1DOF GAIN SCHEDULED PH CONTROL OF CSTR

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ABSTRACT

Motivated by the rich dynamics of chemical processes, we present a gain scheduled control strategy for a pH neutralization occurring inside continuously stirred tank reactor built on a linearization of a nonlinear state equation about selected operating points. Firstly, we address the problem of a selection of scheduling variable. Based on this, an extra scheduling mechanism is presented to simulate the behavior of a nonlinear process using a linear model. Specifically, the proposed step aims at extending the region of validity of linearization by introducing a parametrized linear model, which enables to construct linear controller at each point. Finally, the parameters of resulting family of linear controllers are scheduled as functions of the reference variable, resulting in a single scheduling controller.

INTRODUCTION

Today's world is full of complex systems that try to facilitate our live. More or less complex nonlinear control algorithms play an integral role in advanced flight systems, adaptive strategies has been successfully implemented in robotic manipulators. One can even say that we are heading towards a new industrial revolution of intelligent systems interacting with each other. It is evident that the more complex system is the more challenging control task it brings. From this perspective, the crucial point of the design is to find a balanced way between effectivity and complexity.

When moving from linear to nonlinear spheres superposition principle known from linear systems does not hold any longer and we are offered richer scenarios that are unfortunately difficult to control. However since linear system theory is so much more traceable we can view its mathematics as an effective tool to simplify our design problem. There is no question that whenever possible, we should utilize this useful trick. Basically, there is only one limitation we must bear in mind. The fact that such a controller can only operate in the neighborhood of a single operating point, predicting the local behavior of the nonlinear system. Interestingly enough, in many cases, it is possible to capture how the dynamics of a system change in its equilibrium. Repeating this idea in multiple operating points we are given a whole family of linearized systems that act as parameterized linear model (PLM). Moreover, it may be even possible to find one or more variables that parameterize this equilibrium points. In such cases, it is intuitively reasonable to linearize the nonlinear model about selected operating points, capturing key states of a system, design a linear controller at each point, and interpolate the resulting family of linear controllers by monitoring scheduling variables.

Early scheduling theories revealed a crucial point associated with selection of scheduling variables. Although there has been a great deal of research discussion about scheduling guidelines it did not bring any general clue. We refer the interest reader to (Rugh 1991; Shamma and Athans 1991; Shamma and Athans 1992; Lawrence and Rugh 1995) for deeper and more insightful into problematics. Moreover, most efforts have been concentrated on nonlinear equations of motion of airplanes or missiles (Khalil 2002), except few applications in car engines (Jiang 1994; Kaminer et al. 1995).

However, nonlinear phenomena are more than typical for chemical processes that may even occur in living cells. We have heard of studies, claiming that metabolism of cancer cells is significantly affected by pH value (Kroemer and Pouyssegur 2008).
From this view point, it is very important to maintain its value inside the boundaries.
In order to reflex richness of pH processes, we have stressed to illustrate gain scheduling strategy for pH neutralization running inside continuously stirred tank reactor (CSTR). Throughout the paper we gradually reveal the scheduling procedure satisfying a tracking problem as well as the design of a control trajectory for the CSTR. We will see that it allows us to smoothly move from one design to another, even though the process exhibits significant nonlinearities.

MODEL OF THE CSTR

A simplified model of the CSTR (Corriou 2004) shown in Figure 1 illustrates neutralization of waste water. As can be seen, process consists of two inlet streams that are perfectly mixed inside reactor.

The first stream represents waste water that enters the reactor with the constant feedrate of q_w at pH_w. Pump with a flow rate q_a that discharges acid serve as actuator to neutralize waste water.

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Both parameters of the CSTR and initial conditions of the neutralization process are captured in Table 1.

