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Control of the Steady-State Gradient of an Ammonia Reactor using Transient Measurements

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Abstract

This paper presents the application of a steady-state real-time optimization strategy using transient measurements to an ammonia synthesis reactor case. We apply a new method for estimating the steady-state gradient of the cost function based on linearizing a dynamic model at the present operating point. The gradient is controlled to zero using a standard feedback controller, for example, a PI-controller. The applied method is able to adjust fast to the new optimal operation in case of disturbances. The advantage 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. It is significantly faster than classical extremum-seeking control and does not require the measurement of the cost function and additional process excitation. Compared to self-optimizing control, it allows the process to achieve the true optimum.

Keywords: Optimal Control, Extremum-Seeking Control, Reactor Control, Measurement Based Optimization

1. Introduction

The general aim of a process plant is to operate at the economic optimum. Different approaches are available in the literature for driving a process to its optimal operation point. The traditional approach is steady-state real-time optimization (RTO) in which a rigorous steady-state model is used for computing optimal setpoints. The necessary model reconciliation requires however that the plant is at steady-state before each reoptimization. This is a fundamental limitation of RTO as it may lead to subopimal operation most of the time (Darby et al., 2011).

Self-optimizing control (SOC) (Skogestad, 2000) alleviates this problem through keeping the operation close to the optimum at all times by controlling selected controlled variable at a constant setpoint. Therefore, it can be used for close to optimal operation while waiting for the steady-state. The implementation is very fast and simple, but in case of unknown or large disturbances, the setpoints need to be updated using some other approach.

An alternative to RTO is a data-based approach, e.g. extremum-seeking control (ESC), which uses the plant measurements to drive the process to its optimal operation (Krstić and Wang, 2000). This is achieved by estimating the steady-state gradient from the input to the cost and using a small I-controller to drive the gradient to zero. Closely related approaches are the “hill-climbing” controller of Shinskey used recently by Kumar and Kaistha (2014) and the NCO-tracking approach of Bonvin and coauthors (Franois et al., 2005). Their main advantage is that they are model free. The main challenge in these methods is the accurate estimation of the steady-state gradient from dynamic measurements. This normally requires constant excitations that are slow enough such that the dynamic system can be approximated as a static map (Krstić and Wang, 2000). As a result the convergence to the optimum is usually very slow. In the presence of abrupt disturbances, extremum-seeking control also causes unwanted deviations as discussed by Kumar and Kaistha (2014) andKrishnamoorthy et al. (2016).

A newer method for optimal operation is economic nonlinear model predictive control (E-NMPC), which handles the dynamic process behaviour, operational constraints, and leads to the optimal inputs for multivariable processes. Nevertheless, solving the optimization problem for a large-scale problem is computationally intensive and can potentially lead to computational delay.

In this paper, a new model-based dynamic gradient estimation (Krishnamoorthy et al., 2018, in preparation) is applied to drive the process to optimal operation. In contrast to standard ESC, the exact steady-state gradients is estimated based on the dynamic model of the process and hence no excitations are required. For the proposed method there is no need to measure the cost directly. Moreover, reoptimization is done by feedback control and solving the optimization problem is not necessary.

Heat-integrated processes, like the ammonia synthesis reactor (Morud and Skogestad, 1998) considered in this paper, are widespread in case of exothermic reactions to utilize the reaction heat. However, limit-cycle behaviour and reaction extinction may occur in the case of disturbances due to the positive feedback imposed through the heat integration (Morud and Skogestad, 1998). Straus and Skogestad (2017) proposed the application of E-NMPC for optimal control of the ammonia reactor to avoid this behaviour. In this paper, the application of the new feedback method is suggested to drive this process to optimal operation without the need of nonlinear dynamic optimization as is the case with E-NMPC or dynamic RTO.

2. Steady-state gradient control using transient measurements

We consider a process that can be modelled as a nonlinear dynamic system of the form

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

$$\mathbf{y} = \mathbf{h}_{\mathbf{y}}(\mathbf{x}, \mathbf{u}) \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{u} \in \mathbb{R}^{n_u}$, $\mathbf{d} \in \mathbb{R}^{n_d}$, and $\mathbf{y} \in \mathbb{R}^{n_y}$ are the states, available control inputs, disturbances, and measurements. The cost does not need to be directly measured. In the proposed method, a state estimator such as an extended Kalman filter (EKF) (Simon, 2006) is applied to estimate the states $\mathbf{x}$ of the system by using the measurements and the dynamic model, given in Eqs. (1) and (2).

Let the cost be modelled as $J = h_J(\mathbf{x}, \mathbf{u})$ with $h_J : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}$. A local linear state-space model, given by the Eqs. (3) and (4), can be obtained through linearization around the current operation point, as shown by Krishnamoorthy et al. (2018, in preparation).

