

## REFERENTIAL PROCESS REACTION CURVE FOR BATCH OPERATIONS

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**Abstract:** This paper shows 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 non-stationary batch processes. The basic idea is to isolate the dynamics associated to 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 non-stationary 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.

**Keywords:** reaction-curve method, controller tuning, batch process systems, process systems engineering.

## INTRODUCTION

Process control specialists have dedicated more time to the analysis, design and tuning of controllers for processes operating under stationary mode than for non-stationary processes like batch processes. Traditional methods for adjusting classic controllers like PI and PID assume they will be dedicated to disturbance rejection from a stationary state, or to setpoint changes if the process must go from one stationary state to another. This is the type of control task mostly expected when Ziegler-Nichols (1949), Cohen and Coon (1953), or more closely, when Rivera et al. (1986) or Chien and Fruehauf (1990) tuning rules are adopted. Traditional texts for teaching process control like Stephanopoulos (1984) and Seborg, et al. (1989) emphasize on 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 start-up or shut-down “until the operation is close to the desired condition.” Hence, 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, i.e., the open-loop response of the process to a step change in the controller output. This test continues to be very popular since not only 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 and the easy 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 non-linear evolution the system follows during a standard or nominal run. The proposal tries to keep the simplicity expected by practitioners from model-

ing 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 perceptible 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 in order to reach the maximum product concentration at the end of the operation.

In the next section, the fundamentals 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 to 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 finally section presents the conclusions of this work.

## **REFERENTIAL PROCESS REACTION CURVE**

The outstanding feature of batch or semi-batch 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 non-linear 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. Since 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, have 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

$$\begin{aligned}\dot{x}(t) &= f\{x(t), t\} + g\{x(t)\}u(t), \quad x(0) = x_0 \\ y(t) &= h\{x(t)\}.\end{aligned}\quad (1)$$

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

Let us assume, that as part of the batch recipe, an specific  $u(t) = u_r(t)$  input trajectory is available all along the operative time interval  $[0, t_f]$ , i.e., a sequence of manipulated-variable changes are scheduled in order 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

$$\begin{aligned}\dot{x}_r(t) &= f\{x_r(t), t\} + g\{x_r(t)\}u_r(t), \quad x_r(0) = x_0 \\ y_r(t) &= h\{x_r(t)\}.\end{aligned}\quad (2)$$

Notice that the control input in Eqn. (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

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

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 (3), are predetermined time functions, i.e., they are not time variables capable to react 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 like temperature or concentration; this means that in many regular SISO control problems  $h\{x(t)\}$  is a very simple function providing some simplicity to (3). There are also no doubts that (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 an strict theoretical approach.

In a batch reactor for instance, most of the variables of interest evolve due to 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 one, with only minor changes due to many hardly controllable causes; this is basically what happens when the reactor temperature rises due to the released heat of reaction. Hence, 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 to 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 than the process-reaction curve for stationary processes and leads to reduced-complexity models for designing and tuning feedback controllers. Besides, due to 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. Since a plant is generally of relatively high order, identification for controller design and tuning purposes means also a model reduction exercise. The temperature control of a batch bioreactor does not escape to 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. Previ-

ous investigations have determined that the optimal operation of this bioreactor follows a particular temperature profile in order to achieve maximum amount of product in a convenient time interval (Dondo, 2000).

### ***Temperature Control Setup***

Hence, the main objective for the control system is to track the temperature profile shown in solid line in Figure 1, since this allows reaching maximum product concentration after operating about thirty-five hours. Figure 1 also shows the natural temperature evolution when no cooling service is used all along the 35-hours run. When comparing these profiles, a conclusion is that not only cooling is necessary but also - since the reactor temperature rises slowly - a heating stage should be allowed. Hence, the reactor jacket is connected such to receive water at 15 or 80 degrees centigrade. The input of one or the other service is handled by a two-way valve, while the flowrate is regulated by a control valve like shown in Figure 2. In order to fit in this constrained setup, two PI controllers with anti wind-up 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 (taken 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 to achieve the desired tracking. However, it must be emphasized here that this is a secondary issue in this paper; the main concern is the appropriate tuning of the feedback controllers in order 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 flowrate 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 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 most favorable set-point profile. Then, let us take this input-output time evolution as the reference trajectory, i.e., as  $u_r(t)$  and  $T_r(t)$  in equation (2) respectively.

The use of the proposed open-loop response in Figure 3b is supported by the following reasons: i) the closer the output-reference trajectory is to the desired one, the smaller the model mismatch should be, and ii) both, the reference and the perturbed trajectories, should also be safe and economically acceptable runs. These arguments lead also to define time-integral compensated input trajectories when dealing with integrating systems. Figures 4a and 4b exemplifies the concept, where the arrows indicates 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  $T_r(t)$ , i.e., assuming no other disturbance has occurred. This difference is the output response  $\Delta y(t)$  of the referential dynamic system in Eqn. (3) to the input changes in Figure 5a. Each referential responses  $\Delta y(t)$  allows 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

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

This way, the responses in Figure 5b allows to find  $K_p = -0.012$  °C/(kg/h) and  $T_d = 0.17$  h for the cold water, and  $K_p = 0.042$  °C/(kg/h) 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 method has always been a practical model-reduction technique, but also with the naturally expected dynamic associated to a manipulated flowrate variable in a batch system. Appendix B exposes the main assumptions that, from the fundamental model, are necessary to accept (4) as an approximate transfer function for tuning purposes.

