Fractional order PID optimal control in pH neutralization process

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Abstract. This paper proposed a fractional order PID (FOPID) optimal control scheme for pH neutralization process which is modeled as a discrete state equation with disturbance. In order to enhance the stability of the outlet-pH as well as minimize the consumption of chemicals, the design of the fractional order PID controller is transformed into a discrete nonconvex optimization problem and solved by the state transition algorithm. Furthermore, a comparative study of the fractional order PID controller with PID controller is carried out, and considering the practical application, the disturbances caused by inlet-flow-rate and inlet-pH are also taken into account to evaluate the performance of the proposed optimal control scheme. The simulation results demonstrate the superior performance of the proposed strategy.

1. Introduction
The control of pH neutralization process plays a vital role in the chemical and biotechnological engineering processes [1]. Particularly, in wastewater treatment plants, the pH of wastewater must be adjusted and maintained within a stringent range before subsequent biochemical treatment and discharge. However, the control of pH is difficult and often leads to a lot of waste of the chemicals, due to its inherent nonlinearity, high sensitivity near the neutral point and time-varying properties [2]. Therefore, it is important to adopt an optimal control strategy to adjust the pH of wastewater accurately while the least amount of chemicals is consumed.

In theory, the main goal of pH neutralization process is to control the pH of the effluent by manipulating the flow-rate of titrating stream [3]. Hence, in term of practicality, the PID controller is undoubtedly one of the most commonly used control methods [4-5]. In reference [6], the PID controller is used to control dissolved oxygen in the bio-fermenter, but a more accurate model of the dissolved oxygen control process should be required through open-loop experimental data. And many optimal tuning methods have also been developed to design PID controller parameters [7-8]. Yet the PID controller cannot provide effective control for highly nonlinear and time-varying systems with uncertain behavior [9]. In order to improve the dynamic performance and robustness of the PID control system,
Podlubny proposed a novel fractional order PID controller [10]. Because of the additional two parameters $\lambda$ (integral order) and $\mu$ (differential order), fractional order PID controllers are widely applied to engineering practical problems. For example, the fractional order PID controller based on particle swarm optimization algorithm is applied to an automatic voltage regular, the results show that it has higher performance improvement than the PID controller [11]. It is also designed for spherical tank liquid level control based on First Order Plus Dead Time (FOPDT) system [12]. In view of the superior applications of $PI^\lambda D^\mu$-type controller above, we decided to expand it during the pH neutralization process in order to achieve a breakthrough in the control performance. Nevertheless, compared to PID controllers, how to determine the five parameters of the fractional order PID controller remains a challenging problem [13-14].

A discrete fractional order PID controller designed by state transition algorithm (STA) has been applied in this paper. STA treats the solution to a given optimization problem as a state and the optimization solution process as a state transition process [15], which shows a strong global search ability to select the continuous $PI^\lambda D^\mu$ controller parameters [16]. It is also applied to solve the optimal problem in zinc electrowinning process [17]. For instance, taking the computational complexity into account, STA with a fast rotation transformation operator is proposed in reference [18].

In this work, a fractional order PID optimal control scheme for the pH neutralization process is proposed. In order to evaluate the advancement of the scheme, the performance difference between the fractional order PID and the classical PID controller was compared under the same conditions. Considering the dynamic fluctuations in practical applications, the performance of the controller under various disturbance conditions is studied. The simulation results proved the superiority of the proposed optimization scheme.
2. pH neutralization process model

According to our best knowledge, most current studies of the pH neutralization process assume that it occurs in a bench-scale continuous stirred reactor (CSTR), and the pH of the effluent is determined by controlling the flow-rates of the acid, base and buffer streams [19]. However, in the practical application of sewage treatment, the stability of pH control at the drainage outlet is easily and seriously affected due to the disturbances of pH, flow rate, temperature and impurity content of the inlet wastewater. Consequently, in order to meet the actual needs, a better control strategy include modeling, control and optimization is supposed to be applied to the pH neutralization process.