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \tag{3}$$

$$J = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} \tag{4}$$

where $\mathbf{A} = \partial \mathbf{f}/\partial \mathbf{x}$, $\mathbf{B} = \partial \mathbf{f}/\partial \mathbf{u}$, $\mathbf{C} = \partial h_J/\partial \mathbf{x}$, and $\mathbf{D} = \partial h_J/\partial \mathbf{u}$. In order to derive the steady state gradient, we set $\dot{\mathbf{x}} = 0$ and can derive in deviation variables

$$\Delta J = \left(-\mathbf{C}\mathbf{A}^{-1}\mathbf{B} + \mathbf{D}\right)\Delta \mathbf{u} \tag{5}$$

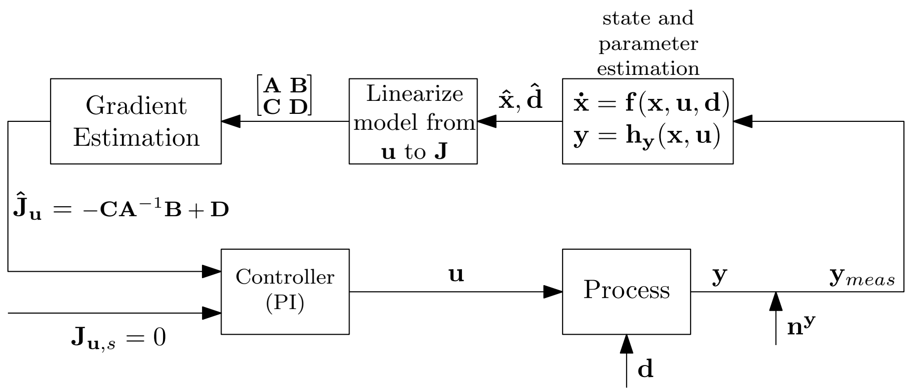

Figure 1: Block diagram of the proposed method.

which, since $\Delta J = \mathbf{J_u}\Delta\mathbf{u}$, gives the following estimate or prediction of the steady-state gradient:

$$\hat{\mathbf{J}}_\mathbf{u} = -\mathbf{C}\mathbf{A}^{-1}\mathbf{B} + \mathbf{D} \tag{6}$$

We want to drive the system to an optimal steady-state where $\mathbf{J_u} = 0$, so even if the system is not at steady-state, we can use feedback control with $\mathbf{y} = \hat{\mathbf{J}}_\mathbf{u}$ as “measurements” to drive the system to the optimal steady-state and by that satisfying the necessary conditions of optimality (Krishnamoorthy et al., 2018, in preparation). Any feedback controller, such as a PI controller, can be used to bring the gradient to zero. It is important to note that by using a nonlinear state estimator and a dynamic model for estimating the steady-state gradient $\mathbf{J_u}$, we can use transient measurements, without the need to wait for steady-state, as in traditional RTO. The scheme of the proposed method is shown in Figure 1. The disturbances can be estimated as well through the extension of Eq. (1) to an augmented system (Simon, 2006).

3. Model and problem formulation

The model of the ammonia reactor and all the model assumptions are based on Morud and Skogestad (1998)’s stability analysis. The process, shown in Figure 2, consists of 3 sequential reactor beds and the feed is split into 4 streams. The model is a differential algebraic system, where the differential equations describe the temperature evolution in the reactor beds and the algebraic equations represent the corresponding mass fraction of ammonia. There are 3 split-ratios or $\mathbf{u}_0 = \begin{bmatrix} u_{0,1} & u_{0,2} & u_{0,3}\end{bmatrix}^\mathsf{T}$ which are controlled by local temperature controllers. This is necessary for stabilizing the process. The temperature controllers are incorporated into the model in contінous time increasing the number of states by 3. This leads to $\mathbf{u} = \begin{bmatrix} T^{sp}_{In,1} & T^{sp}_{In,2} & T^{sp}_{In,3}\end{bmatrix}^\mathsf{T}$. The temperature controllers are modelled as single-input single-output integrator controllers, as the response can be approximated as a proportional process. The SIMC rules (Skogestad and Grimholt, 2012) were applied for the slave controllers tuning.

