Identification and Control of Chemical Processes Using the Anisochronic Modeling Paradigm

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Abstract: An identification methodology is proposed in order to model chemical processes using the anisochronic paradigm. This methodology requires only having the reaction curve of the plant to obtain all the parameters of the model for both over-damped and underdamped processes. On the other hand an optimal tuning for PID controllers considering the closed-loop robustness is also proposed for a given anisochronic model. Both the identification and the control are tested in a pH neutralization process, a well known PID benchmark and in a nonlinear CSTR system, to verify the usefulness of the proposed methodology in chemical processes.

Keywords: Identifications, Anisochronic Model, PID Control, Chemical Processes

1. INTRODUCTION

Even in a decade where advanced control algorithms, mostly based on some kind of optimization procedure, have achieved a high degree of maturity, Proportional-Integral-Derivative (PID) controllers are still widely used in the process industries (Åström and Hägglund, 2001). Their popularity is due to their simplicity - they only have three parameters - and to the satisfactory control performance shown for different kind of processes. However, the adjustable PID controller parameters should be tuned appropriately.

Much of the effort made in the process control field has been focused to chemical processes applications, due to the multiple characteristics that can be found for this kind of systems. Examples of these cases include Continuous Stirred Tank Reactors (CSTR), polymerization reactors, distillation columns with recycling streams and bioreactors that are usually modeled by a low-order model as First-Order-Plus-Time-Delay (FOPTD) transfer function (Zítek and Hlava, 2001).

The availability of FOPTD models in the process industry is a well known fact. The generation of such model just needs for a very simple step-test experiment to be applied to the process. This can be considered as an advantage with respect to other methods that need a more *plant demanding* experiment such as methods based on more complex models or even data-driven methods where a sufficiently rich input needs to be applied to the plant. From this point of view, to maintain the need for plant experimentation to a minimum is a key point when considering industrial application of a technique.

Despite the above, the majority of the systems have a wide range of dynamics that include for example high-order processes, that can be over-damped or under-damped, being this difference an important characteristic that must be represented by the model. In this sense is that the capabilities of the anisochronic model, introduce an alternative form to represent the process with behaviors that can be from low-order to high-order dynamics (Zítek, 1998; Vyhlídal, 2000). It is important to emphasize that even the structure of the anisochronic model is more complex, the procedure to get the parameters depend also of the information of the reaction curve, maintaining the simplicity of the modeling task. Consequently, there has been much interest in the literature in the tuning of industrially standard PID controllers for this kind of identification, applying to chemical processes.

Here in this paper, it is proposed an identification method to achieve the parameters of an anisochronic model, that represents over-damped and under-damped dynamics of different kind of chemical processes. Moreover, it is performed the control design for a PID controller, taking into account the system robustness.

The paper is organized as follows. Section 2 presents the system configuration, where is introduced the anisochronic model and its identification and also is proposed the tuning for the controller. Section 3 describes the results and the analysis of the identification and control of some examples and cases of study as: a pH neutralization process, a CSTR

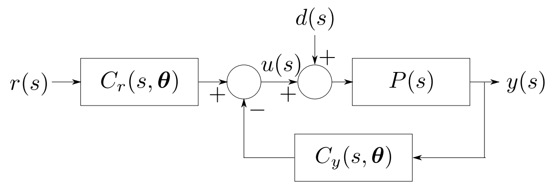

Figure 1. Closed-loop Control System.

and the application of a benchmark system proposed by Åström and Hägglund (2000). The paper ends with some conclusions that are in Section 4.

2. MATERIALS AND METHODS

2.1 Control System Configuration

In this paper, the considered controlled system is presented in Fig. 1 where:

- $C_r(s,\boldsymbol{\theta})$ and $C_y(s,\boldsymbol{\theta})$ are the set-point and feedback controllers respectively, with parameters $\boldsymbol{\theta}$ of a two degree of freedom (2DoF) PID controller.
- $P(s)$ is the process.
- $r(s)$ is the set-point signal.
- $u(s)$ is the control effort.
- $d_i(s)$ is the input-disturbance.
- $y(s)$ is the process output (controlled variable).

