

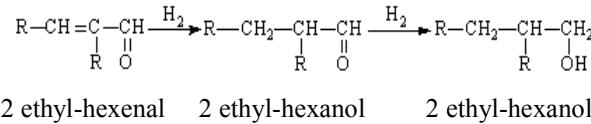
Fractional Order Control for the Temperature Loop in a Chemical Reactor

Cristina I. Muresan, Roxana Both, Clara M. Ionescu, Eva H. Dulf

Abstract— Fractional order control has been used intensively over the last decade in the control of various plants, being considered to enhance the closed loop performance, especially for time delay processes. In this paper, a fractional order PI controller is designed for the temperature control in a chemical reactor. The closed loop performance is evaluated and compared with a simple PI controller. The design approach taken in the paper is based on time domain specifications, rather than the existing frequency domain methods. The simulations show that the fractional order PI controller achieves better performance than the classical PI controller, both under nominal and uncertain conditions.

I. INTRODUCTION

Hydrogenation of 2-ethyl-hexenal is an important step for the industrial synthesis of 2-ethyl-hexanol. The reaction occurs in a hydrogenation reactor, only in the presence of a catalyst, the reaction pathway being expressed as [1]:



The hydrogenation reaction is highly exothermic so the reactor output temperature may become critical and presents a large time delay. The most widely used control structure for time delay processes is the Smith Predictor. In this paper, the authors propose a closed loop control structure based on the Smith Predictor, with the primary controller being a fractional order PI. The choice for the Smith predictor is based on the prediction properties of the control structure, enabling the tuning of the controller based solely on the process transfer function without the associated time delay. Nevertheless, small modeling errors, regarding the time delay, may lead to an unstable behavior of the closed loop system with Smith Predictor. This problem can be avoided by a proper design of the primary controller [2,3,4]. Very few design methods for fractional order controllers combined with Smith Predictors have been proposed so far [2,3], and only few of them consider the robustness issues associated with time delay variations [2].

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The purpose of this paper is to design and evaluate the performance of a Smith Predictor control structure for the temperature loop in a chemical reactor. The robustness of the designed controller is evaluated considering significant time delay variations.

The paper is structured into four main parts. After an introductory section, the following part – *Chemical Reactor Principle of Operation* – describes the process considered in this paper. The problem tackled in this paper is the control of the temperature in a single-input-single-output approach. Section III presents the controller design, while the results obtained for the temperature control loop, both under nominal and uncertain conditions, are given in section IV, *Simulation results*. The advantages of the proposed method are summarized in the final section of the paper, *Conclusions*.

II. CHEMICAL REACTOR PRINCIPLE OF OPERATION

A process flow diagram of a typical 2-ethyl-hexenal hydrogenation process used in industrial plants is presented in Fig.1.

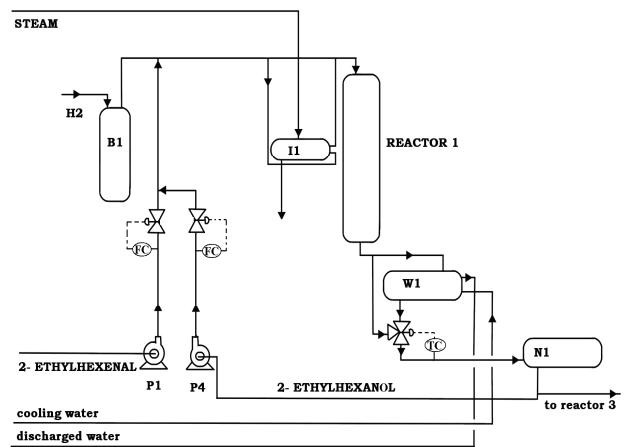


Figure 1. Process flow diagram of a typical 2-ethyl-hexenal hydrogenation process applied in industrial plants

The main feed consists of 2-ethyl-hexenal (liquid) and hydrogen (gas). The reactants are mixed together before they reach the reactor. Another feed is the re-circulated 2-ethyl-hexanol flow. The hydrogenation reaction occurs around 90% in the first third of the reactor. Due to the fact that the hydrogenation reaction is highly exothermic and the 2-ethyl-hexenal concentration in the reaction zone is high the 2-ethyl-hexenal dilution is needed, in order to keep the outlet liquid temperature in a specific range 433K and 453K, depending on the catalyst degree of activity. An increment of the temperature above the critical value will lead to the appearance of secondary products, a decrease of the product

efficiency and also to an increase in the power consumption and production costs. For dilution, a sufficient thermally stable inert is needed. The product itself is chosen for this dilution, namely the re-circulated 2-ethyl-hexanol feed.