![Figure 1. A pH neutralization process.](image)

By the previous analysis, the schematic diagram of pH neutralization process is shown in figure 1. The reactants in this process include an acid (HNO₃) stream, a buffer (NaHNO₃) stream, a base (NaOH) stream and an effluent stream, whose flow-rates are \( q_1, q_2, q_3, q_4 \) respectively. Assuming that the first three streams are thoroughly mixed in the reactor, in which the objective is to control the pH of effluent stream by manipulating the base flow rate \( q_3 \), and define the concentrations of reaction invariants \( W_{a_i} \) and \( W_{b_i} \) for each stream \( (i = 1, 2, 3, 4) \). The dynamic model of state space form and the nonlinear equation to determine the pH value are as follows [20]:

\[
\dot{x} = A_1 x_0 + A_2 x + f(x,u) + g(x,d) = \varphi(x,u,d); \quad z(x,y) = 0
\]

where \( x, x_0, u, d, y \) represent the state variables, initial state, disturbance variable, manipulated variable and outlet-pH respectively, and model parameters \( pK_1 = -\log_{10} K_{a_1}, \quad pK_2 = -\log_{10} K_{a_2}, \quad K_{a_1} \) and \( K_{a_2} \) are equilibrium constants respectively.

\[
x = [W_{a_1}, W_{b_1}]^T, \quad x_0 = [W_{a_2}, W_{b_2}]^T, \quad d = q_2, \quad u = q_3
\]

\[
A_1 = \begin{bmatrix} \frac{q_1}{V} & 0 \\ 0 & \frac{q_1}{V} \end{bmatrix}, \quad A_2 = \begin{bmatrix} -\frac{q_1}{V} & 0 \\ 0 & -\frac{q_1}{V} \end{bmatrix}, \quad f(x,u) = \begin{bmatrix} \frac{u}{V} (W_{a_2} - x_1) \\ \frac{u}{V} (W_{b_2} - x_2) \end{bmatrix}, \quad g(x,d) = \begin{bmatrix} \frac{d}{V} (W_{a_2} - x_1) \\ \frac{d}{V} (W_{b_2} - x_2) \end{bmatrix}
\]
\[
z(x, y) = x_1 + 10^{y+14} + x_2 \frac{1 + 2 \times 10^{y-p_{K_d}}}{1 + 10^{p_{K_d}-y} + 10^{y-p_{K_d}}} - 10^y
\]

Then, we can get the discrete-time equation of equation (1) by the backward-Euler method:

\[
x_k = A_x h x_{0,k-1} + (A_z h + 1)x_{k-1} + h f(x_{k-1}, u_{k-1}) + h g(x_{k-1}, d_{k-1}) := \varphi(x_{k-1}, u_{k-1}, d_{k-1}) \quad (2)
\]

where \( k \) is the sampling time, \( h \) is the step size.

3. **Structures of fractional order PID controllers**

We discuss the structure of fractional order PID controller in this section. The fractional order PID is a controller with five adjustable parameters whose transfer function can be expressed as follows [10]:

\[
G(s) = k_p + \frac{k_i}{s^\alpha} + k_d s^\mu
\]

(3)

where \( k_p, k_i, k_d, \lambda, \mu \) are five adjustable parameters, represent the proportional gain, integral gain, differential gain, integral order and differential orders respectively.

It is not difficult to find that a classical integer-order PID controller can be obtained when the two additional parameters \( \lambda=1, \mu=1 \):

\[
G(s) = k_p + \frac{k_i}{s} + k_d s
\]

(4)

At the same time, in order to design a discrete form \( PI^\lambda D^\mu \) controller that meets the requirements of industrial applications, it is necessary to introduce some basic principles of fractional calculus.

3.1. **Fractional order calculus**

Consider a differential equation \( y(t) = D^\alpha u(t) + u(t) \) with fractional order \( \alpha \), in order to describe the fractional calculus, we stated the two most widely used Riemann-Liouville and Grünwald-Letnikov definitions.

(1) Riemann-Liouville definition (RL)

\[
D^\alpha f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} f(\tau) d\tau
\]

(5)

Where \( t > 0, n \) is an integer which satisfies the condition \( n-1 < \alpha < n \), and \( \Gamma(\cdot) \) is the renowned Euler’s gamma function.

(2) Grünwald-Letnikov definition (GL)

\[
D^\alpha f(t)_{\tau=h} = \lim_{h \to 0} \tau^{-\alpha} \sum_{j=0}^k (-1)^j \binom{\alpha}{j} f(t - j\tau)
\]

(6)

where \( \binom{\alpha}{j} \) represents binomial coefficient.