Table 1: Model parameters

Waste water inlet stream	q_w= 2000 l/h
Waste water OH^- concentration	$C_w^{OH^-}$ = 10^{-13} mol/l
Waste water H^+ concentration	$C_w^{H^+}$ = 10^{-1} mol/l
Acid pump OH^- concentration	$C_a^{OH^-}$ = $1.29\cdot10^{-15}$ mol/l
Acid pump H^+ concentration	$C_a^{H^+}$ = 7.7371 mol/l
Initial pH	pH(t = 0) = 13
Reactor volume	V = 4000 l

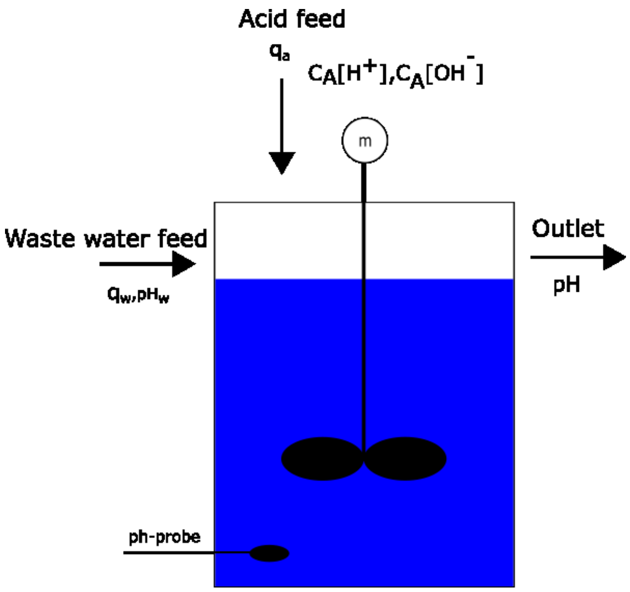

Figure 1: Continuously stirred tank reactor

The only step needed to develop the model of CSTR is to write conservation equation (Richardson 1989), representing material balance for a single material. Recall that the general form of a mass balance is given.

INPUT = OUTPUT + ACCUMULATION

It is easy to see that the simplified dynamic behavior of the CSTR can be modeled by

$$V\frac{d}{dt}C^{OH^-} = q_w C_w^{OH^-} - (q_w + q_a)C^{OH^-} + q_a C_a^{OH^-} \quad (1)$$

$$V\frac{d}{dt}C^{H^+} = q_w C_w^{H^+} - (q_w + q_a)C^{H^+} + q_a C_a^{H^+} \quad (2)$$

where V represents reactor volume, C stands for the concentration of H^+ and OH^- ions q_w and q_a are waste and acid feedrates, respectively.

The main problem of neutralization is that autoprotolysis of water occurs.

$$H^+ + OH^- \Leftrightarrow H_2 0 \quad (3)$$

Assuming the constant temperature, this reaction has the approximate equilibrium constant

$$C^{H^+} \cdot C^{OH^-} = 10^{-14} \quad (4)$$

In order to simplify our task, let us suppose that this reaction does not take place and concentration of both ions remain in the solution. Indeed, since our control task is to track pH value we will find the equilibrium of the autoprotolysis.

To put it in another way, we known that reaction (4) consumes or produces a certain amount of ΔH, until it reaches steady state.

$$(C^{H^+} + \Delta H)\cdot(C^{OH^-} + \Delta H) = 10^{-14} \quad (5)$$

Substitution of $\tilde{C}^{H^+}$ for $(C^{H^+} + \Delta H)$ in (5) yields

$$(\tilde{C}^{H^+})\cdot(C^{OH^-} + \tilde{C}^{H^+} - C^{H^+}) = 10^{-14}, \quad (6)$$

which can be easily rewritten into the standard form as

$$0 = \underbrace{-1}_{a}(\tilde{C}^{H^+})^2 + \underbrace{(C^{H^+} - C^{OH^-})}_{b}\cdot\tilde{C}^{H^+} + \underbrace{10^{-14}}_{c} \quad (7)$$

It can be easily seen that the above equation must be solved for unknown $\tilde{C}^{H^+}$. Fortunatelly, (7) is quadratic equation, producing straight forward solution.