Because detailed nonlinear mathematical models are too complex to be used in the design of controllers, an alternative approach is to use a simple model of the process which describes its most important properties. Based on the analysis of the hydrogenation reaction and the plant data acquired, the main connections between the input and output variables were determined. The main input variables of the entire process are: the 2-ethyl-hexenal input flow, the 2-ethyl-hexanol re-circulated flow (Q_{oct}) and the input temperature of the reactants. The main output variables are: the output temperature of the product (T_{out}) and the output concentration of the product. For controlling the output temperature, the manipulated variable is the re-circulated 2-ethyl-hexanol flow rate (Q_{oct}), with the transfer function presented below:

$$T_{out}(s) = \frac{-2.1}{1422s^2 + 65.41s + 1} e^{-27.5s} \cdot Q_{oct}(s)$$

III. FRACTIONAL ORDER PI CONTROLLER

Fractional order calculus has been used intensively to solve control problems [5,6]. Fractional order PIDs (FO-PID) are in fact a generalization of the classical integer order PID controllers, being considered to ensure an increased robustness of the resulting closed loop system [7-11]. The FO-PID controller consists in an integrator of order λ and a differentiator of order μ , yielding a $PI^\lambda D^\mu$ controller. The general approach for designing such fractional order PID controllers consists in a frequency domain specification for gain and phase margins and crossover frequencies [12]. The parameters of the FO-PID controller are then found using different optimization routines [8, 13], which are generally time consuming.

In this paper, the authors use a time domain specification approach [9] unlike the previously mentioned controller design strategies. The method used in this paper has the secondary advantage of being more appealing to the industry engineer since it is based on time domain performance specifications, such as settling time and overshoot, rather than the more abstract notions of phase margin, gain margin and crossover frequencies.

The robustness of the proposed method is evaluated for variations in the time delay of the temperature loop in the chemical reactor. It is expected that the design method tackles intrinsically the problem of robustness to time delay uncertainties, in the framework of Smith Predictor control structure [9].

The general form of fractional order PI controller is given by:

$$C_{FO-PI}(s) = k_p + \frac{k_i}{s^\lambda} \quad (1)$$

with $\lambda \in \Re$ being the fractional order. For $\lambda=1$, the controller in (1) becomes the classical PI controller. For $\lambda \neq 1$, the FO-PI controller design parameters are: k_p , k_i and the fractional order λ .

For the temperature control loop, the Smith Predictor control strategy is used, given in Fig. 2, where the primary controller is in fact the fractional order PI controller from (1).

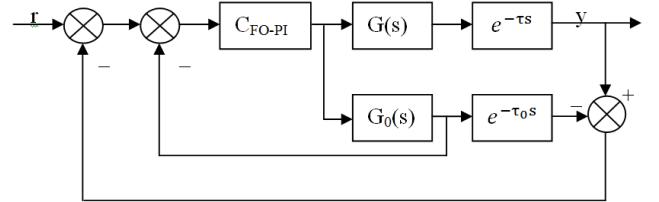


Figure 2. Closed loop control structure with Smith Predictor and fractional order PI

The process transfer function in Fig. 2, corresponding to the input-output relation presented in Section II, is [14]:

$$H(s) = G(s)e^{-st} = \frac{-2.1}{1422s^2 + 65.41s + 1} e^{-27.5s} \quad (2)$$

The model of the process is assumed to be:

$$H_0(s) = G_0(s)e^{-st_0} = \frac{-2.1}{1422s^2 + 65.41s + 1} e^{-27.5s} \quad (3)$$

being equal to the process transfer function in (2), under nominal conditions. The corresponding time delay is 27.5 minutes.

The main problem with Smith predictor structures consists in the possible lack of robustness, especially in terms of time delay variations. In this paper, the authors use a design method for a special class of FO-PI controllers to be used in Smith Predictor structures for time delay compensation, the classical approach for designing FO-PI controllers [8,12] being altered in order to enhance robustness against time delay variations [9].