For analysis purposes (but not for implementation), the controller's output can be described as:

$$u(s) = C_r(s,\boldsymbol{\theta})r(s) - C_y(s,\boldsymbol{\theta})y(s), \tag{1}$$

where $C_r(s,\boldsymbol{\theta})$ is the set-point controller given by:

$$C_r(s,\boldsymbol{\theta}) = K_p\left(\beta + \frac{1}{T_i s}\right), \tag{2}$$

and $C_y(s,\boldsymbol{\theta})$ is the feedback controller given by:

$$C_y(s,\boldsymbol{\theta}) = K_p\left(1 + \frac{1}{T_i s} + \frac{T_d s}{\alpha T_d s + 1}\right). \tag{3}$$

The controller parameters K_p, T_i, T_d and β are the proportional gain, the integral time constant, the derivative time constant and the proportional set-point weight factor, respectively. It is common to have a constant $\alpha = 0.1$ in order to have a physically realizable derivative term. These parameters can be grouped in a single vector given by $\boldsymbol{\theta} = [K_p, T_i, T_d, \beta]^T$.

In this work, the use of anisochronic first order models plus time delay (AFOPTD) is presented for chemical processes. This model has the characteristic to have a time delay at the input and another internal delay in the state. Its differential equation is given by Vyhlídal (2000):

$$T\frac{dy(t)}{dt} + y(t-\phi) = Ku(t-\tau), \tag{4}$$

where T in the time constant, ϕ is the internal delay and τ is the external delay. The corresponding transfer function is given by:

$$P(s) = \frac{Ke^{-s\tau}}{Ts + e^{-s\phi}}. \tag{5}$$

The exponential term in the denominator makes the model to be able to represent both over-damped and under-damped systems since, this model has an infinite number of poles. Because of this, it is said that the anisochronic model is able to represent first and second order dynamics with the same topology.

It is common to normalize the model and the controller in order to simplify the analysis (Skogestad and Postlethwaite, 2007). With the transformation $\hat{s} = Ts$, the normalized plant $\hat{P}(\hat{s})$ is given by:

$$\hat{P}(\hat{s}) = \frac{e^{-\hat{s}\tau_0}}{\hat{s} + e^{-s\phi_0}}, \tag{6}$$

where the normalized time delay τ_0 is defined as:

$$\tau_0 = \frac{\tau}{T}, \tag{7}$$

and the normalized internal time delay ϕ_0 is defined as:

$$\phi_0 = \frac{\phi}{T}. \tag{8}$$

The gain of the plant is introduced in the controller in order to obtain the normalized controller given by:

$$\begin{aligned}\hat{C}_r(\hat{s},\hat{\boldsymbol{\theta}}) &= \kappa_p\left(\beta + \frac{1}{\tau_i\hat{s}}\right),\\ \hat{C}_y(\hat{s},\hat{\boldsymbol{\theta}}) &= \kappa_p\left(1 + \frac{1}{\tau_i\hat{s}} + \frac{\tau_d s}{\alpha\tau_d s + 1}\right),\end{aligned} \tag{9}$$

with the following normalized parameters $\hat{\boldsymbol{\theta}}=[\kappa_p, \tau_i, \tau_d, \beta]^T$:

$$\kappa_p \doteq KK_p, \quad \tau_i \doteq \frac{T_i}{T}, \quad \tau_d \doteq \frac{T_d}{T}. \tag{10}$$

With this controller, the closed-loop response, is given by

$$\begin{aligned}y(\hat{s}) = &\frac{\hat{C}_r(\hat{s},\hat{\boldsymbol{\theta}})\hat{P}(\hat{s})}{1+\hat{P}(\hat{s})\hat{C}_y(\hat{s},\hat{\boldsymbol{\theta}})}r(\hat{s})\\ &+ \frac{\hat{P}(\hat{s})}{1+\hat{P}(\hat{s})\hat{C}_y(\hat{s},\hat{\boldsymbol{\theta}})}d_i(\hat{s})\end{aligned} \tag{11}$$

As it can be seen from (11), the closed-loop response to a reference change, can be independently tuned from the disturbance responses, due to the $C_r(\hat{s},\hat{\theta})$ controller. In fact, some filter can be added in order to obtain a more independent response (Hägglund, 2012).