Having calculated (7), the pH value is given by

$$pH = -\log(\tilde{C}^{H^+}) \quad (8)$$

We can now see, that the equilibrium concentration $\tilde{C}^{H^+}$ depends only on the term b.

This leads us to the simple modification. By substracting (1) from (2) we obtain neutralization model

$$V\frac{d}{dt}b = q_w b_w - (q_w + q_a)b + q_a b_a \quad (9)$$

where b represents correponding difference between hydrogen and hydroxyl ions.

MODEL STRUCTURE FOR GS DESIGN

In the process of designing and implementing a gain scheduled controller for a nonlinear system, we have to find its approximations about the family of operating (equilibrium) points. Thus, the nonlinear first-order ordinary differential equation (9) capturing the dynamics of the neutralization process has to be transformed into its linearized form.

In view of our example, we shall deal with single-input single-output linearizable nonlinear system represented by

$$\dot{x} = f(x,u) \quad (10)$$

$$y = g(x) \quad (11)$$

where $\dot{x}$ denotes derivative of x with respect to time variable and u are specified input variables. We call the variable x the state variable and y the output variable. We shall refer to (10) and (11) together as the state-space model.

To obtain a state-space model of the CSTR, let us take $x = b$ as a state variable and $u = q_a$ as a control input. Then the state equation is

$$\frac{dx(t)}{dt} = \frac{1}{V}\left[q_w b_w - q_w x(t) - x(t)u(t) + b_a u(t)\right] \quad (12)$$

Because the output of the process is pH value, the output equation takes the form

$$y = -\log\left\{\frac{1}{2}\left[x(t) + \sqrt{x(t)^2 - 4\cdot 10^{-14}}\right]\right\} \quad (13)$$

One can easily sketch the trajectory of steady-state characteristic by setting $\dot{x} = 0$ and solving for unknown x.

Therefore the equilibrium points correspond to the solution of

$$0 = \frac{1}{V}\left[q_w b_w - q_w x(t) - x(t)u(t) + b_a u(t)\right] \quad (14)$$

Having calculated equilibrium points of state equation, our goal now is to approximate (12) about selected single operating point. Suppose $\bar{x} \neq 0$ and $\bar{u} \neq 0$, and consider the change of variables

$$x_\delta(t) = x(t) - \bar{x} \quad (15)$$

$$u_\delta(t) = u(t) - \bar{u} \quad (16)$$

$$y_\delta(t) = y(t) - \bar{y} \quad (17)$$

It should be noted that in the new variables system has equilibrium in origin.
Expanding the right hand side of (12) about point $(\bar{x},\bar{u})$, we obtain

$$f(x,u) \approx f(\bar{x},\bar{u}) + \frac{\partial f(\bar{x},\bar{u})}{\partial x} + \frac{\partial f(\bar{x},\bar{u})}{\partial u} + \text{H.O.T.} \quad (18)$$

If we restrict our attention to a sufficiently small neighborhood of the equilibrium point such that the Higher-Order Terms are negligible, then we may drop these terms and approximate the nonlinear state equation by the linear state equation.

$$\dot{x}_\delta = Ax_\delta + Bu_\delta \quad (19)$$

where

$$A = \left.\frac{\partial f}{\partial x}\right|_{x=\bar{x},u=\bar{u}} \qquad B = \left.\frac{\partial f}{\partial u}\right|_{x=\bar{x},u=\bar{u}} \quad (20)$$

PARAMETRIZATION OF LINEAR MODELS

Before we present a parametrization via scheduling variable, let us first examine configuration of the gain scheduled control system captured in Figure 2. From the figure, it can be easily seen that controller parameters are automatically changed in open loop fashion by monitoring operating conditions. From this point of view, presented gain scheduled control system can be understand as a feedback control system in which the feedback gains are adjusted using feedforward gain scheduler.