### ***Controller Tuning***

No too many references 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. Hence, once the normalized slope  $S^*$  and the time delay  $\theta$  is 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  $K_p = S^*$  and  $T_d = \theta$  in this article.

Alternatively, Chien and Fruehauf (1990) propose tuning rules for PI and PID controllers using the 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 y Luyben (1992) use classical frequency response methods to propose an 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 closely, Luyben (1996) extends 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 settings given by Ziegler-Nichols 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. Hence, the following parameter values for the PI controllers are determined:  $K_c = -441.2$  kg/h °C and  $T_I = 0.56$  h; and  $K_c = 153.0$  kg/h °C, 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  $T(0) = T_d(0) = 28.5$  °C,



i.e., 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 batch evolution can be observed in Figures 7a to 7c; in particular Figure 7b shows the effective cooling and heating periods since crossing points between jacket and reactor temperature are clearly determined. Since 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 minutes. This is followed by a cooling period that lasts until the hour 24 approximately, when an important transition has to be done 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 in ahead, cooling is again necessary to compensate the heat of reaction.

The robustness of this tuning approach is exposed in Figure 8a that 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 beginning of the run. In addition, a step change from 15 °C 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 flowrate variations in Figure 8b with those in Figure 7c.

Furthermore, it is worth to mention that the overshoot observed after abruptly raising the reactor temperature is mainly due 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, since occasionally the desired output profile might be modified due to operative reasons or to online optimization, the sensitivity to changes in the profile of Figure 1 was also evaluated. Figure 10 shows the response obtained by arbitrarily maintaining the setpoint in 28.5 °C along 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 setpoint trajectory is similar to the original one.

Several questions remain to be answered in regard to the effectiveness of the proposed procedure. This paper discusses the main concepts from a practical point of view only, leaving additional analysis and evaluations for a future work. Topics like the effect of noise or

disturbances in the collected data, the sensitive to different input-reference sequences or the importance of online adaptation are significant issues that should be evaluated in several batch-process systems besides the bioreactor used in this work.

## **CONCLUSIONS**

This paper proposes a referential process reaction curve method to identify dominant dynamics relating manipulated variables with outputs 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 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 on 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 like exposed in this paper or as part of a hierarchical optimizing structure; it also provides a reference performance when more sophisticated control systems are analyzed.

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## APPENDIX A

### *Nonlinear Model of the Xanthan-Gum Production*

The following are the fundamental relationships used for describing the Xanthan-gum production. The model uses the “logistic equation” for representing the biomass ( $X$ ) kinetics, the “Luedeking-Piret equations” for the product ( $P$ ), and the total substrate ( $S$ )

$$\frac{dX}{dt} = \mu_M \left( 1 - \frac{X}{X_s} \right) X \quad (\text{A1})$$

$$\frac{dP}{dt} = \left( a \frac{dX}{dt} + bX \right) \left( \frac{S}{S + k_s} \right) \quad (\text{A2})$$

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

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

where,

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

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

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

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

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

In this equations,  $c_{\mu 1}$ ,  $c_{\mu 2}$ ,  $T_{\min \mu}$ ,  $T_{\max \mu}$ ,  $c_{a1}$ ,  $c_{a2}$ ,  $T_{\min a}$ ,  $T_{\max a}$ ,  $a_b$ ,  $e_b$ , are constant kinetic parameters.  $K_{ATP}$  is the maintenance coefficient,  $P/O$  the oxidation level,  $k_s$  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 in this paper use the parameter values shown in Table 1.

### *Energy Balances.*

The reactor energy balance is given by

$$m_r \cdot cp_r \cdot \frac{dT}{dt} = \Delta H_r - Q_a, \quad (\text{A5})$$

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,  $\Delta H_r$  is the heat of reaction,  $Q_a = UA \cdot \Delta T_m$  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  $Q_{O_2}$  (g O<sub>2</sub> /h L ) as

$$\Delta H_r(P, S_{cat}) = Q_{O_2}(P, S_{cat}) \cdot \lambda_{O_2} \cdot V \cdot \frac{1}{PM_{O_2}}, \quad (A6)$$

where  $\lambda_{O_2}$  represents the released energy (kJ/mol O<sub>2</sub>),  $V$  stands for the reactor volume (L) and  $PM_{O_2}$  the oxygen molecular weight (g O<sub>2</sub>/mol O<sub>2</sub>). Besides, the energy balance for the cooling water can be written as follows:

$$m_a \cdot cp_a \frac{dT_a}{dt} = w_a \cdot cp_a (T_a^o - T_a) + UA \cdot \Delta T_m, \quad (A7)$$

where  $T_a^o$  is the inlet temperature,  $T_a$  stands for the outlet temperature,  $m_a$  is the mass of water in the jacket,  $w_a$  is the mass flow rate, and  $cp_a$ : the water heat capacity.