The peak of the sensitivity function is commonly used as a measure of the robustness of the closed-loop controlled system:

$$M_S(\boldsymbol{\theta}) = \max_{\omega}|S(j\omega,\boldsymbol{\theta})| = \max_{\omega}\left|\frac{1}{1+P(j\omega)C_y(j\omega,\boldsymbol{\theta})}\right|. \tag{12}$$

It is common to consider a maximum sensitivity value $M_S \leq 2$ as a good robustness indicator.

It may be possible to define a controller using also an anisochronic strategy. However, since PID controllers are common in industry, in this paper a methodology for finding the optimal tuning parameters for PID based on anisochronic models.

2.2 System Identification

The first step to control a chemical process is to find a suitable model, in order to incorporate this information into the controller. According to Vyhlídal (2000), it is possible to find the parameters of the anisochronic model by applying the relay test proposed by Åström and Hägglund. (1984). However, an apriori estimation of the external time delay is needed in order to find the rest of the parameters. In Vyhlídal and Zítek (2001) a method using a tangent of the reaction curve is proposed. They proposed that the value of ϕ affects the position of the inflection point in

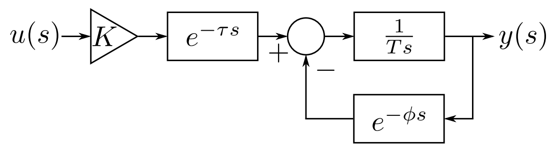

Figure 2. Alternative structure for the anisochronic model.

which the tangent curve is drawn. Knowing the position and the slope of the tangent, it is possible to find the value of the anisochronic parameters. But it is not said how to relate the position of the tangent with the value of ϕ.
In this work, a non-linear optimization problem is proposed to find the parameters of the plant by writing the objective function as:

$$S_{cr}(\mathbf{\Psi}) = \int_0^\infty |y(t) - y_m(t, \mathbf{\Psi})| \, \mathrm{d}t, \tag{13}$$

where $y(t)$ is the response of the plant to step change in open loop and $y_m(t)$ is the response of the model given by (5), with parameters $\mathbf{\Psi} = [\ K, \quad T, \quad \tau, \quad \phi\ ]^T$ to the same input. The value of the steady state gain K is computed by measuring the change in steady state of the output for a particular step change in the input. The identification procedure s given by the following steps:

- The step response of the plant is considered to have reached the new steady state of the process and that the data has been sampled with a constant sampling time and normalized in such a way that both the input and the output has a change in magnitude of one.
- In order to accelerate the optimization and considering Vyhlídal and Zítek (2001), the starting point of the optimization is computed as follows:
  - Approximate the external delay time as the time needed to reach the 7.5% of the output signal. This consideration is based in the fact that the process dynamics are not exactly the same as the model and that, in general, the anisochronic model has a larger external delay time than the process.
  - An approximation of the constant time of the process can be found by considering the alternative structure of the anisochronic model shown in Fig. 2. Before, ϕ units of time has passed from the instant of the step change, the model dynamics are the same as a pure integral process with time delay. The response to a step response of this kind of system is a delayed ramp with a slope equal to K/T. Taking this into account, an approximation of the time delay of the system can be found by computing the slope of the line that joins the points at 20% and 50% of the output response as shown in Fig. 3.
  - Finally, the internal time delay is approximated as the time needed to reach the 50% of the output signal.
- With this starting point, the objective function (13) is minimized using a nonlinear optimization algorithm.

2.3 Controller Design

Once an optimal model has been defined for the process, another optimization can be computed in order to find the controller parameters. Consider the 2DoF PID controller of Fig. 1, but applying the transformation $\hat{s} = Ts$ and equations (5) and (9). In a chemical process, the reference signal does not change as often as the disturbance, therefore to optimize the response to a disturbance is more important than the set-point change response Shinskey (2002). Therefore, the procedure to follow is to first optimize the κ, τ_i and τ_d parameters of the $\hat{C}_y(\hat{s}, \hat{\boldsymbol{\theta}})$ controller and in a second stage, optimize the β value in the $\hat{C}_r(\hat{s}, \hat{\boldsymbol{\theta}})$ controller for set-point tracking.