Since the approximate form of GL definition below is of great beneficial to obtain the numerical solutions [21].
\[ D^\alpha f(t) = \tau^{-\alpha} \sum_{j=0}^{N(t)} w^\alpha_j f(t - j\tau) \]  

(7)

where \( a \) and \( t \) are the limits of the operator, \( N(t) = \frac{t - a}{\tau} \), \( w^\alpha_j \) is the binomial coefficient, and \( w^\alpha_0 = 1 \), \( w^\alpha_j = (1 - \frac{1+\alpha}{j})w^\alpha_{j-1}, j = 1,2,..., \), and this method is used to define the following discrete fractional order PID controller.

3.2. Discrete-time Fractional order PID controller

Considering the continuous time domain equation of fractional order PID controller which is developed on the basis of fractional order calculus:

\[ u(t) = k_p e(t) + k_i \int e(t) dt + k_d \frac{de(t)}{dt} \]  

(8)

Where GL definition is used to approximate the D operator, the discrete-time form can be described as:

\[ u(k) = K_p e(k) + K_i \sum_{j=0}^{k} w\alpha_j e(k - j) + K_d \sum_{j=0}^{k} w\alpha_j^\mu e(k - j) \]  

(9)

where \( K_p = k_p \), \( K_i = k_i(\frac{1}{T})^\lambda \), \( K_d = k_d(\frac{1}{T})^\mu \), \( T \) is the sampling interval.

Then an incremental form of fractional-order PID is obtained as follows:

\[ u(k) = u(k-1) + \Delta u(k) \]  

(10)

\[ u(k-1) = K_p e(k-1) + K_i \sum_{j=0}^{k-1} w\alpha_j e(k-1 - j) + K_d \sum_{j=0}^{k-1} w\alpha_j^\mu e(k-1 - j) \]

\[ \Rightarrow \Delta u(k) = u(k) - u(k-1) = K_p \Delta e(k) + K_i \sum_{j=1}^{k} w\alpha_j e(k - j) + K_d \sum_{j=1}^{k} w\alpha_j^\mu e(k - j) \]  

(11)

where \( \tilde{K}_i = K_i + K_d \), \( \tilde{K}_d = -(K_i \frac{1+\lambda}{j} w\alpha_{j-1} + K_d \frac{1-\mu}{j} w\alpha_j^\mu) \).

4. Optimization problem formulation and optimization of pH neutralization process

In practical applications, the pH of the wastewater is controlled by the addition of base or acid, which we called them chemicals. Due to the inherent characteristic of the pH neutralization process, it’s not an easy task to properly add the chemicals. Therefore, this process is designed as an optimization problem to be solved with the aim of keeping the outlet pH within the required range while minimizing chemical consumption. The framework of the fractional order PID optimal control strategy is as shown in the following figure 2.
4.1. Optimal problem formulation of pH neutralization process

4.1.1. Objective function. Based on the reference [16], it is shown that the ITAE criterion has superior performance in the optimization of continuous fractional order PID controller parameters. Therefore, the objective function to be optimized is designed as follows:

$$\min J = \int_0^T [w_1 |e(t)| + w_2 u(t)] \, dt$$

and the discrete form is:

$$\min J = \sum_{k=0}^{N} [w_1 |e(k)| + w_2 u(k)]$$

where \(w_1, w_2\) are the weighting factors, \(N\) is the sample size.

4.1.2. Terminal constraint. In this paper we assume that the outlet-pH \(y\) is equal to the set-point \(y_{sp}\) and the manipulated variables are bounded as: \(u_{min} \leq u(t) \leq u_{max}\).

Therefore, combining equation (2) and equation (10), the fractional order PID optimal control in pH neutralization process is to find the optimal values of these five parameters of the fractional order PID controller through the discrete-time state equation of the pH neutralization process, so that the objective function \(J\) is minimized and the constraints are all satisfied.

Since the above optimization problem is a non-convex optimization problem, STA is selected because of its strong global optimization ability [22]. At the same time, considering the complexity of the pH neutralization process dynamic model, STA with fast rotation transformation operator is introduced [18], which has better computing power.

4.2. Optimization method of pH neutralization
4.2.1. Continuous state transition algorithm (STA). STA is a stochastic optimal method that considers the solution as a state, and the transformation of a solution is a state transition process. Generally, the uniform form based on state space representation is defined as follows:

\[
\begin{align*}
    x_{k+1} &= A_k x_k + B_k u_k \\
    y_{k+1} &= f(x_{k+1})
\end{align*}
\]

(14)

where \( x_k \in R^n \) is a state, which corresponds to a solution of the optimization problem, \( A_k \) and \( B_k \) are state transition matrices with suitable dimensions, \( u_k \) is a function of \( x_k \) and \( f \) is considered as the objective function.

