraints	no	no	no	yes	yes	yes
numerical solver	no	no	no	static	static	dynamic
computational cost	very low	very low	low	intermediate	intermediate	high

[a]SOC is complementary to the other methods that should ideally be used in combination. [b]NCO tracking has similar properties but also can track changes in active constraints. [c]Economic MPC typically has noneconomic control objectives in addition to the economic objectives in the cost function, whereas DRTO has only economic objectives. [d]If model is structurally correct. [e]Requires time scale separation between system dynamics, dither and convergence. Suboptimal operation for long periods following disturbances. [f]Slow due to steady-state wait time. Suboptimal operation for long periods following disturbances. [g]Limited by computation time.

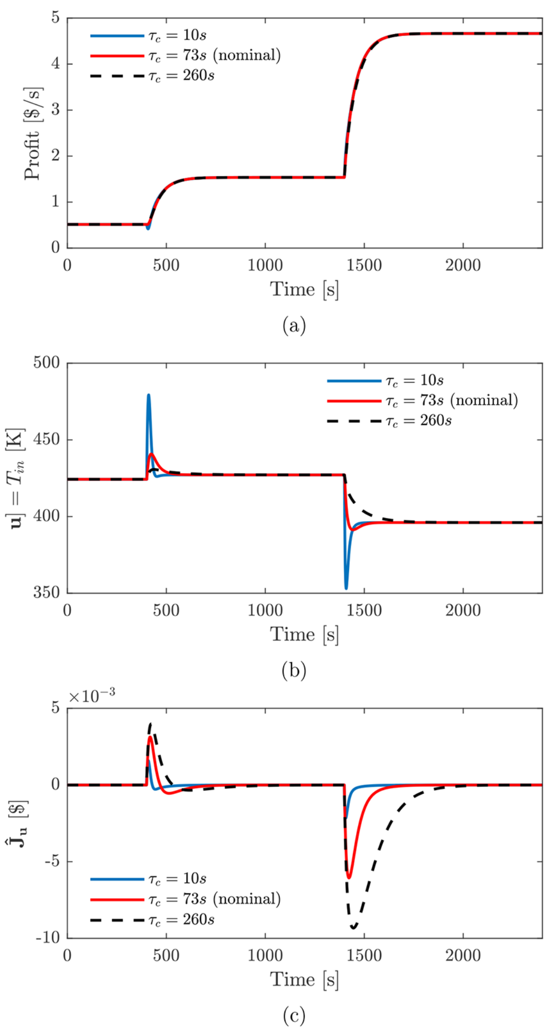

Figure 8. Effect of controller tuning (τ_c) for the new method. (a) Objective function J. (b) Control input $\mathbf{u}$. (c) Estimated gradient $\hat{\mathbf{J}}_\mathbf{u}$.

Stability Robustness. The stability of the system is determined by the closed-loop stability involving the plant input $\mathbf{u}$ (manipulated variable) and the estimated gradient $\mathbf{J}_\mathbf{u}$ as the plant output $\mathbf{y}$. Thus, the overall plant for this analysis includes the real process, the estimator (extended Kalman Filter in our case) and the "measurement" $\mathbf{y} = \mathbf{J}_\mathbf{u} = CA^{-1}B + D$. In this case we use a simple PI-controller and the conventional linear measures for analyzing robustness to compute the gain margin, phase margin or delay margin, or H-infinity measures such as the peak of the sensitivity function, M_S.

The gain and phase margins at the three different steady states are shown for the three alternative PI-controllers in Table 3. The gain margin varies from 17.3 to 6.14 for the least robust controller with $\tau_c = 10$ s, which is still much larger than the expected variations in the process gain (which is about a factor of 3 from 2.25×10^{-4} to 6.33×10^{-4}). This is of course a nonlinear plant, and the conventional linear analysis of closed-loop stability will have the same limitations as it has for any nonlinear plant. It is also possible to consider nonlinear controllers for the plant, but it does not seem necessary because of the large robustness margins for the linear controllers.

In summary, stability is not an important concern for the tuning of the controllers in our case. The important issue is the trade-off between input usage and the speed of response. This was also observed in the other case studies.[23,24]

■ CONCLUSION

To conclude, we propose a novel model-based direct input adaptation approach, where the steady-state gradient $\mathbf{J}_\mathbf{u}$ is estimated as $\hat{\mathbf{J}}_\mathbf{u} = -CA^{-1}B + D$ by linearizing the nonlinear model around the current operating point. The nonlinear model, and thus the steady-state gradient, is updated using transient measurements. It is based on well-known components in the control theory, namely, state estimation and simple feedback control. Since a dynamic model is linearized around the current operating point, the method does not need to wait for the process to reach steady-state before updating the next move. The proposed method also does not require additional perturbations for the gradient estimation as opposed to extremum-seeking control. By using the model online, the proposed method can reduce steady-state losses associated with self-optimizing control. The proposed feedback RTO method is similar to the recently proposed HRTO,[4] but involves a novel way of estimating the steady-state gradient and instead solves the optimization by feedback. This is robust and simple and avoids maintaining a steady-state model. The

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proposed method is tested in simulations, and compared to commonly used optimization-based approaches and direct-input adaptation-based approaches. The simulation results show that the proposed method is accurate, fast and easy to implement. The proposed method thus adds on to the existing toolbox of approaches for real-time optimization, and can be useful for certain cases.

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Notes

The authors declare no competing financial interest.

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