The closed loop specifications for the temperature loop are: a desired overshoot of less than 10% and a settling time of less than 300 min. The controller design is given in what follows being based on an approximation of the final closed loop system with a second order system. The imposed overshoot $\sigma^* = 10\%$, yields a damping factor of:

$$\xi = \frac{|\ln(\sigma^*)|}{\sqrt{\ln^2(\sigma^*) + \pi^2}} = 0.59 \quad (4)$$

The required phase margin is computed based on the value derived for the damping factor:

$$\varphi_m = \cos^{-1} \frac{1}{2\xi^2 + \sqrt{1+4\xi^4}} = 60^\circ \quad (5)$$

From the imposed settling time $t_s < 300$ min, the natural frequency is computed as:

$$\omega_n = \frac{4}{t_s \xi} = 0.022 \quad (6)$$

The closed loop bandwidth, ω_b , is obtained as [15]:

$$\omega_b = \omega_n \sqrt{1 - 2\xi^2 + \sqrt{2 - 4\xi^2 + 4\xi^4}} = 0.026 \quad (7)$$

Then, the gain crossover frequency is obtained as [15]:

$$\omega_{cg} \equiv \frac{1.6}{\omega_b} = 0.016 \quad (8)$$

For the time delay process in (2), the maximum time delay for which the closed loop system remains stable is given by $\hat{\tau}$ [2]:

$$\hat{\tau} = \frac{\varphi_m}{\omega_{cg}} + \tau_0 = 91 \text{ min} \quad (9)$$

where φ_m is the desired phase margin and ω_{cg} is the desired gain crossover frequency. The imposed φ_m is used to guarantee damping and robustness to changes in time delays, while ω_{cg} guarantees nominal speed of the closed loop response [9]. Thus, with this approach the robust stability of the closed loop system is ensured for a maximum value of the time delay of 91 min.

The robust stability condition in (9) can be written as [9]:

$$G_0(j\omega_{cg}) C_{FO-PI}(j\omega_{cg}) = -e^{(\varphi_m + \tau_0 \omega_{cg})} \quad (10)$$

Using (1) and (10), yields:

$$k_p + \frac{k_i}{(j\omega_{cg})^\lambda} = -\frac{e^{(\varphi_m + \tau_0 \omega_{cg})}}{G_0(j\omega_{cg})} \quad (11)$$

The parameters of the FO-PI controller can be obtained as follows:

$$k_p = -\Re(X_{sp}(j\omega_{cg})) - \cot\left(\frac{\pi}{2}\lambda\right) \Im(X_{sp}(j\omega_{cg})) \quad (12)$$

$$k_i = \frac{\omega_{cg}^\lambda}{\sin\left(\frac{\pi}{2}\lambda\right)} \Im(X_{sp}(j\omega_{cg})) \quad (13)$$

where $X_{sp}(j\omega_{cg}) = -\frac{e^{(\varphi_m + \tau_0 \omega_{cg})}}{G_0(j\omega_{cg})}$ and

$$(j\omega_{cg})^{-\lambda} = (\omega_{cg})^{-\lambda} \left(\cos \frac{\pi\lambda}{2} - j \sin \frac{\pi\lambda}{2} \right).$$

The fractional order λ in (2) was chosen according to the following algorithm:

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for λ = 0:0.1:2;
    compute k_p using (12), k_i using (13)
    compute (2)
    compute the corresponding gain margin g_m
end
select max(g_m)
select λ corresponding cu max(g_m)

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The algorithm is based on an iterative procedure. The controller parameters are computed for different values of the fractional order λ . Then, based on the computed values, for each λ , the corresponding gain margin of the open loop system is computed. From the entire set of gain margins, the maximum value is determined and the corresponding value of the fractional order λ . The algorithm runs until the results considering all possible values of the fractional order λ are evaluated.

Fig. 3 shows the result of the algorithm. The maximum value of the gain margin was obtained for $\lambda=1.4$. The corresponding parameters of the FO-PI controller were determined using (12) and (13) to be:

$$k_p = -0.3947 \quad (14)$$

$$k_i = 7.97 \cdot 10^{-4} \quad (15)$$

Using the same performance specifications, but for a classical PI controller, with $\lambda=1$, the controller parameters are obtained based on equation (12) and (13) as:

$$k_p = -0.5643 \quad (16)$$

$$k_i = 0.0033 \quad (17)$$

Fig. 3 presents the absolute values of the gain margin computed for different values of the fractional order parameter λ ranging from 0 to 2. The results in Fig. 3 show that the maximum gain margin is achieved with $\lambda=1.4$, being more than twice larger than the gain margin achieved with the traditional integer order controller ($\lambda=1$). Thus, the FO-PI controller is expected to achieve better results in uncertain closed loop simulations.