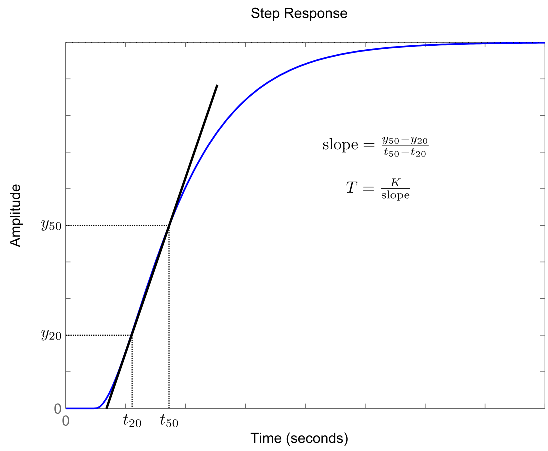

Figure 3. Procedure to find the approximation of the constant time of the process.

Defining $y_d(t, \hat{\boldsymbol{\theta}})$ as the closed-loop system response in the time domain given a step change in $d_i(t)$ and $r(t) = 0$ for a given set of parameters $\hat{\boldsymbol{\theta}}$ and M_S^t as the desired maximum sensitivity of the closed-loop system, the optimization problem can be defined as:

$$\min_{\hat{\boldsymbol{\theta}}} J_{ed}(\hat{\boldsymbol{\theta}}) = \int_0^\infty \left| -y_d(t, \hat{\boldsymbol{\theta}}) \right| \mathrm{d}t, \tag{14}$$
$$\text{subject to} \left| M_S^t - M_S(\hat{\boldsymbol{\theta}}) \right| = 0.$$

Once the problem in (15) is solved, the $\hat{C}_r(\hat{s}, \hat{\boldsymbol{\theta}})$ is optimized by solving:

$$\min_{\beta} J_{er}(\hat{\boldsymbol{\theta}}) = \int_0^\infty \left| r(t) - y_r(t, \hat{\boldsymbol{\theta}}) \right| \mathrm{d}t, \tag{15}$$

where $y_r(t, \hat{\boldsymbol{\theta}})$ is the closed-loop system response to a step change in the reference signal while maintaining $d_i(t) = 0$. Problems (15) and (15) are solved for normalized anisochronic models with parameters varying as follows: $0.1 \leq \tau_0 \leq 2.0$ and $0 \leq \phi_0 \leq 2e^{-1}$. The values of ϕ_0 comprises cases with over-damped and underdamped dynamics. The considered sensitivity values where $M_S^t = 1.4$ to $M_S^t = 2.0$ in steps of 0.1. The optimal parameters are computed and stored in a data base. Then, the user is able to interpolate the PID controller tuning from this data base, given the anisochronic model parameters.

3. RESULTS AND DISCUSSIONS

In order to test the anisochronic identification and optimal PID tuning, two representative chemical processes were considered.

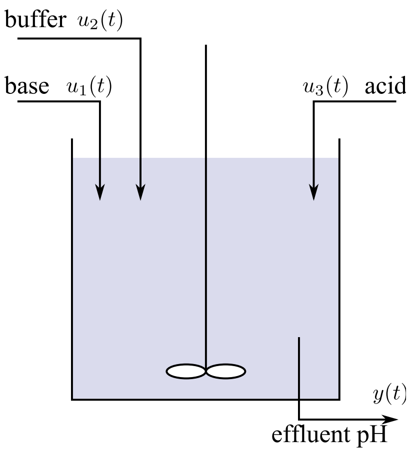

Figure 4. pH neutralization process.

3.1 Identification of the pH Neutralization Process

The first one is a pH neutralization process shown in Fig. 4. The system have three inputs: $u_1(t)$ is a base (NaOH) stream (which is considered to be a disturbance), $u_2(t)$ is a constant buffer stream ($NaHCO_3$) and $u_3(t)$ is the acid stream (HNO_3). The output $y(t)$ is the measured effluent pH. The non-linear model used for simulation is given by:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})u_1 + \mathbf{p}(\mathbf{x})u_2, \tag{16}$$

$$h(\mathbf{x}, y) = 0, \tag{17}$$

with $\mathbf{x} = [x_1, x_2]^T$ and:

$$\mathbf{f}(\mathbf{x}) = \left[\frac{u_3}{V}(W_{a3} - x_1), \frac{u_3}{V}(W_{b3} - x_2)\right]^T,$$

$$\mathbf{g}(\mathbf{x}) = \left[\frac{1}{V}(W_{a1} - x_1), \frac{1}{V}(W_{b1} - x_2)\right]^T,$$