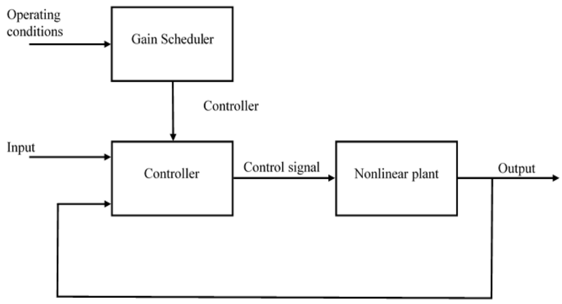

Figure 2: Gain scheduled control

Then it comes as no surprise that first and the most important step in designing a controller is to find an appropriate scheduling strategy. Once the strategy is found, it can be directly embedded into the controller design.

In order to understand the idea behind the gain scheduling let us first consider the nonlinear system

$$\dot{x} = f(x,u,\alpha) \quad (21)$$

$$y = g(x,\alpha) \quad (22)$$

We can see that the nonlinear system is basically same as the system that we have introduced in the previous section by equations (10) and (11). The only difference here is that both state and output equations are parameterized by a new *scheduling variable α* representing the operating conditions.

To illustrate this motivating discussion let us consider this crucial point in the context of our example.

Suppose the system is operating at steady state and we want to design controller such that *y* tracks a reference signal *w*. In order to maintain the output of the plant at the value $\bar{y}$, we have to generate the corresponding input signal to the system at $\bar{u} = q_w \frac{\bar{x} - b_w}{b_a - \bar{x}}$. This implies that for every value of *w* in the operating range, we can define the desired operating point by

$$\bar{y} = w \quad (23)$$

$$\bar{u} = q_w \frac{\bar{x}(w) - b_w}{b_a - \bar{x}(w)} \quad (24)$$

In other words, this leads us to the simply conclusion that we can directly schedule on a reference pH trajectory.

Having identified a scheduling variable, the common scheduling scenario takes this form

$$\dot{x}_\delta = A(\alpha)x_\delta + B(\alpha)u_\delta \quad (25)$$

Intuitively speaking, the parameters of (19) are scheduled as functions of the scheduling variable α. Since our model is simple nonlinear SISO system, we need to calculate constants of A, B. In other words, the key how to move from one operating point to another is given by

$$
\begin{aligned}
A(\alpha) &= \left.\frac{\partial f}{\partial x}\right|_{x=\bar{x},u=\bar{u}} = -\frac{q_w + u(\alpha)}{V} \\
B(\alpha) &= \left.\frac{\partial f}{\partial u}\right|_{x=\bar{x},u=\bar{u}} = -\frac{b_a - x(\alpha)}{V}
\end{aligned}
\tag{26}
$$

An important feature of our analysis is that even if α represents reference vector, the equations (24) still capture the behavior of the system around equilibria. We can also observe that both x and u are functions of α. This is no problem since we have defined our scheduling variable as a desired pH value. Interested reader has certainly noticed that we can easily calculate them from (23) and (24).

GAIN SCHEDULED CONTROLLER DESIGN

Since the basis for the construction of family of parametrized linear models has been previously explored, we would like to look more closely at the derivation of the linear controller at each operating point that is a prescription for designing u such that y asymptotically tracks w with all generated signals remaining bounded. In order to achieve this control objective, we analyze one degree of freedom configuration. The configuration arrangement is shown in Figure 3 and includes one degree of freedom that is represented by feedback controller G_Q.
In this configuration, w represents the reference signal, v is the load disturbance, y is the controlled output and u is the control input

