Referential Process–Reaction Curve for Batch Operations

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An extension of the well-known process–reaction curve method to empirically determine reduced-complexity models aimed to the design and tuning of feedback controllers for nonstationary batch processes is reported. The basic idea is to isolate the dynamics associated with the manipulated variable from the main time-variable behavior that characterizes the operation, by taking the time evolution of a previous run as reference. One or more input-perturbed evolutions can then be compared to the previous dynamic pattern yielding referential reaction curves. This modeling approach cancels out most of the nonstationary behavior, allows capturing the dominant manipulated-variable dynamics, and the use of available tuning rules for integrating systems. The effectiveness of this procedure is illustrated by using a nonlinear model of a bioreactor that simulates the production of xanthan gum. © 2004 American Institute of Chemical Engineers *AIChE J,* 50: 3160–3168, 2004

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Introduction

Process control specialists have dedicated more time to the analysis, design, and tuning of controllers for processes operating under stationary mode than for nonstationary processes such as batch processes. Traditional methods for adjusting classic controllers, such as proportional integral (PI) and proportional integrative derivative (PID), assume they will be dedicated to disturbance rejection from a stationary state, or to set-point changes if the process must go from one stationary state to another. This is the type of control task mostly expected when Ziegler and Nichols (1949), Cohen and Coon (1953), or more recently, when Rivera et al. (1986) or Chien and Fruehauf (1990) tuning rules are adopted. Traditional texts for teaching process control, such as those by Stephanopoulos (1984) and Seborg et al. (1989), emphasize the dynamics of stationary processes. The references to modeling and control of batch processes or transient operations are sporadic or quite scarce. In this regard, it is frequent to find references to programmable logic controllers (PLC), or to the proportional control as the principal resource during startup or shutdown "until the operation is close to the desired condition." Thus, there is a need for determining practical tuning guidelines for industrial PI or PID controllers, not only for immediate commissioning but also to provide a reference performance when more sophisticated control systems are analyzed.

If a tuning technique is to be applied to any process encountered in practice, a method is required for obtaining numerical parameters that sufficiently describe the particular process to which the tuning technique is to be applied. Perhaps one of the easiest tests to perform on a typical stationary process is to determine the process–reaction curve, that is, the open-loop response of the process to a step change in the controller output. This test continues to be very popular not only because many engineers are very familiar with it, but also because the method is particularly appealing when the dynamics of the main process including measuring sensor and final control element are poorly known. Of the methods available for setting controllers, those based on the process–reaction curve have a tremendous advantage over others because of the simplicity

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and the ease with which the necessary experimental data can be obtained.

This work proposes to extend the use of the process–reaction curve and the application of some tuning rules, originally developed for "dynamics valid in the neighborhood of stationary operating points," to operations "in the neighborhood of a reference transient evolution" like those occurring in chemical batch reactors. This extension is done by referencing the output response curve to the nonlinear evolution the system follows during a standard or nominal run. The proposal tries to keep the simplicity expected by practitioners from modeling methods dedicated to designing and tuning plant controllers. In this article the application case is the temperature control of a batch bioreactor for the production of xanthan gum, but it is conceivable that the procedure is applicable to numerous batch processes. The example is appropriated because it is desired not only to keep regulatory control, but also a reactor temperature profile has to be maintained to reach the maximum product concentration at the end of the operation.

In the next section, the fundaments of the proposed methodology are presented through the analysis of a general nonlinear representation of the dynamic system. After that, this article describes the application example and the tracking control objective. It explains the adaptation of the auxiliary cooling/heating system, and the control setup required to achieve the desired tracking. The open-loop input trajectories used to model the dynamics associated with the manipulated variable are discussed, as well as available tuning rules for adjusting feedback controllers based on integrator-plus-time-delay process models. The remainder of this article is devoted to show the results obtained by simulating the closed-loop system during the set-point tracking routine. The nonlinear model used to simulate the bioreactor is presented in Appendix A, and a complementary linear analysis is presented in Appendix B that partially justifies the results obtained in this application. The final section presents the conclusions of this work.

Referential Process–Reaction Curve

The outstanding feature of batch or semibatch processes is that the operation starts at a given time instant, follows a sort of recipe, and stops when a given condition is reached. The operating condition changes during all this time, frequently following nonlinear characteristics that are hard to model. This type of behavior is very common during the operation of batch reactors or bioreactors in many pharmaceutical, biotechnological, chemical, or food industries.

Process engineers have frequently derived fundamental models for these batch processes, mostly for process design or simulation purposes. Because they never reach a stationary state and a continuous dynamic evolution is instead observed, it is not possible to apply the typical open-loop test to obtain the reaction curve that shows the effect of the manipulated variable on the process output. Consequently, the simple linear modeling approach for control design and tuning, available for stationary processes, has not been a common resource in these cases.

It is intuitively acceptable that, in general terms, the dynamic characteristics mentioned before can be represented by

$$\dot{x}(t) = f\{x(t), t\} + g\{x(t)\}u(t) \qquad x(0) = x_0$$
$$y(t) = h\{x(t)\} \tag{1}$$

In a single-input, single-output (SISO) system, $y(t)$ is a single-output variable, $u(t)$ is the control variable, and the dimension of the state vector $x(t)$ allows us to think in terms of a generic order n. Note that the way in which Eq. 1 represents the relationship with $u(t)$ is quite consistent with most real chemical processes where actual manipulated variables are flow-rate variables appearing as factors in convective nonlinear terms.