Then the following four special operators are used to generate candidate solution. Particularly, a fast rotation transformation operator is introduced to reduce computational complexity [18].

(1) Fast Rotation Transformation (RT)

\[
x_{k+1} = x_k + \alpha \bar{R}_r \frac{u}{\|u\|_2}
\]

(15)

where \( \alpha \) is a rotation factor, also a positive constant, \( \bar{R}_r \in R \) is a random variable, the elements are uniformly distributed within [-1, 1], \( u \in R \) is a vector of which elements are also uniformly distributed within [-1.1], \( \| \cdot \|_2 \) is a 2-norm of the vector. The computational complexity of the fast rotation operator is much lower than the old one because the new random variable \( \bar{R}_r \) is a scalar rather than a matrix.

(2) Translation Transformation (TT)

\[
x_{k+1} = x_k + \beta R_t \frac{x_k - x_{k-1}}{\|x_k - x_{k-1}\|}
\]

(16)

where \( \beta \) is a translation factor, also a positive constant, \( R_t \in R \) is a random variable, the elements are uniformly distributed within [0, 1].

(3) Expansion Transformation (ET)

\[
x_{k+1} = x_k + \gamma \bar{R_e} x_k
\]

(17)

where \( \gamma \) is an expansion factor, also a positive constant, \( \bar{R_e} \in R^{n \times n} \) is a random diagonal matrix, the elements follow the Gaussian distribution.

(4) Axesion Transformation (AT)

\[
x_{k+1} = x_k + \delta \bar{R_a} x_k
\]

(18)

where \( \delta \) is an axesion factor, also a positive constant, \( \bar{R_a} \in R^{n \times n} \) is a random diagonal matrix with only one random position for nonzero value, the elements of which follow the Gaussian distribution.

Now, the steps to solve the optimization problem through STA can be described as follows:

Step 1: Randomly generate an initial solution \( \text{Best}_k = \text{Best} \) and set the algorithm parameter \( \alpha = \alpha_{\text{max}} = 1, \quad \alpha_{\text{min}} = 1 e^{-4}, \quad \beta = 1, \quad \gamma = 1, \quad \delta = 1, \quad f_c = 2, \quad k = 0, \)

Step 2: Based on the current best solution \( \text{Best}_k \), use the expansion transformation operation to generate SE samples, and update the current best solution with the update strategy. If the current best
solution has changes, perform the translation transformation operation and update the current best solution $\text{Best}_k$ with the same method. Then, use the remaining three operators to perform the transformation operation.

Step 3: Set $k = k + 1$, if $\alpha < \alpha_{\text{min}}$, $\alpha = \alpha_{\text{max}}$, otherwise $\alpha = \alpha / f_c$, then return to step 2 and repeat until the termination condition is satisfied.

5. Simulation and results

In this section, both the PID and fractional order PID controllers are applied to the proposed optimal control scheme based on the state model of pH neutralization process. Some simulation results of the proposed optimal control scheme are presented in this section.

5.1. Comparative study of PID and fractional order PID

Based on the nominal plant parameters in table 1, the PID and fractional order FPI controllers are applied to the simulation of the process to bring the outlet-pH to a set-point and minimize chemicals consumption. The response of the closed-loop system under the two controllers is shown in figure 3. Both controllers allow the system to reach the set-point, but it is clear that the fractional order PID controller can make the system more responsive. Table 2 shows the simulation results of controller parameter values and other parameters obtained by the STA with fast rotation operator, and sampling time $t_s=0.1$. In addition, figure 4 shows the chemical consumption within 2 hours under the nominal plant parameters and two different control strategies. As can be seen from the figure 4, the control strategy proposed in this paper has a significant contribution to reducing chemicals consumption.
Figure 4. The chemicals consumption within 2 hours under three different conditions.