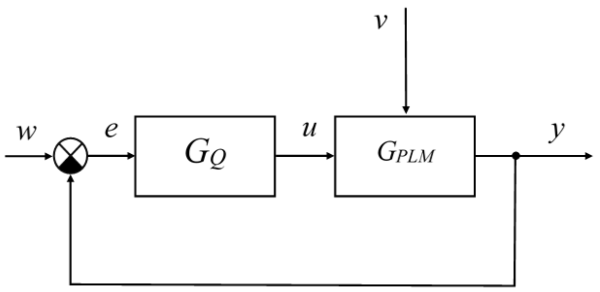

Figure 3: 1DOF control system configuration

Consider now the single-input single output linearized system described by equation (19) or, equivalently, by the transfer function model

$$Y(s) = G_{PLM}(s)U(s) = \frac{b(s)}{a(s)}U(s) \tag{27}$$

where $U(s)$ and $Y(s)$ are Laplace transforms of the control input $u(t)$ and measured output $y(t)$**,** respectively.

From the equation (19) it can be seen that the polynomials a and b are monic having following structure

$$a(s) = s + a_0 \tag{28}$$

$$b(s) = b_0 \tag{29}$$

To aid insight into controller

$$G_Q(s) = \frac{q(s)}{p(s)}, \tag{30}$$

where q and p represents polynomials in s, we will work with both reference signal and disturbance signal as follows

$$W(s) = \frac{w_0}{s}, \; V(s) = \frac{v_0}{s} \tag{31}$$

As is well known we have to use integral control such that polynomial p takes the form

$$p(s) = s\tilde{p}(s) \tag{32}$$

To proceed with the design of the controllers, we leave it as an exercise for the reader to verify that both closed-loop linear systems has the characteristic equation. The reader may consult (Kučera 1993).

$$a(s)\,p(s) + b(s)\,q(s) = d(s) \tag{33}$$

One can intuitively expect that the control system is stable if we design d to be Hurwitz polynomial.

Toward the goal suppose we have succeeded in finding polynomials of the transfer functions

$$G_Q(s) = \frac{q(s)}{s\tilde{p}(s)} = \frac{q_1 s + q_0}{s p_0} \tag{34}$$

that satisfy (33) for the stable polynomial

$$d(s) = (s + \beta_1)(s + \beta_2) \tag{35}$$

Recalling the basis of linear algebra, we can obtain the controller parameters from the solution of the matrix equation

$$\begin{bmatrix} 1 & 0 & 0 \\ a_0 & b_0 & 0 \\ 0 & 0 & b_0 \end{bmatrix} \begin{bmatrix} p_0 \\ q_1 \\ q_0 \end{bmatrix} = \begin{bmatrix} d_2 \\ d_1 \\ d_0 \end{bmatrix} \tag{36}$$

where the coefficients of polynomial d are given by

$$d_2 = 1, d_2 = \beta_1 + \beta_2, d_0 = \beta_1\beta_2 \tag{37}$$

It is important to emphasize that selectable poles β_1 and β_2 are the only parameters through which the controller parameters can be adjusted.

The resulting gain scheduled controller can be obtained by scheduling coefficients of $q(s)$ as functions of α; that is, α is replaced by w, so that the gains vary directly with the desired pH value.

From this, the linear control law, which is prescribed by controller (34) can be rewritten in terms of scheduling variables as

$$u = q_1(\alpha)e + q_0(\alpha)\sigma \tag{38}$$

where

$$e = \sigma$$

So far, we have formed the basic idea of construction of gain scheduled control law. All that remains now is to show, that for a desired Hurwitz polynomial d, the gains are taken as

$$q_1(\alpha) = \frac{\beta_1 + \beta_2 - a_0(\alpha)}{b_0(\alpha)}$$
$$q_0(\alpha) = \frac{\beta_1 \beta_2}{b_0(\alpha)} \qquad (39)$$

When the control (38) is applied to the nonlinear state equation (12) it results in the closed-loop system

$$\dot{x} = \frac{1}{V}\left[q_w b_w - q_w x + q_1(b_a - x)q_1\left(e + \frac{q_0}{q_1}\sigma\right)\right] \qquad (40)$$

In view of the procedure that we have just described, one can notice that three main issues are involved in the development of gain scheduled controller; namely linearization of neutralization process about the family of operating regions, design of a parametrized family of linear controllers for the parametrized family of linear systems and construction of gain scheduled controller.