Let us assume that, as part of the batch recipe, a specific $u(t) = u_r(t)$ input trajectory is available all along the operative time interval $[0, t_f]$, that is, a sequence of manipulated-variable changes are scheduled to approximately follow a desired convenient trajectory during the operation. This sort of open-loop tracking is frequently implemented using time-programmable controllers to approach an acceptable time evolution that can be described by

$$\dot{x}_r(t) = f\{x_r(t), t\} + g\{x_r(t)\}u_r(t) \qquad x_r(0) = x_0$$
$$y_r(t) = h\{x_r(t)\} \tag{2}$$

Notice that the control input in Eq. 1 can be adopted such that $u(t) = u_r(t) + \Delta u(t)$, where $\Delta u(t)$ is a known step change introduced at a given time $t \in [0, t_f]$. Then, the dynamic effect of $u(t)$ can be isolated from the general system dynamics by observing the relative time evolution of the concerning variables. In other words, from the manipulated-variable viewpoint, the system response is determined by

$$\frac{d\Delta x(t)}{dt} = \Delta f\{x(t), x_r(t), t\} + \Delta g\{x(t), x_r(t)\}u_r(t) + g\{x(t)\}\Delta u(t)$$
$$\Delta y(t) = h\{x(t)\} - h\{x_r(t)\} \tag{3}$$

where $\Delta x(t) = x(t) - x_r(t)$, $\Delta f(x, x_r, t) = f(x, t) - f(x_r, t)$ and $\Delta g(x, x_r) = g(x) - g(x_r)$. Observe that $x_r(t)$ and $u_r(t)$ in Eq. 3 are predetermined time functions, that is, they are not time variables capable of reacting to process changes or disturbances occurring during the testing run.

When working with batch processes, it is frequent that every state variable represents a real physical variable such as temperature or concentration; this means that in many regular SISO control problems $h\{x(t)\}$ is a very simple function providing some simplicity to Eq. 3. There are also no doubts that Eq. 3 can be rewritten in other convenient ways if a theoretical type of development is intended. However, the interest here is to show an application-oriented type of result by simple inspection of the response $\Delta y(t)$ rather than a strict theoretical approach.

In a batch reactor, for instance, most of the variables of interest evolve as the result of an internal force–function term included in $f(x, t)$. This internal force basically comes up from a source of free energy that remains with variable intensity during the whole operation and repeats itself from one run to the next, with only minor changes resulting from many

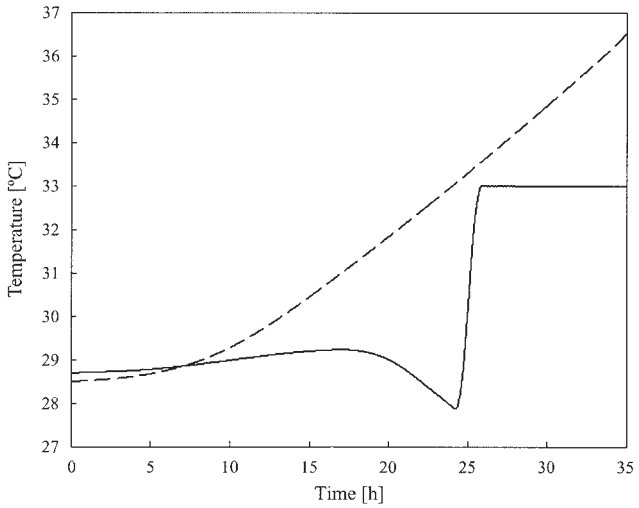

Figure 1. The solid line shows the desired temperature evolution; the dashed line is the temperature evolution for null water flow rate in the jacket.

scarcely controllable causes; this is basically what happens when the reactor temperature rises as a result of the released heat of reaction. Thus, it is expected here that, even if this force function is the most important term in $f(x, t)$, the difference $\Delta f(x, x_r, t)$ cancels out most of it. In addition, a significant cancellation of nonlinearities occurs in $\Delta g(x, x_r)$, leaving only residual dynamics associated with the change $\Delta u(t)$.

The claim in presenting this approach is that the above referential evolution for batch systems gives the same type of information as that of the process–reaction curve for stationary processes and leads to reduced-complexity models for designing and tuning feedback controllers. Besides, because of the non-self-regulating nature of most batch systems, it should not be a surprise to find out that the dominant dynamic corresponds to an integrating behavior.

Application Example

In the majority of the model-based control schemes used in the chemical process industry, reduced-complexity models are generated to capture the most dominant dynamic of the process. Because a plant is generally of relatively high order, identification for controller design and tuning purposes also means a model reduction exercise. The temperature control of a batch bioreactor does not avoid this characteristic.

In the following, the referential output response of a nonlinear simulator of a batch bioreactor for xanthan gum production is determined as described in the previous section. The kinetics expressions describing the dynamic evolutions of biomass (X), product (P), and substrate (S) are presented in Appendix A, as well as the two main energy balances: one for the matter in the reactor and the other for the cooling/heating service utility in the jacket. Previous investigations have determined that the optimal operation of this bioreactor follows a particular temperature profile to achieve the maximum amount of product in a convenient time interval (Dondo, 2000).

Temperature control setup

Thus, the main objective for the control system is to track the temperature profile, shown as a solid line in Figure 1, because this allows reaching maximum product concentration after operating about 35 h. Figure 1 also shows the natural temperature evolution when no cooling service is used all along the 35-h run. When comparing these profiles, a conclusion is that not only cooling is necessary but also—because the reactor temperature rises slowly—a heating stage should be allowed. Thus, the reactor jacket is connected such that it receives water at 15 or 80°C. The input of one or the other service is handled by a two-way valve, whereas the flow rate is regulated by a control valve like that shown in Figure 2. To fit in this constrained setup, two PI controllers with anti-windup devices are used; they work alternately depending on which type of control action is necessary: cooling or heating. The controller selection is made by comparing the error (difference between the set point and the reactor temperature) with a threshold (0.1 in this case) that avoids switching controllers continuously. When the error changes sign, its absolute value must be larger than the threshold to change the control loop.

The described setup, which belongs to the category of flexible-structure control systems, confers the physical possibility of achieving the desired tracking. However, it must be emphasized here that this is a secondary issue in this report; the main concern is the appropriate tuning of the feedback controllers to track the desired temperature profile.