Table 1. The nominal parameters of the pH neutralization reactor.

| Variable | Value       |
|----------|-------------|
| $P_{k_1}$ | 6.35        |
| $P_{k_2}$ | 10.25       |
| $W_{a_1}$ | $3 \times 10^{-3} \text{mol}$ |
| $W_{a_2}$ | -0.03 \text{mol} |
| $W_{a_3}$ | $-3.05 \times 10^{-3} \text{mol}$ |
| $W_{b_1}$ | 0.0 \text{mol} |
| $W_{b_2}$ | 0.03 \text{mol} |
| $W_{b_3}$ | $5 \times 10^{-5} \text{mol}$ |
| $q_1$    | 16.6 ml/s   |
| $q_1(d)$ | 0.55 ml/s   |
| $q_1(u)$ | 15.8 ml/s   |
| $y_{sp}$ | 7           |
| $V$      | 2900 ml     |

Table 2. Optimal tuning results for controllers.

| Controller | $k_p$   | $k_i$   | $k_d$   | $\lambda$ | $\mu$ | Steady-state errors |
|------------|---------|---------|---------|-----------|-------|---------------------|
| PID        | 812.5526| 133.5016| 68.4643 | -         | -     | 3.36e-4             |
| FOPID      | 986.5877| 739.3450| 551.0219| 0.9991    | 0.0467| 6.13e-4             |

5.2 Disturbance rejection

In this paper, the CSTR model proposed by Heson in 1994 is used, but in industrial processes, there are disturbances such as inlet-flow-rate and inlet-pH of wastewater, which may have some impacts on the system stability. Therefore, the disturbances mentioned above should be considered when evaluating the performance of the controller.

5.2.1. Disturbance changed in inlet-flow-rate. Fluctuations in inlet-flow-rate tend to oscillate the outlet-pH. From the following equations:

\[
\frac{W_{a_1}}{V} (q_1 + \Delta) + \frac{W_{a_2}}{V} q_2 = \frac{W_{a_1}}{V} q_1 + \frac{W_{a_2}}{V} (q_2 + \frac{W_{a_1}}{W_{a_2}} \Delta) \\
\frac{W_{b_1}}{V} (q_1 + \Delta) + \frac{W_{b_2}}{V} q_2 = \frac{W_{b_1}}{V} q_1 + \frac{W_{b_2}}{V} (q_2 + \frac{W_{b_1}}{W_{b_2}} \Delta)
\]

(19)

where $\Delta$ is the change value of the inlet-flow-rate $q_1$. It can be seen that the change value of the inlet-flow-rate is directly related to the buffer-flow-rate. Therefore, in this paper, the disturbance variable $d$ is used to represent the changeable inlet-flow-rate. Figure 5 shows the corresponding results when the disturbance variable becomes 25%, 50% of the inlet-flow-rate. Obviously, the stability of the system under fractional order PID control is superior to that under PID control.
5.2.2. Disturbance changed in inlet-pH. In practice, due to the diversity of the input wastewater sources, the inlet-pH often fluctuates. From the following equations [23]:

\[
\begin{align*}
\frac{q_1}{V} (W_{a1} + \Delta_1) + \frac{q_2}{V} W_{a2} &= \frac{q_1}{V} W_{a1} + \frac{q_2}{V} (W_{a2} + \frac{q_1}{q_2} \Delta_1) \\
\frac{q_1}{V} (W_{b1} + \Delta_2) + \frac{q_2}{V} W_{b2} &= \frac{q_1}{V} W_{b1} + \frac{q_2}{V} (W_{b2} + \frac{q_1}{q_2} \Delta_2)
\end{align*}
\]

where \(\Delta_1, \Delta_2\) is the change value of the reaction invariants \(W_{a1}, W_{b1}\) of inlet-stream \(q_1\), in other words, the varying inlet-pH value. It is obvious that the change value of the inlet-pH is directly related to the pH change of buffer stream. Similarly, the pH change of the disturbance variable \(d\) is used to represent the above disturbance. Figure 6 and figure 7 show the corresponding results when the pH changes by \(\pm 25\%\) of its nominal value, the fractional order PID controller has better control effect than the PID controller when the inlet-pH changes.
Figure 7. The pH-value change of buffer stream in FOPID control.

Figure 8. The pH-value change of buffer stream in PID control.

6. Conclusion
This paper proposes an optimal control method based on fractional order PID controller, which aims to make simple, fast and accurate pH control for complex industrial processes such as wastewater treatment plants. Here is a brief summary of this paper.

(1) The reaction mechanism of pH neutralization process is analyzed, and the discrete state equation with disturbance is obtained.

(2) A fractional order PID controller is introduced to control the pH neutralization process, the design problem of the controller parameters is transformed into a discrete nonconvex optimization problem, and the objective function that minimizes chemical consumption is introduced.

(3) Based on practical considerations, the disturbance caused by the change of inlet-flow-rate and inlet-pH is studied to prove the robustness and effectiveness of the proposed controller, and all the simulation results support that the proposed optimal control scheme has certain practicability in pH neutralization process.
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