$$\mathbf{g}(\mathbf{x}) = \left[\frac{1}{V}(W_{a2} - x_1), \frac{1}{V}(W_{b2} - x_2)\right]^T,$$

$$h(\mathbf{x}, y) = x_1 + 10^{y-14} - 10^{-y} + x_2 \frac{1 + 2 \times 10^{y-pK_2}}{1 + 10^{pK_1 - y} + 10^{y - pK_2}},$$

where V is the volume of the tank, pK_1 and pK_2 are the first and second disassociation constant of the weak acid H_2CO_3 and W_{a1}, W_{a2}, W_{a3}, W_{b1}, W_{b2}, W_{b3} are the reaction invariants. The details on the model and the parameters values can be found in Gomez et al. (2004) and references therein. As it is known, a pH neutralization process has highly non-linear dynamics. Using the proposed identification procedure shown in Section 2.2, it was possible to find an anisochronic model that fits the dynamics of the pH neutralization process within a certain range.

The identification was computed for the case in which the input (the acid stream) is changed 5%, 20% and 30% from its operating point. The integral of the absolute value of the error quantify how good is the response of the model in comparison with the plant. In Fig. 5, the identification of the anisochronic plant for positive changes in the acid stream are presented. As it can be seen, for changes up to 20%, the identification procedure is able to find suitable model parameters for this particular plant. However, the non-linearity of the plant affects the identification during the transient. However, the identification procedure is able to accurately model the time constant of the plant.

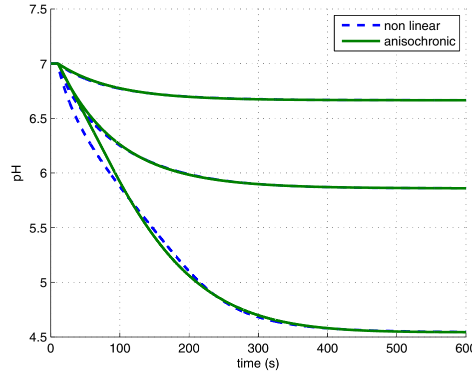

Figure 5. Different identification results for the pH neutralization process.

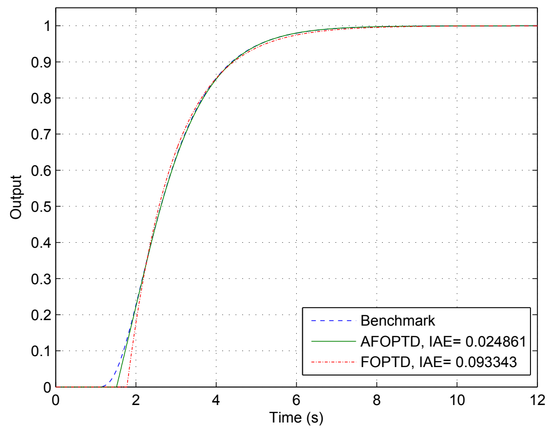

Figure 6. Comparison of the identification for a benchmark process.

However, given the non-linearity of the plant, a linear PID controller would not be attempt to be found since it is already known that, to control this plant, more advanced controllers have to be implemented Benny et al. (2013).

3.2 Identification and Control of a Benchmark Process

In order to test the capabilities of the proposed control procedure, a benchmark process presented in Åström and Hägglund (2000) is used for comparison. It is a fourth order plant given by:

$$P(s) = \frac{1}{\prod_{n=0}^{3}(0.5^n s + 1)}. \tag{18}$$

An optimal First Order Plus Time Delay (FOPTD) plant model was also identified using an optimization procedure. It was found that the procedure using the AFOPTD model gives a better approximation in the IAE (Integral Absolute Error) sense, as can be seen in Fig 6, where the proposed AFOPTD identification procedure gives a result that is almost four times lower compared with the FOPTD.