Referential process modeling

As described before, the method basically consists on using a standard or nominal time evolution as reference dynamic to determine by contrast the effect of changing the manipulated variable (the water flow rate in this example) on the controlled one (the reactor temperature). For instance, the open-loop temperature profile for $w_a = 0$ shown in Figure 1 can be taken as a reference trajectory, and the perturbed response can be the divergent response resulting from a single-step input change at any selected time instant.

However, let us assume that a sequence of manipulated-variable movements like the one shown in Figure 3a is typically executed when running the process with the purpose of maintaining the reactor temperature (in Figure 3b) close to the

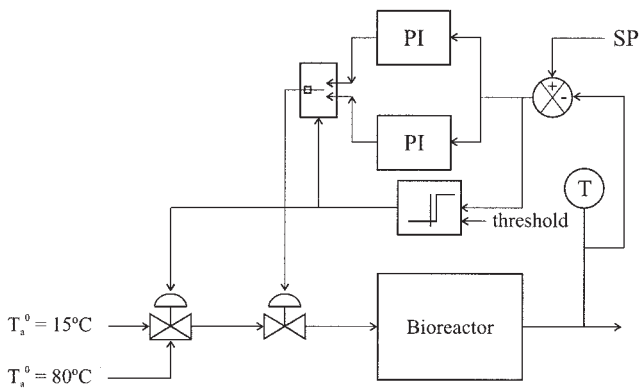

Figure 2. Switching PI control system adopted for the bioreactor temperature-tracking problem.

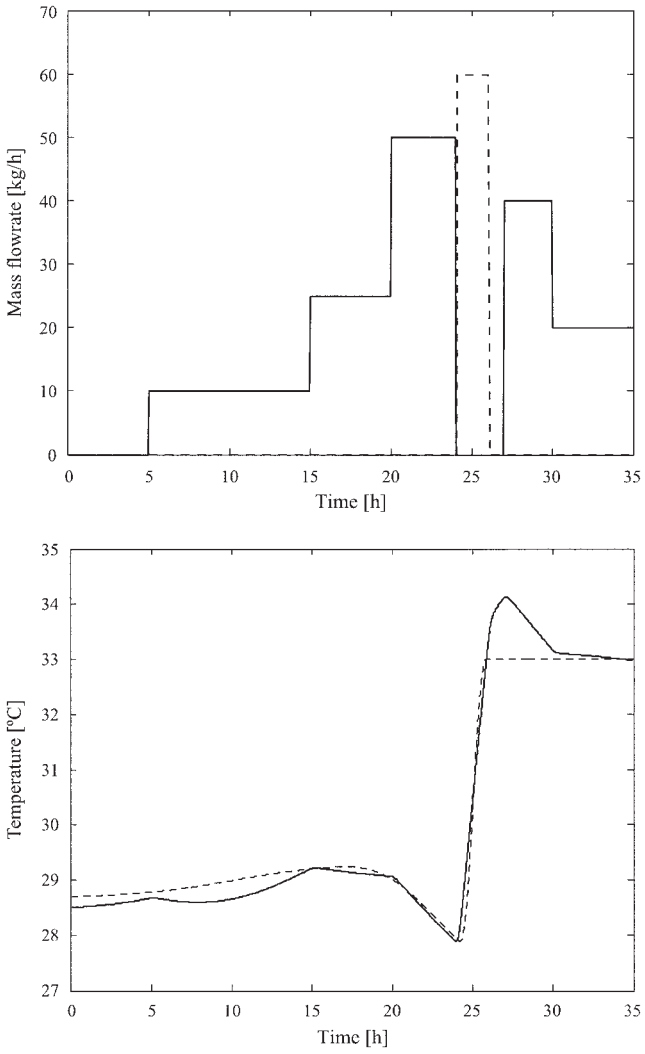

Figure 3. (a) Nominal input profile: the solid line shows the programmed sequence of cooling-water flow rates; the dashed line shows the use of hot water; (b) solid line: temperature profile obtained with the open-loop program shown in (a); the desired profile is shown in dashed line.

most favorable set-point profile. Then, let us take this input–output time evolution as the reference trajectory, that is, as $u_r(t)$ and $T_r(t)$ in Eq. 2, respectively.

The use of the proposed open-loop response in Figure 3b is supported by the following reasons: (1) the closer the output-reference trajectory is to the desired one, the smaller the model mismatch should be, and (2) both the reference and the perturbed trajectories should also be safe and economically acceptable runs. These arguments also lead to definition of time-integral–compensated input trajectories when dealing with integrating systems. Figures 4a and b exemplify the concept, where the arrows indicate the changes made to the input-reference trajectory $u_r(t)$ to obtain the input-perturbed $u(t)$. Note that the perturbed trajectory $u(t)$ is designed such that the difference of accumulated energy is finally compensated.

Figure 5a shows the net input changes $\Delta u(t)$, and Figure 5b shows the referential process–reaction curves or referential temperature evolutions determined by the difference between the perturbed responses $T(t)$ and the reference $T_r(t)$, that is, assuming no other disturbance has occurred. This difference is the output response $\Delta y(t)$ of the referential dynamic system in Eq. 3 to the input changes in Figure 5a. Each referential responses $\Delta y(t)$ allows one to determine the slope and the delay from the reaction to the first step change, as indicated in Figure 6; these yield representative parameters values of the integrator/dead time process model

$$\tilde{G}_p(s) = \frac{K_p e^{-T_d s}}{s} \tag{4}$$

This way, the responses in Figure 5b enable one to determine $K_p = -0.012°\text{C kg}^{-1}$ and $T_d = 0.17$ h for the cold water, and $K_p = 0.042°\text{C kg}^{-1}$ and $T_d = 0.14$ h for the hot water, respectively. Although this is a quite simple result, it is consistent not only with the fact that the process–reaction curve