IV. SIMULATION RESULTS

To demonstrate the effectiveness of using a FO-PI controller for the temperature control loop in the chemical reactor, instead of the classical integer order PI controller, the following case studies were considered: a nominal case scenario, in which the temperature setpoint is incremented 3.5 degrees from its stationary point and some uncertain case studies in which the temperature setpoint is incremented 3.5

degrees from its stationary point, but the time delay associated varies in the range of approximately [-50%, +50%].

Fig. 4 shows the simulation results obtained under nominal conditions. The temperature reaches its new setpoint within less than 300 minutes and with a corresponding overshoot of less than 10% as specified in the performance requirements. The two controllers designed achieve similar performance considering these nominal conditions, with the time delay of 27.5 minutes.

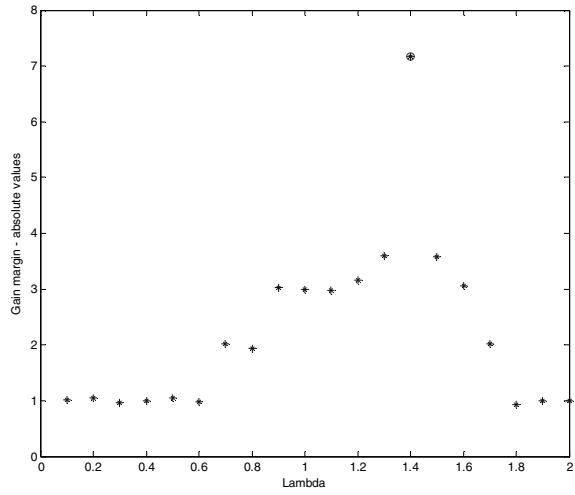


Figure 3. Gain margin in absolute value as a function of the fractional order parameter λ

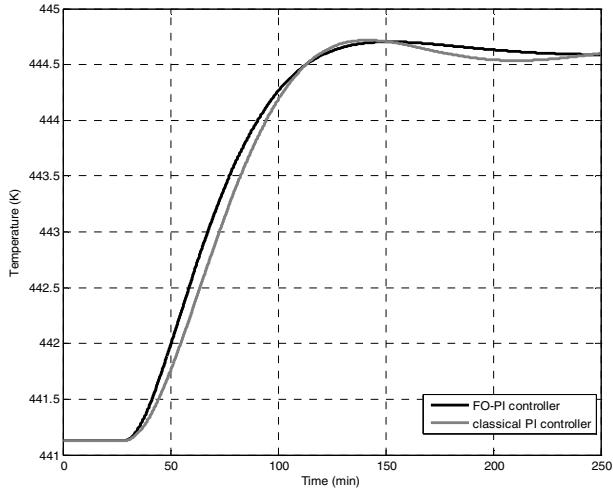


Figure 4. Temperature evolution under nominal conditions using FO-PI controller and classical integer order controller

Fig. 5 and 6 present the temperature evolution and the re-circulated 2-ethyl-hexanol flow considering significant variations of the time delay. The closed loop simulations are performed using the fractional order PI controller. Fig. 6 shows that the temperature reaches its new prescribed setpoint within less than 300 minutes, while the maximum overshoot is 8.5%, still below the imposed design specifications.

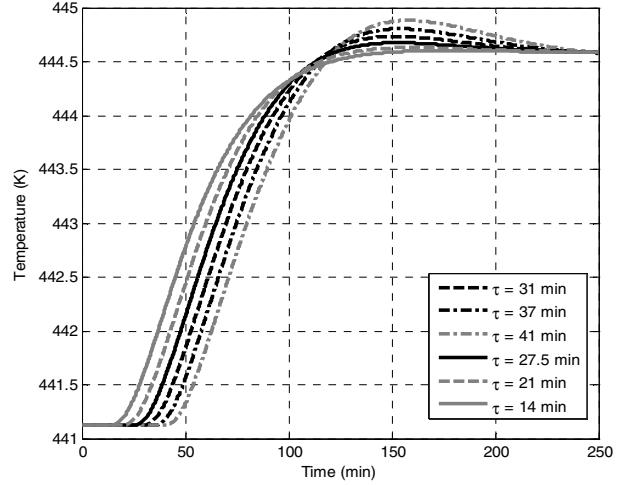


Figure 5. Temperature evolution considering time delay variations using FO-PI controller