The state estimation is performed using an EKF (Simon, 2006). To this end, the model was reformulated as a system of ordinary differential equations. Each reactor bed in the model consists of n discrete volumes, which can be modelled as a CSTR cascade. This leads for each reactor bed to a total of $2n$ state variables per time step. For any CSTR reactor j in the CSTR cascade, the differential equations for the ammonia weight fractions $w_{NH_3,j}$ can be formulated as seen in Eq. (7), in which $\alpha = 0.33$ represents the bed void fraction, $\rho_g = 50$ kg/m^3 the density of the gas,

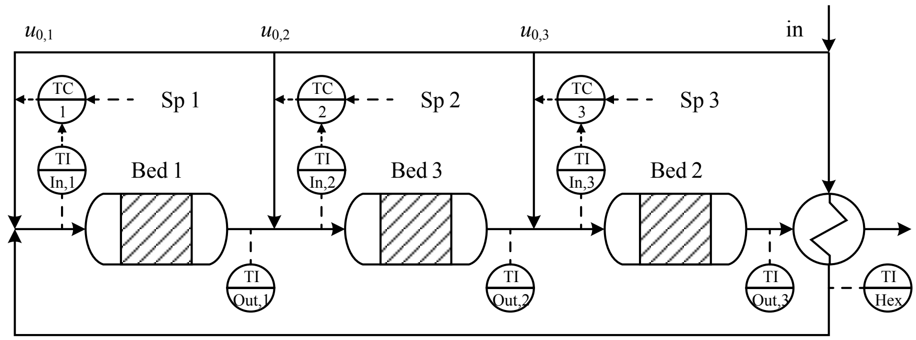

Figure 2: Heat-integrated 3 bed ammonia synthesis reactor with cascade control. The setpoint of the slave temperature loop is given by the proposed method.

and $V_j = V_{bed}/n$ the volume of each CSTR reactor j (Morud, 1995).

$$\frac{\mathrm{d}w_{\mathrm{NH}_3,j}}{\mathrm{d}t} = \frac{\dot{m}_{j-1}w_{\mathrm{NH}_3,j-1} - \dot{m}_j w_{\mathrm{NH}_3,j} + m_{cat,j} r_{NH_3,j}}{V_j \rho_g \alpha} \tag{7}$$

To summarize, we can write, $\mathbf{x} \in \mathbb{R}^{6n+3}$, $\mathbf{u} \in \mathbb{R}^3$ in the system, given in Eqs. (1) and (2).

In contrast to Straus and Skogestad (2017), full state knowledge is not assumed in this paper. The measurement set for state estimation is given by the inlet and outlet temperature of each reactor as well as the outlet temperature of the heat exchanger (see Figure 2). In real plants the catalyst activity is changing over time, which is difficult or impossible to measure and leads to a plant-model mismatch. To take into account industrial applicability, we assume, that the catalyst activity is not measured, but included in the model as an uncertain parameter. Hence, the states and the uncertain parameter are combined to the augmented states with $d = [a_{cat}]$, what results in an augmented system. To optimize the operation, we want to maximize the (mass) extent of reaction.

$$\xi = \dot{m}_{in}(w_{\mathrm{NH}_3,3n} - w_{\mathrm{NH}_3,in}) \tag{8}$$

This results in a cost function $J = -\xi$. In this case, a cascade control is used, where the master controllers drive the three gradients to zero by giving new set points to three slave control loops. The EKF and the proposed method were implemented in discrete time. The controller of the proposed method are single-input single-output controllers. The continuous time process model, given in Eq. (1), was modelled using CasADi (Andersson, 2013) and integrated with CVODES, which is part of the SUNDIALS package (Hindmarsh et al., 2005)

4. Results

In the following section, we consider a disturbance in the feed flow and a plant-model mismatch, given by a mismatch in the catalyst activity. In all cases, we have three inner stabilizing temperature loops as indicated by the letter "T" on the plots. In addition, the results are compared to pure self-optimizing control (SOC) and extremum-seeking control (ESC) in the optimization layer. The integrated cost difference (loss) J_{int} is used for comparison of the different methods,

$$J_{int}(t) = \int_0^t \left[\xi_{opt,SS}(t') - \xi(t')\right] \mathrm{d}t' \tag{9}$$