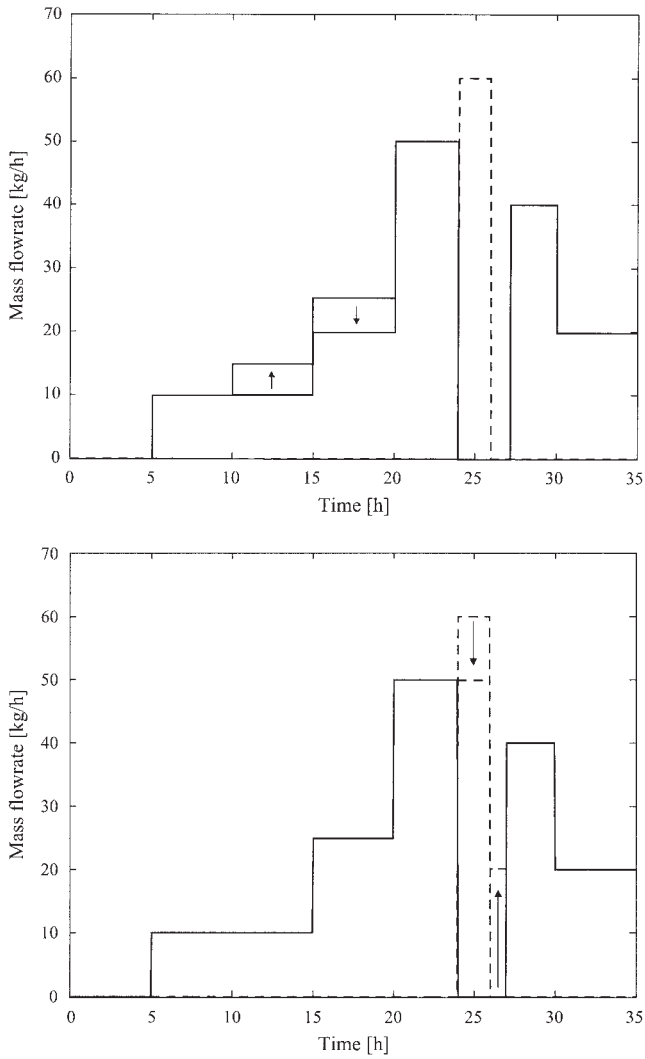

Figure 4. (a) The arrows show two compensating changes made in the cooling-water flow rate; (b) the arrows show two compensating changes made in the heating-water flow rate.

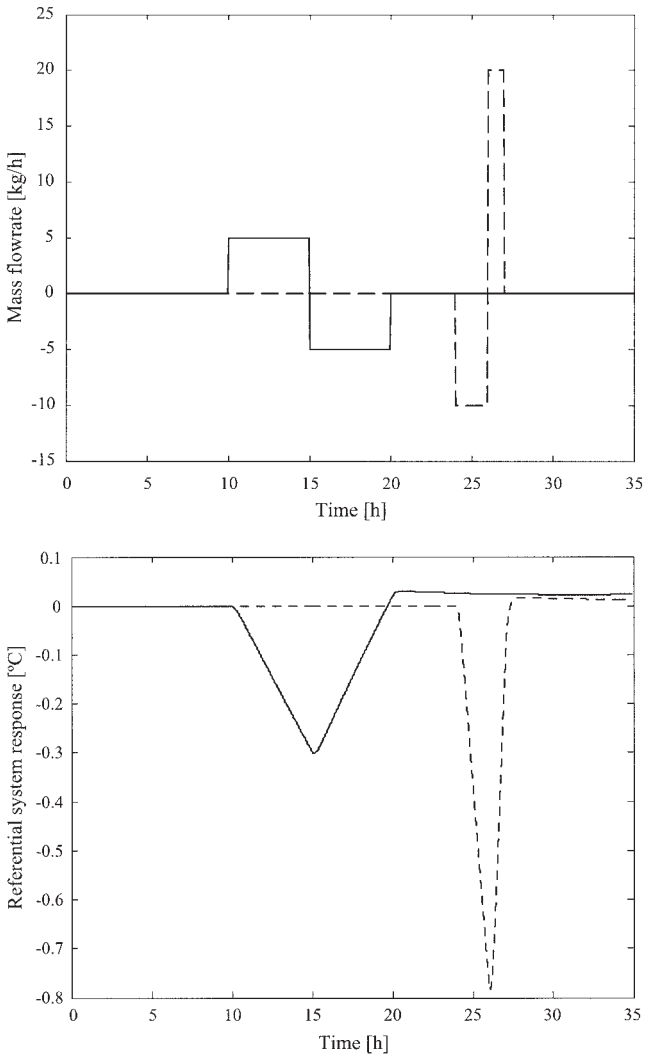

Figure 5. (a) Net input changes in the referential process system; (b) referential process–reaction curves obtained from the referential changes in (a).

method has always been a practical model-reduction technique, but also with the naturally expected dynamic associated with a manipulated flow rate variable in a batch system. Appendix B exposes the main assumptions that, from the fundamental model, are necessary to accept Eq. 4 as an approximate transfer function for tuning purposes.

Controller tuning

Only a few references from the literature can be given that deal with tuning industrial PI or PID controllers for integrating plants. First, it is fair to mention that Seborg et al. (1989) remarks that the process–reaction curve method can be used for both self-regulating and non-self-regulating systems. Thus, once the normalized slope S^* and the time delay θ are determined from the curve, the Ziegler and Nichols (1942) tuning relations can be used for P, PI, and PID controllers. In particular, for PI controllers: $K_c = 0.9/(\theta S^*)$ and $T_I = 3.33\theta$. Note that herein $K_p = S^*$ and $T_d = \theta$.

Alternatively, Chien and Fruehauf (1990) proposed tuning rules for PI and PID controllers using the internal model control (IMC) parameterization for several transfer functions representing process dynamics. In particular, for time-constant dominant processes, the authors suggest to approximate the model with an integrator plus time delay. This way, the controller designed based on this model maintains the controlled variable near the initial response operating region.