SIMULATIONS AND RESULTS

In this section, we simulate the gain scheduled control of CSTR. We have developed a custom MATLAB function based on the simulator introduced by (Krhovják et al. 2015) that simulates adequately the behavior of CSTR. Idealistic model has been implemented according to equation (8) and (9). The popular ODE solver using based on Runge-Kutta methods (Hairer et al. 1993) was considered to calculate numerical solution.

The simulation results of gain scheduled control are presented in Figures 4-6. Figure 4 clearly illustrates how the linearized plant dynamics vary with the operating conditions that are given by scheduling variable α.

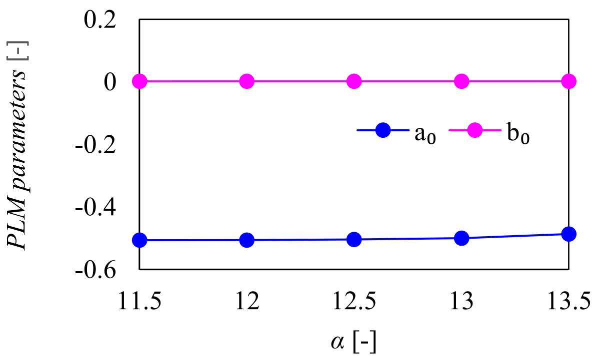

Figure 4 Parameter evolution

Figure 5 shows the responses of the control system to the sequence of step changes in reference signal. As can be seen from Figure 6, we have found such a combination of parameters β_1 and β_2 that results in reasonably good responses.

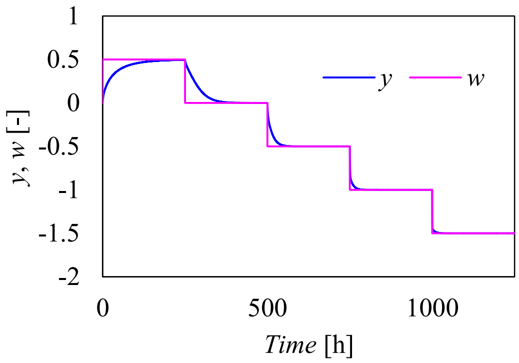

Figure 5: The responses of the closed-loop system to a sequence of step changes

From a gain-scheduling viewpoint, a step change in reference signals causes a new calculation of the equilibrium point of the system. This claim is also supported by Figure 6 in which the gain adjustment is captured. It is important to notice that the change of controller parameters occurs with the step change in reference trajectory.

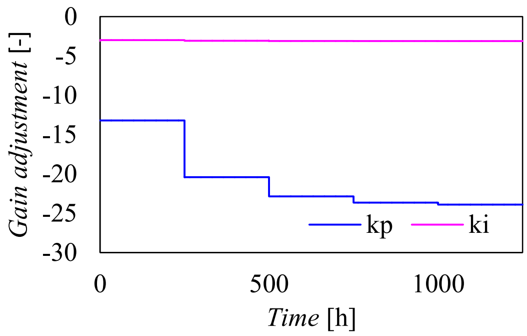

Figure 6: Gain adjustment during control

CONCLUSION

This paper addressed the control problem of neutralization processes. Excited by their dynamics, we presented a promising gain scheduling strategy that overcomes a highly nonlinear behavior. First, we have detailed studied the simplified model of the neutralization process. Based on the model, we have followed a general analytical framework for gain scheduling. The most importantly, we outlined a possible way how to select an appropriate scheduling variable. The main advantage of this approach is that linear design methods can be applied to the linearized system at each operating point. Thanks to this feature, the presented procedure leaves room for many linear control methods We have demonstrated that a gain scheduled control system has the potential to respond rapidly changing operating conditions

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