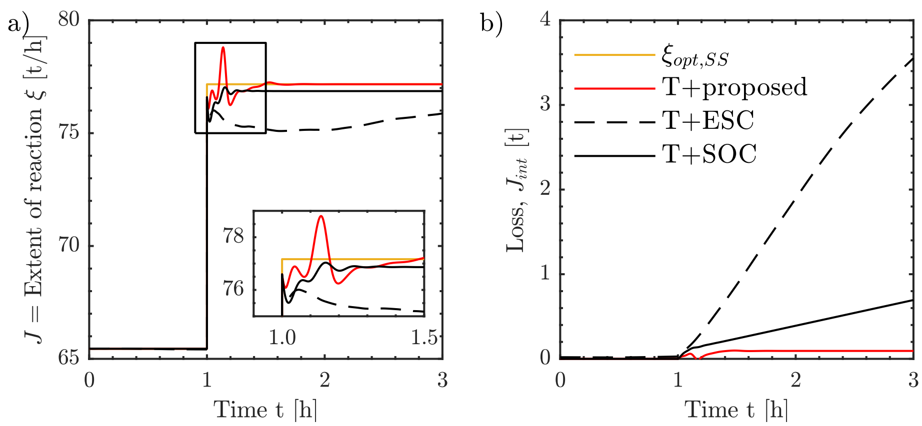

Figure 3: Responses of the alternative methods in a) the extent of reaction and b) the integrated loss to a disturbance in the feed flowrate of $\Delta\dot{m}_{in} = -15$ kg/s at time $t = 1$ h. $\xi_{opt,SS}$ represents the steady-state optimal extent of reaction.

First we simulate a disturbance change in the inlet flowrate $\dot{m}_{in}$ to evaluate the performance of the control structure. The results for a decrease in the feed flowrate of $\Delta\dot{m}_{in} = -15$ kg/s at time $t = 1$ h are presented in Figure 3. The new proposed method gives fast disturbance rejection and settles down at the new optimal operation after about 30 min, as seen Figure 3 a). SOC is equally fast, but it does not quite reach the new optimum. This leads to a continous increase in the integrated loss for SOC as seen in Figure 3 b). If we compare the proposed method to ESC as optimizing control, the proposed method is much faster and therefore causes a lower integrated cost difference of $J_{int}\left(t_{end}\right) = 0.1$ t. This is because the data-based gradient estimation takes longer time for accurate gradient estimation and the controller gain has to be small to satisfy stability. The application of extremum-seeking controllers does not converge to the steady-state optimum in the investigate time frame and requires 13 h.

In the second simulation, we consider plant-model mismatch. The results for a decreased catalyst activity Δa_{cat} by 20 % at time $t = 1$ h, which normally occurs slowly over a longer period of time, are presented in Figure 4. Therefore, the activity of the catalyst, or more specifically the

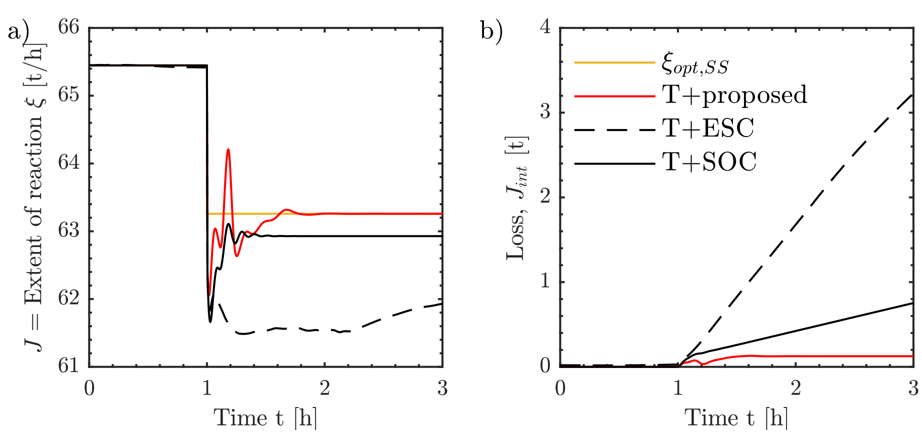

Figure 4: Responses of the alternative methods in a) the extent of reaction and b) the integrated loss to a plant-model mismatch of $\Delta a_{cat} = -20$ % at time $t = 1$ h. $\xi_{opt,SS}$ represents the steady-state optimal extent of reaction.

pre-exponential factor of the Arrhenius equation, spontaneously changes between the model used for the simulations and the model for the state estimation. The simulation shows that the proposed method is performing well even in the presence of a plant-model mismatch. This is because we are able to estimate the real value of the catalyst activity using the augmented EKF framework. About 1.5 minutes after the activity change, the mismatch as well as the states are estimated correctly. The proposed method is much faster than T+ESC, which in turn results in a lower total loss as seen in Figure 4 b). Again, SOC is equally fast, but the real optimum is not reached. The proposed method causes a total integrated cost difference of about $J_{int}(t_{end}) = 0.12$ t of ammonia for the considered case with plant-model mismatch.

5. Conclusion

We have applied a new method of utilizing transient measurements and a dynamic estimator to estimate the steady-state gradient and then using a simple PI controller for driving the process to its optimal operation. For an ammonia synthesis reactor with both disturbances and plant-model mismatch, the proposed method outperforms comparable control strategies. The industrial applicability is conceivable due to the usage of only seven measurements of the process besides the used dynamic model. An extended Kalman filter (EKF) allows the estimation of the steady-state gradients, even in case of plant-model mismatch by including unmeasured but modelled parameters in the estimator.

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