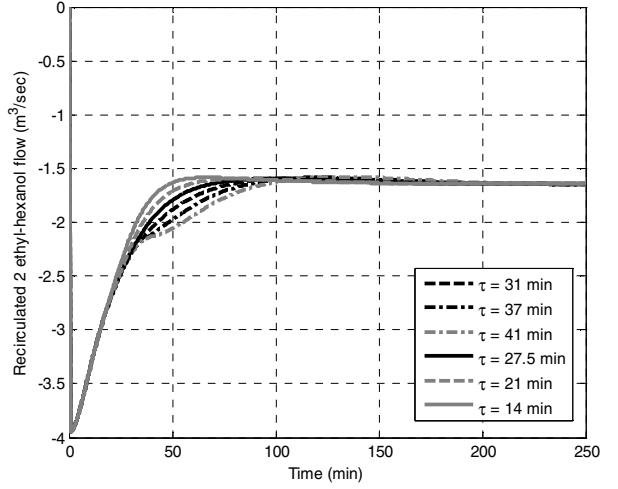


Figure 6. Re-circulated 2-ethyl-hexanol flow considering time delay variations using FO-PI controller

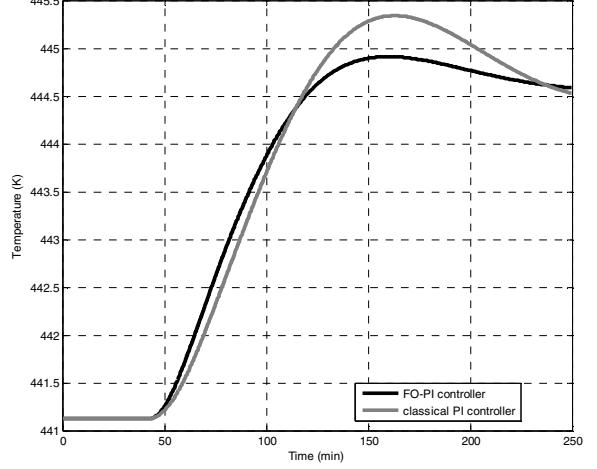


Figure 7. Temperature evolution considering +50% variation of the time delay using FO-PI controller and classical integer order controller

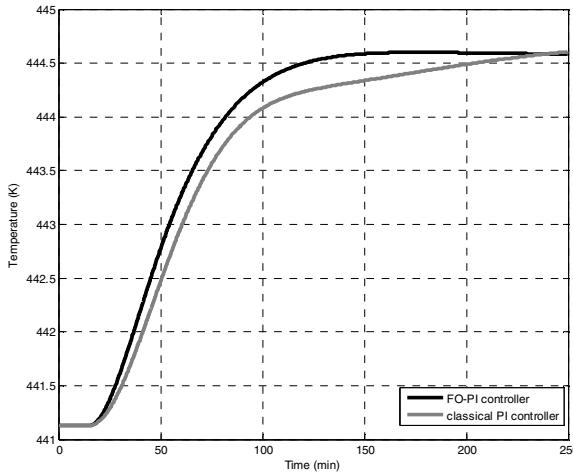


Figure 8. Temperature evolution considering -50% variation of the time delay using FO-PI controller and classical integer order controller

To compare the robustness of the two controllers designed, Fig. 7 presents the temperature evolution, considering a +50% variation of the time delay, while Fig. 8 presents the temperature evolution considering a -50% variation of the time delay, both using a fractional order and an integer order PI controller.

Fig. 7 and 8 show that the FO-PI controller achieves better closed loop performance compared to a classical integer order controller, with a reduced settling time (Fig. 8) and a reduced overshoot (Fig. 7).

V. CONCLUSION

The method implemented in this paper is designed specifically for time delay robustness, in the framework of Smith Predictor closed loop schemes. The choice for the fractional order parameter is based on a maximization of the open loop gain margin, done in an iterative procedure to avoid the complicated and time consuming optimization routines. An important advantage is that the control algorithm is based on a time domain approach, with performance specifications in terms of closed loop overshoot and settling time, rather than frequency domain specifications, which are generally used in fractional order controller tuning.

Under nominal conditions, the designed fractional order controller offers similar results as the classical integer order controller, however the robustness of the fractional order controller to time delay changes is higher than that of the classical PI controller, as shown when considering +50% and -50% variations of the time delay.

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