Besides, Tyreus and Luyben (1992) used classical frequency response methods to propose a specific tuning rule to adjust the PI controller when the response of the process looks almost like the response of a pure integrator. The method basically yields the best settings achievable for a given degree of closed-loop damping; in particular, for a maximum log modulus of +2 dB the following relations are determined: $K_c = 0.487/(K_p T_d)$ and $T_I = 8.75T_d$.

More recently, Luyben (1996) extended the previous work with PI control to include the tuning of PID controllers; this three-mode alternative provides tighter control but requires the signals to be almost noise free.

In this work, the Ziegler–Nichols settings are used for the feedback controllers of Figure 2. Although there are no changes in the jacket capacity, in the heat-exchange area or the actuator dynamics, the difference between controller settings comes up through the referential process–reaction curves, revealing different dynamic effects of the inlet-water temperature. Thus, the following parameter values for the PI controllers are determined: $K_c = -441.2$ kg h^{-1}°C^{-1} and $T_I = 0.56$ h; and $K_c = 153.0$ kg h^{-1}°C^{-1} and $T_I = 0.46$ h for cooling and heating duties, respectively.

Closed-loop simulation

The control system sketched in Figure 2 is simulated using PI controllers adjusted as indicated above. To accomplish the simulation the bioreactor is represented by the nonlinear model detailed in Appendix A, taken as initial temperature conditions $T(0) = T_a(0) = 28.5$°C, that is, the service fluid in the jacket and the material in the reactor are at thermal equilibrium. All the control steps occurring along the simulated closed-loop

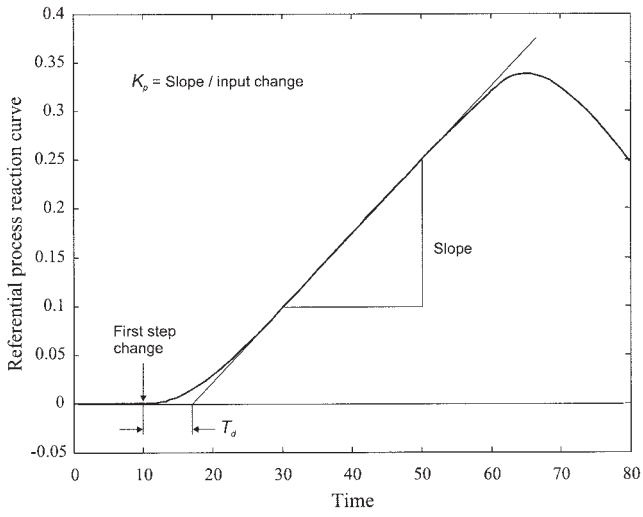

Figure 6. Typical referential process–reaction curve and estimation of parameters.

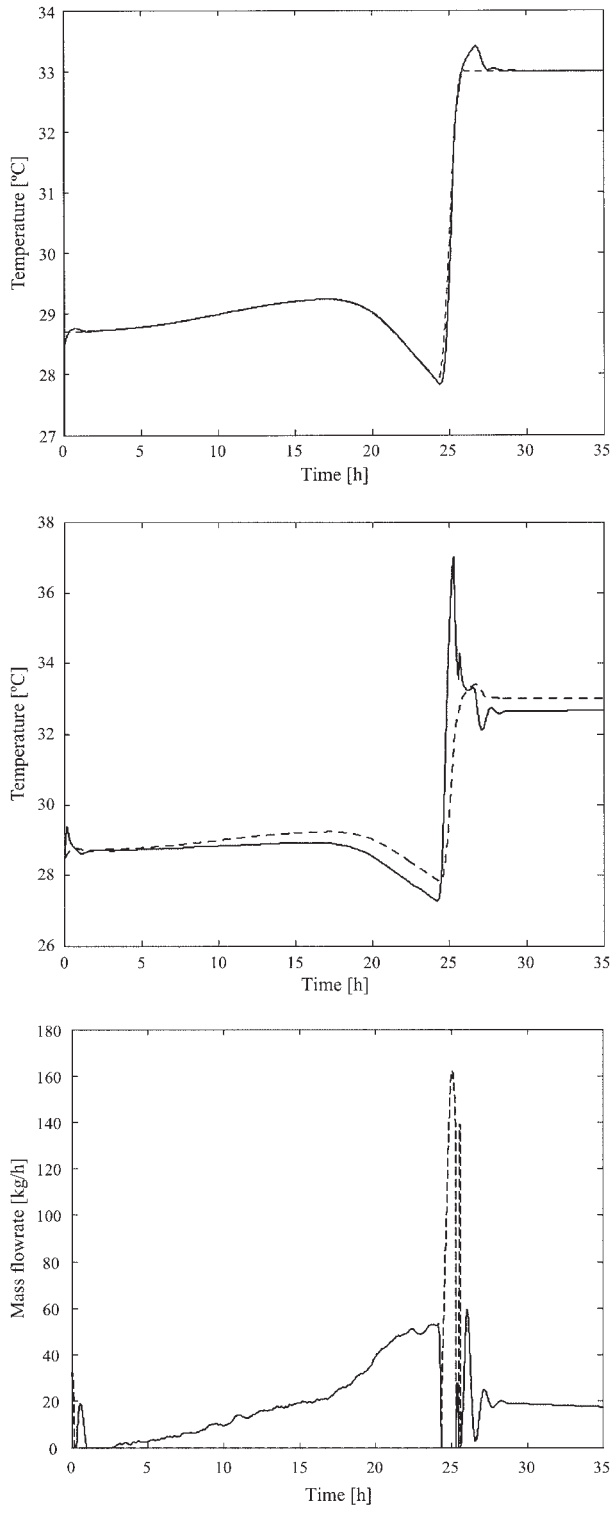

Figure 7. (a) Closed-loop tracking response obtained with the PI controllers adjusted using the referential process models and Ziegler–Nichols settings; (b) the solid line is the water temperature in the jacket; the dashed line is the reactor temperature; (c) control actions corresponding to the evolutions in (a) and (b).