## APPENDIX B

This appendix is aimed to highlight several hypothesis 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 only pursued, let us take merely those relationships arising from the energy balances. In other words, let us assume the expression (1) is given by

$$\begin{bmatrix} \frac{dx_1(t)}{dt} \\ \frac{dx_2(t)}{dt} \end{bmatrix} = \begin{bmatrix} \frac{1}{m_r \cdot cp_r} \cdot \Delta H_r(t) - \frac{UA}{m_r \cdot cp_r} \cdot (x_1(t) - x_2(t)) \\ \frac{UA}{m_a \cdot cp_a} \cdot (x_1(t) - x_2(t)) \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{m_a} (x_2^{in} - x_2(t)) \end{bmatrix} u(t) \quad (B1)$$

$y(t) = x_1(t)$

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

If the second term in equation (B1) is changed by a first order approximation to separate the effects of  $w_a$  and  $T_a$ , the referential process reaction (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 repeat itself from one run to the next one. The elements of matrix  $A$  are

$$\begin{aligned}a_{11} &= -\frac{UA}{m_r \cdot cp_r}, & a_{12} &= \frac{UA}{m_r \cdot cp_r}, \\ a_{21} &= \frac{UA}{m_a \cdot cp_a}, & a_{22} &= -\left[ \frac{UA}{m_a \cdot cp_a} + \frac{\bar{w}_a}{m_a} \right],\end{aligned}$$

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

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

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 (B3) is that the exothermic heat generation is independent of the state-variable path. Hence, an extra term associated to 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  $\Delta w_a$ . This reasoning allows us to rewrite (B3) as

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

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

According to (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 look as coming from an integral-plus-delay dynamic, particularly for relatively short times. This is the case for this bioreactor since under conditions determined by Tables 1 and 2, and for  $\bar{w}_a = 10$  kg/h and  $\bar{T}_a = 16-17$  °C, one time constant is about 106 h while the other one is around 0.17 h.

Table 1. Nonlinear model parameters

Variable	Value	Variable	Value
$c_{\mu 1}$	0.0405 h <sup>-1</sup> °C <sup>-1</sup>	$e_b$	-9580 °C <sup>-1</sup>
$c_{\mu 2}$	0.26 °C <sup>-1</sup>	$X_1$	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 <sup>-1</sup>	$K_{ATP}$	0.7 h <sup>-1</sup>
$c_{a2}$	0.486 °C <sup>-1</sup>	$P/O$	1.3
$T_{mina}$	20.44 °C	$k_S$	1.8 g/L
$T_{maxa}$	32.75 °C	$Y_{X/ATP}$	10.5 g/g
$a_b$	1.61e+13 h <sup>-1</sup>	$Y_{ATP}^0$	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



Table 2. Main parameters of the bioreactor

Variable	Value
$m_r$	1000 kg
$cp_r$	3.55 kJ/kg °C
$V$	1000 L
$m_a$	210 kg
$cp_a$	4.18 kJ/kg °C
$UA$	4000 kJ/hr °C
$T_a^o$	15 - 80 °C
$\lambda_{o_2}$	451.44 kJ/mol

## Figure Captions

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

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

Figure 3a. Nominal input profile: the solid line shows the programmed sequence of cooling-water flowrates; the dashed line shows the use of hot water.

Figure 3b. Solid line: temperature profile obtained with the open-loop program shown in Figure 3a; the desired profile is shown in dashed line.

Figure 4a. The arrows show two compensating changes made in the cooling-water flowrate.

Figure 4b. The arrows show two compensating changes made in the heating-water flowrate.

Figure 5a. Net input changes in the referential process system.

Figure 5b. Referential process reaction curves obtained from the referential changes in Figure 5a.

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

Figure 7a. Closed-loop tracking response obtained with the PI controllers adjusted using the referential process models and Ziegler-Nichols settings.

Figure 7b. The solid line is the water temperature in the jacket; the dashed line is the reactor temperature.

Figure 7c. Control actions corresponding to the evolutions in Figures 7a and 7b. The solid line represents the cold-water flowrate, the dashed line is the hot-water flowrate.

Figure 8a. The solid line shows the controlled temperature when a  $+5\text{ }^{\circ}\text{C}$  load change at  $t = 15\text{ h}$  is made in the cooling water, and the hot water is at  $70\text{ }^{\circ}\text{C}$ . The dashed line is the previous response in Figure 7a.

Figure 8b. Control actions corresponding to the closed-loop response in Figure 8a.

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

Figure 10. Controlled temperature following an arbitrary setpoint trajectory.