With these results, a PID controller was tuned using the tuning procedure of section 2.3. In order to compare the results, another PID controller was tuned solving the same optimization problem (15) and (15), but with the FOPTD model. In both cases, the desired maximum sensitivity was set as $M_S^t = 1.8$. In Fig. 7, the response of the two PID tunings are tested for the plant given in 18. Both

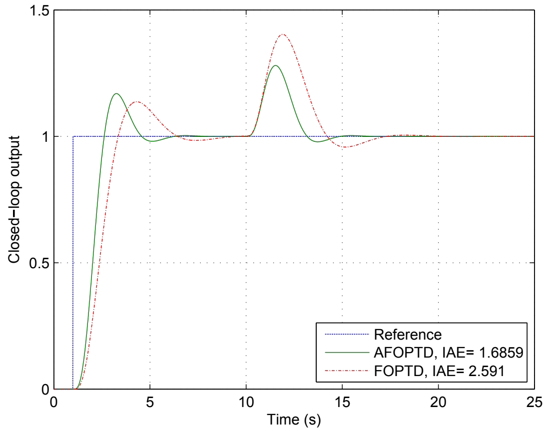

Figure 7. Response of the controlled system using optimal PID controllers.

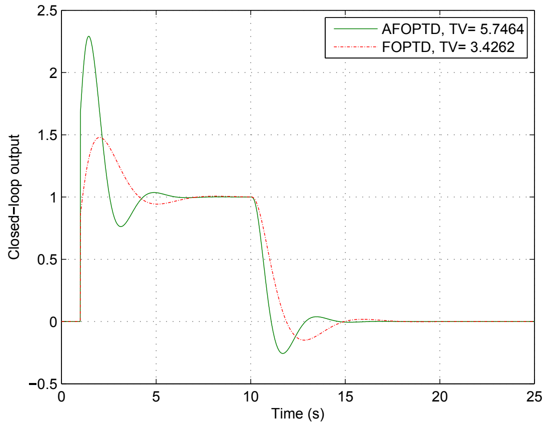

Figure 8. Control effort of the PID controller for the benchmark process.

methods depends heavily in the model obtained during the optimization phase. The PID controller obtained with the AFOPTD model, was able to control the system, for both a change in the reference signal and an input disturbance, with a reduction of almost 35% in the IAE indicator. This improvement have a price of course: since the same controller topology is used for both cases, a better response of the controlled system requires a "stronger" control effort, as can be seen in Fig. 8. If the Total Variation (TV) defined as:

$$TV := \sum_{i=1}^{\infty} (u_i - u_{i-1}), \tag{19}$$

with a sampling time of $t_s = 0.01$ s is considered as a measure of the effort of the controller, the PID controller tuned with the AFOPTD model requires 68% more effort than in the other case. It has to be noticed that, for both controllers, the optimization took into account the robustness constraint. Since the model used for the optimization is different, the $M_S(\boldsymbol{\theta})$ computed is also different, and that is the reason why two optimization procedures with the same controller topology and constraint has different response and control effort signal.

3.3 Identification and Control of a CSTR

Continuous Stirred Tanks Reactors (CSTR) are one of the most common sub-system in the chemical process field.

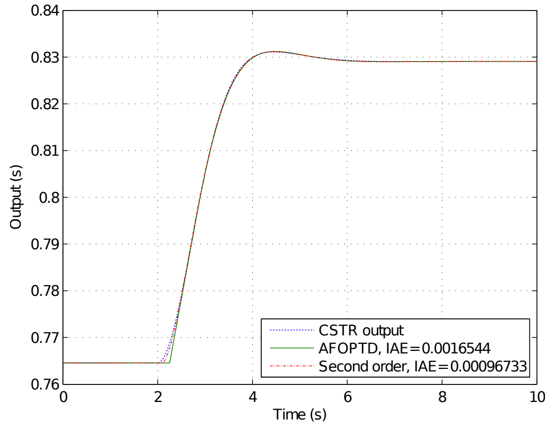

Figure 9. Identification results for the CSTR process.

Depending on the reaction, the dynamic of this plant can be highly non-linear, however, it is common to operate them in a given operational point with the controllers tuned for disturbances rejection. In order to shown the effectiveness of the AFOPTD model and associated PID tuning procedure, a CSTR model is identified and controlled.
Consider the CSTR non-linear model given by Chang (2013) and references therein:

$$\dot{x}_1 = -x_1 + D_a(1 - x_1)e^{\frac{x_2}{1+x_2/\varphi}}, \tag{20}$$

$$\dot{x}_2 = -(1 + \delta)x_2 + BD_a(1 - x_1)e^{\frac{x_2}{1+x_2/\varphi}} + \delta u, \tag{21}$$