The solid line represents the cold-water flow rate; the dashed line is the hot-water flow rate.

batch evolution can be observed in Figures 7a–c; in particular, Figure 7b shows the effective cooling and heating periods, given that crossing points between jacket and reactor temperature are clearly determined. Because 28.5°C is 0.2°C lower than what is required by the desired profile, the first control action is a short heating for about 15 to 20 min. This is followed by a cooling period that lasts for about 24 h, when an important transition has to occur to obtain maximum gum production. At this point, the change to a reactor temperature close to 33°C requires an important heating action that is interrupted only when the desired temperature is reached. From this point forward, cooling is again necessary to compensate the heat of reaction.

The robustness of this tuning approach in shown in Figure 8a, which compares the closed-loop reactor temperature evolution in Figure 7a with the closed-loop evolution obtained when the inlet hot water is 70°C instead of 80°C from the

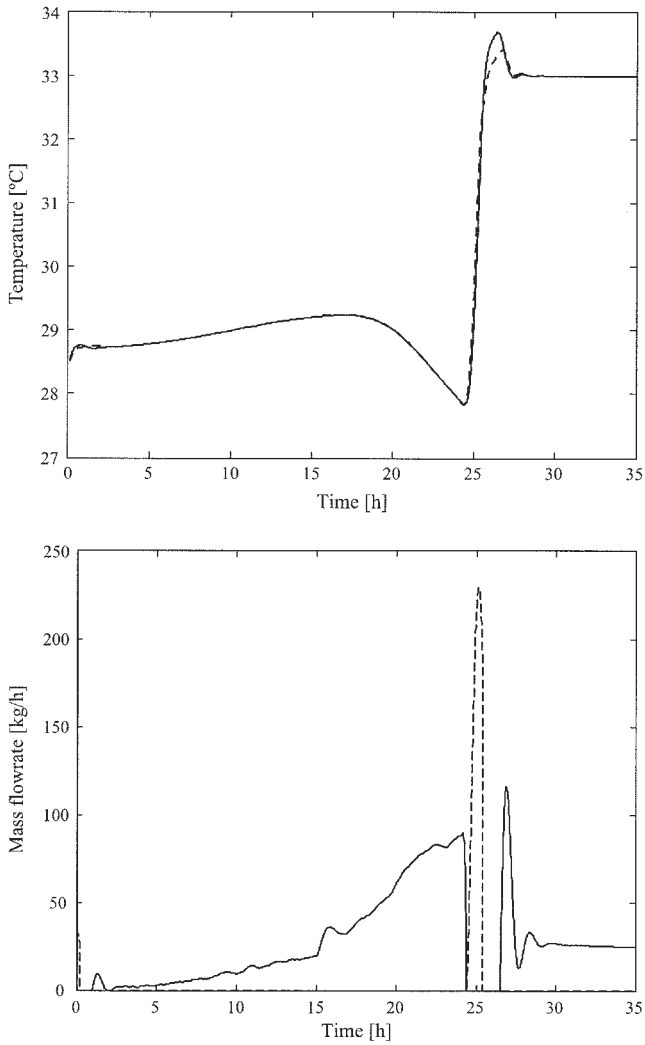

Figure 8. (a) The solid line shows the controlled temperature when a +5°C load change at t = 15 h is made in the cooling water, and the hot water is at 70°C (the dashed line is the previous response in Figure 7a); (b) control actions corresponding to the closed-loop response in (a).

beginning of the run. In addition, a step change from 15 to 20°C is made in the cold water entering at $t = 15$ h. In fact, the major differences between these runs are better observed by comparing the water flow rate variations in Figure 8b with those in Figure 7c.

Furthermore, it is worth mentioning that the overshoot observed after abruptly raising the reactor temperature is mainly attributed to the reset windup in the PI controller handling the cooling water. This undesirable effect is eliminated by using an antireset windup configuration that temporarily halts the integral action (Riggs, 2001). Figure 9 shows the results of running under similar conditions to those corresponding to Figures 7a, but using antireset windup in both controllers.

Finally, because occasionally the desired output profile might be modified as a result of operative reasons or to on-line optimization, the sensitivity to changes in the profile of Figure 1 was also evaluated. Figure 10 shows the response obtained by arbitrarily maintaining the set point in 28.5°C during the first 5 h, and then including two step changes to 29.5°C and back to 28.5°C at the time instants 5 and 15 h, respectively. After about 23 h, the set-point trajectory is similar to the original one.

Several questions remain to be answered with respect to the effectiveness of the proposed procedure. This report discusses the main concepts from a practical point of view only, leaving additional analysis and evaluations for a future work. Topics such as the effect of noise or disturbances in the collected data, the sensitive to different input-reference sequences, or the importance of on-line adaptation are significant issues that should be evaluated in several batch-process systems besides the bioreactor used in this work.

Conclusions

This article proposes a referential process–reaction curve method to identify dominant dynamics relating manipulated variables with output variables characterized by a permanent transition, as typically occurs in batch-process systems. Following the same philosophy supporting the traditional reaction curve method for stationary processes, this extension allows us to determine reduced-complexity models valid in the neighborhood of a reference evolution in processes that never reach a steady state. This way, the approach provides a simple modeling procedure for the systematic tuning of industrial PI or PID controllers that was still missing when facing control problems in transient processes or batch-process operations.

The proposed method was tested with a nonlinear simulator of a batch bioreactor where the control problem consists of tracking a predetermined temperature profile. The balance between the method simplicity and the performance obtained suggests the usefulness of the referential process–reaction curve, for not only immediate implementations in low-level controllers such as those discussed in this article or as part of a hierarchical optimizing structure; it also provides a reference performance when more sophisticated control systems are analyzed.

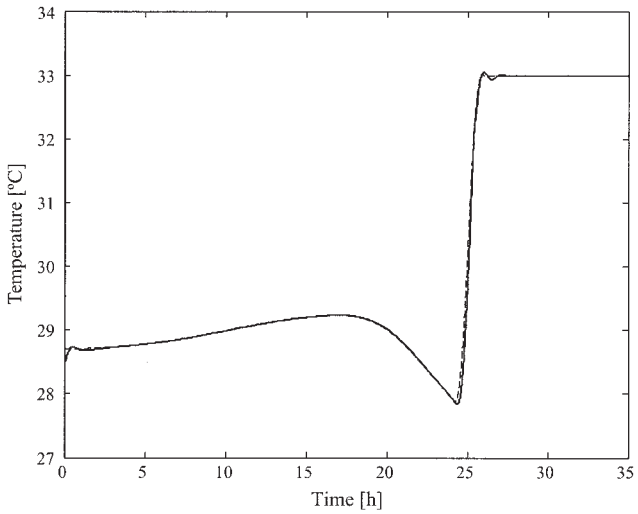

Figure 9. Closed-loop response obtained using antiwindup protection in both PI controllers.

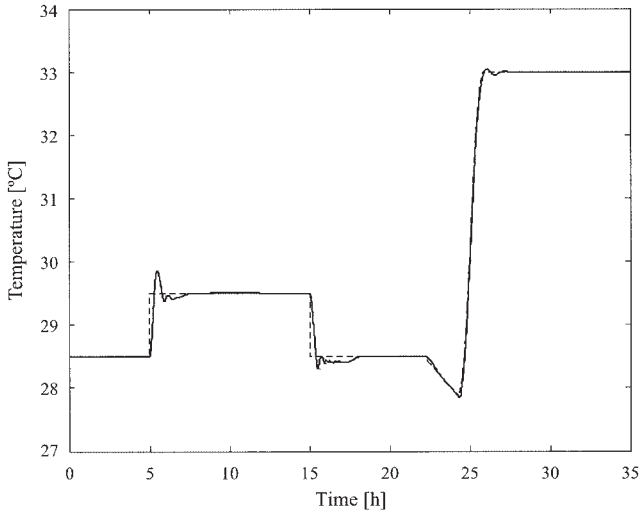

Figure 10. Controlled temperature following an arbitrary set-point trajectory.

Acknowledgments

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Appendix A

Nonlinear model of xanthan gum production

The following are the fundamental relationships used for describing the production of xanthan gum. The model uses the "logistic equation" for representing the biomass (X) kinetics, the "Luedeking–Piret equations" for the product (P), and the total substrate (S) as follows

$$\frac{dX}{dt} = \mu_M\left(1 - \frac{X}{X_S}\right)X \tag{A1}$$

$$\frac{dP}{dt} = \left(a\,\frac{dX}{dt} + bX\right)\left(\frac{S}{S + k_S}\right) \tag{A2}$$

$$\frac{dS_{cat}}{dt} = \left\{\frac{1}{Y_{X/ATP}}\frac{dX}{dt} + \frac{1}{Y_{P/ATP}}\frac{dP}{dt} + K_{ATP}X\left(\frac{S}{S + k_S}\right)\right\} \times \frac{1}{3 + 12P/O} \tag{A3}$$

$$\frac{dS}{dt} = -\left(\frac{1}{Y_{X/S}}\frac{dX}{dt} + \frac{1}{Y_{P/S}}\frac{dP}{dt} + \frac{dS_{cat}}{dt}\right) \tag{A4}$$

where

$$\mu_M = c_{\mu 1}(T - T_{\min \mu})(1 - e^{c_{\mu 2}(T - T_{\max \mu})})$$

$$X_s = \frac{x_1 + x_2 e^{(T_0 - T)}}{1 + e^{(T_0 - T)}}$$

$$a = c_{a1}(T - T_{\min a})(1 - e^{c_{a2}(T - T_{\max a})})$$

$$b = a_b e^{e_b/(T + 273)}$$

$$Y_{P/ATP} = \frac{PM_{gum}}{Y^0_{ATP} - Y_{NADH2/P}P/O}$$

In this system of equations, $c_{\mu 1}$, $c_{\mu 2}$, $T_{\min \mu}$, $T_{\max \mu}$, c_{a1}, c_{a2}, $T_{\min a}$, $T_{\max a}$, a_b, and e_b are constant kinetic parameters; K_{ATP} is the maintenance coefficient; P/O is the oxidation level; k_S is the Monod coefficient; S_{cat} represents the main substrate catabolism; $Y_{I/J}$ stands for a stoichiometric yield of component I on component J; and ATP stands for adenosine 5-triphosphate. A more detailed explanation of this model can be found in Dondo (2000) and Shu and Yang (1990, 1991). The simulations presented herein use the parameter values shown in Table A1.

Table A1. Nonlinear Model Parameters

Variable	Value	Variable	Value
$c_{\mu 1}$	0.0405 h^{-1} $°C^{-1}$	e_b	−9580 $°C^{-1}$
$c_{\mu 2}$	0.26 $°C^{-1}$	x_1	1.58 g/L
$T_{\min \mu}$	11.69°C	x_2	2.02 g/L
$T_{\max \mu}$	35.17°C	T_0	29.0°C
c_{a1}	0.209 $°C^{-1}$	K_{ATP}	0.7 h^{-1}
c_{a2}	0.486 $°C^{-1}$	P/O	1.3
$T_{\min a}$	20.44°C	k_S	1.8 g/L
$T_{\max a}$	32.75°C	$Y_{X/ATP}$	10.5 g/g
a_b	1.61e+13 h^{-1}	Y^0_{ATP}	10.9 mol/mol
$Y_{P/S}$	0.917 g/g	$Y_{NADH2/P}$	3.58 mol/mol
$Y_{X/S}$	1.78 g/g	PM_{gum}	906 g/mol