$$y = x_1, \tag{22}$$

where x_1 and x_2 represents dimensionless reactant concentration and reactor temperature, u is the dimensionless cooling jacket temperature which is considered as the control input, y is the output of the system, D_a is the Damköhler number, φ is the activated energy, B is the heat of the reaction and δ is the heat transfer coefficient. The value of the parameters The system is considered to be controlled from the equilibrium point $x_1 = 0.765$ and $x_2 = 4.705$.
A step change in u is applied to the system for identification purposes. Using the same data set, an AFOPTD model and a second order underdamped plus time delay (SOUPTD) model are computed for comparison. The results are as given in Fig. 9. A FOPTD model can't fit the response of the model, because, as it can be seen, the response is underdamped. However, it is clear that the AFOPTD is able to find a suitable model for the process. to surpass the identification results of the AFOPTD, it is necessary to identify a second order model, thus increasing the complexity of the model (two states instead of one state in the case of the AFOPTD).
As in the case of the Benchmark model, a PID controller is tuned using the AFOPTD model using the procedure presented in Section 2.3. In Fig. 10, the response of the controlled system to a step disturbance at the input and a change if 5% in the setpoint, is compared for the AFOPTD, SOUPTD and FOPTD models. In all cases, the controller parameters were found by solving an optimization problem using the respective model as if it were the real process dynamics and constraining the resulting closed-loop to have a $M_S^t = 1.8$. The controller tuned using the AFOPTD have an 66.58% lower IAE than the controller tuned using the FOPTD. The controller that

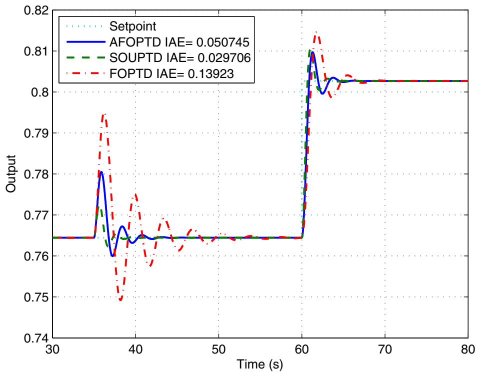

Figure 10. CSTR controlled output for three different PID tuning.

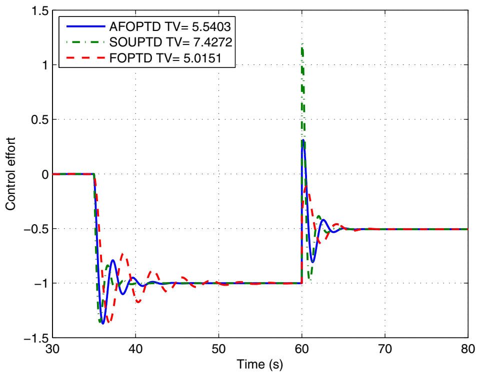

Figure 11. Control effort of three different PID tuning for the CSTR process.

was tuned based on the more complex SOUPTD model gives an IAE that is 41.46% lower than the AFOPTD controller. This result was expected since the SOUPTD model is a better approximation to the plant. Of course the TV of this controller is higher (34.06%) than in the AFOPTD controller, but a special mention has to be given to the FOPTD controller: it has a poor performance compared with the AFOPTD controller but almost the same TV (9.5% in difference).

With this example it was shown that using an AFOPTD, it is possible to model underdamped responses using the same first order model. The controlled response is acceptable, improved only by using a more complex model. It is clear then, that AFOPTD can be successfully applied to model chemical processes within a range and that this model can then be used to optimally tune a PID controller.

4. CONCLUSIONS

In this work, a procedure for optimal identification and optimal tuning of PID controllers for chemical processes was proposed, using the anisochronic framework. It was shown that this model is able to represent both over-damped and underdamped processes using the same structure.

The methodology was successfully applied to two important chemical processes: a pH neutralization plant and a non-isothermal CSTR. Also, the identification was tested in a benchmark system process.

It was found that the AFOPTD based controller gives a better response than a controller, also optimally tuned, but based on a FOPTD model. Only if the model complexity is increased to a SOUPTD model, the obtained controller gives a better performance than AFOPTD. The results shown the suitability of this modeling framework to be applied in chemical processes.

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