Energy balances

The reactor energy balance is given by

$$m_r cp_r \frac{dT}{dt} = \Delta H_r - Q_a \tag{A5}$$

where m_r is the mass in the reactor, cp_r is the heat capacity of the material in the reactor, T stands for the reactor temperature, ΔH_r is the heat of reaction, $Q_a = UA\Delta T_m$ is the energy given to the cooling fluid, $\Delta T_m = T - T_a$ is the overall temperature difference to the jacket fluid, and UA is the global heat transfer coefficient times the exchange area. The heat of reaction is described based on the oxygen consumption Q_{O2} (g O_2 h^{-1} L^{-1}) as

$$\Delta H_r(P, S_{cat}) = Q_{O2}(P, S_{cat})\lambda_{O2}V\frac{1}{PM_{O2}} \tag{A6}$$

where λ_{O2} represents the released energy (kJ/mol O_2), V is the reactor volume (L), and PM_{O2} is the oxygen molecular weight (g O_2/mol O_2). Besides, the energy balance for the cooling water can be written as follows

$$m_a cp_a \frac{dT_a}{dt} = w_a cp_a(T^0_a - T_a) + UA\Delta T_m \tag{A7}$$

where T^0_a is the inlet temperature, T_a is the outlet temperature, m_a is the mass of water in the jacket, w_a is the mass flow rate, and cp_a is the water heat capacity.

Appendix B

This appendix was prepared to highlight several hypotheses or simplifications indirectly assumed when the referential reaction curve is used to approach a referential linear model, and to provide few considerations to improve the reliability of the representation. The analysis is based on the xanthan gum bioreactor presented in Appendix A. Although the kinetics expressions describing the dynamic evolutions of biomass (X), product (P), and substrate (S) should be included to consider the complete model, for the benefit of simplicity and because temperature-tracking control is pursued, let us take merely

those relationships arising from the energy balances. In other words, let us assume that Eq. 1 is given by

$$\begin{bmatrix} \frac{dx_1(t)}{dt} \\ \frac{dx_2(t)}{dt} \end{bmatrix} = \begin{Bmatrix} \frac{1}{m_r cp_r}\Delta H_r(t) - \frac{UA}{m_r cp_r}[x_1(t) - x_2(t)] \\ \frac{UA}{m_a cp_a}[x_1(t) - x_2(t)] \end{Bmatrix} + \begin{Bmatrix} 0 \\ \frac{1}{m_a}[x_2^{in} - x_2(t)] \end{Bmatrix} u(t)$$

$$y(t) = x_1(t) \tag{B1}$$

where $x_1 = T$ is the reactor temperature, and $x_2 = T_a$ and $u = w_a$ are the jacket-side fluid temperature and flow rate, respectively. Notice also that ΔT_m is approached here by $T(t) - T_a(t)$ and because state variables P and S_{cat} are not included, ΔH_r is assumed to be time dependent only.

If the second term in Eq. B1 is changed by a first-order approximation to separate the effects of w_a and T_a, the referential process reaction in Eq. 3 takes the linear form

$$\begin{aligned} \Delta\dot{x}(t) &= A\Delta x(t) + B\Delta u(t) \\ \Delta y(t) &= C\Delta x(t) \end{aligned} \tag{B2}$$

where the heat-of-reaction term cancels out, assuming it repeats itself from one run to the next. The elements of matrix A are

$$a_{11} = -\frac{UA}{m_r cp_r} \qquad a_{12} = \frac{UA}{m_r cp_r}$$

$$a_{21} = \frac{UA}{m_a cp_a} \qquad a_{22} = -\left[\frac{UA}{m_a cp_a} + \frac{\bar{w}_a}{m_a}\right]$$

Matrix $B = [0 \quad b_2]^T$, and matrix $C = [1 \quad 0]$, where

$$b_2 = \frac{(T_a^0 - \bar{T}_a)}{m_a}$$

Table B1. Main Parameters of the Bioreactor

Variable	Value
m_r	1000 kg
cp_r	3.55 kJ kg^{-1} °C^{-1}
V	1000 L
m_a	210 kg
cp_a	4.18 kJ kg^{-1} °C^{-1}
UA	4000 kJ h^{-1} °C^{-1}
T_a^0	15–80°C
λ_{O2}	451.44 kJ/mol

In these expressions, $\bar{w}_a$and $\bar{T}_a$ stand for reference values used in the linear approximation of the second term. Applying Laplace transforms and rearranging, the following expression for the process reaction is obtained:

$$\Delta T(s) = \frac{a_{12}b_2}{s^2 - (a_{11} + a_{22})s + (a_{11}a_{22} - a_{12}a_{21})}\Delta w_a(s) \tag{B3}$$

It is apparent that the most important assumption included to arrive at Eq. B3 is that the exothermic heat generation is independent of the state-variable path. Thus, an extra term associated with expected inaccuracies in the above transfer function must be accepted. It can also be assumed that this mismatch increases proportionally to the amplitude of the deviation Δw_a. This reasoning allows us to rewrite Eq. B3 as

$$\Delta T(s) = [\tilde{G}_p(s) + \Delta\tilde{G}_p(s)]\Delta w_a(s) \tag{B4}$$

where $\tilde{G}_p(s)$ is the transfer function approximated by the referential process–reaction curve. Equation B4 also suggests that a set of experiments using different perturbed paths can help to determine limits to the model uncertainty.

According to Eq. B3, $\tilde{G}_p(s)$ should be a second-order transfer function, occasionally with a time delay included. However, if one of the two time constants is very large compared to the other one, the observed response might appear to be coming from an integral-plus-delay dynamic, particularly for relatively short times. This is the case for this bioreactor, given that under conditions determined by Tables A1 and B1, and for $\bar{w}_a = 10$ kg h^{-1} and $\bar{T}_a = 16$–17°C, one time constant is about 106 h, whereas the other is around 0.17 h.

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