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Certain Investigation on Concentration Control of CSTR - A Comparative Approach

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Abstract

In this paper the design of a nonlinear feedback controller is analyzed for concentration control of continuous stirred tank reactors (CSTR) which have strong nonlinearities. Continuous Stirred Tank Reactor (CSTR) is one of the common reactors in chemical process and all industrial process requires a solution of specific chemical strength of chemicals considered for analysis. Here Particle Swarm Optimization (PSO) algorithm based PID controller tuning is attempted for the concentration control of Continuous Stirred tank reactor (CSTR). Based on the Performance indexes and criterion controller can be estimated. The Integral Square Error (ISE) criterion is used to guide PSO algorithm to search the controller parameters like Kp, Ki, Kd. A comprehensive simulation is carried out with PID and I-PD controller Structures. The simulation results shows that the PSO based PID controller tuning approach provides better performance compared to other conventional PID tuning methods.

Keywords**:** ***PID controller, I-PD controller, Particle Swarm Optimization Algorithm, Chemical Concentration, CSTR***

1. Introduction

The Continuous Stirred Tank Reactor system (CSTR) is a complex nonlinear system. Due to its strong nonlinear behavior, the problem of identification and control of CSTR is always a challenging task for control systems engineer[1]. Chemical reactors often have significant heat effects, so it is important to be able to add or remove heat from them. In a CSTR (continuously stirred tank reactor) the heat is add or removed by virtue of the temperature difference between a jacked fluid and the reactor fluid. Often, the heat transfer fluid is pumped through agitation nozzle that circulates the fluid through the jacket at a high velocity. The reactant conversion in a chemical reactor is a function of a residence time or its inverse, the space velocity. For a CSTR, the product concentration can be controlled by manipulating the feed flow rate, which change the residence time for a constant chemical reactor[3]

In the conventional PID controller, the proportional, integral and derivative actions on error are placed in the forward path. The proportional or derivative action on the error cause an abrupt change in the controller output when the set point change is introduced. This one is the addressed drawbacks of conventional PID controller [4]. This proportional and derivative kick can be avoided by I-PD controller where the proportional and derivative terms are given in the feedback path to avoid the set point kick. In this paper parameters of I-PD controller for a second order time delayed system are optimized using Particle Swarm Intelligence.[5]

The model based controller tuning also requires complex computations to identify the controller parameters. To overcome this, it is necessary to use soft computing based auto tuning methods[14]. Particle Swarm Optimization is a population based stochastic optimization technique first introduced by Kennedy and Ebert in 1995 [6], inspired by social behavior of bird flocking or fish schooling, and it is widely used in engineering applications due to its high computational efficiency, easy implementation and stable convergence. PSO algorithm is easy to implement and there are few parameters to adjust and has been successfully applied in many areas such as function optimization, fuzzy gain scheduling, PID Auto-tuning and fractional order PID controller design [9].

In this paper, CSTR has been used to mix ethylene oxide with water to make ethylene glycol. Here the purpose is to control the concentration of ethylene glycol with the help of concentration of ethylene oxide. But undershoot, overshoot and inverse response come in the considered system while performing in a conventional way. But after implementation of PID controller to the process, removing of those shoots can be seen but still the design requirement is not achieved. So finally auto tuning method of PID controller is implemented in order to achieve the design requirement [3].

2.Continuous Stirred Tank Reactor (CSTR) Modeling

The Continuous Stirred Tank Reactor with single input and single output is shown in Fig. 1. The Continuous Stirred Tank Reactor system (CSTR) is a complex nonlinear system. Due to its strong nonlinear behavior, the problem of identification and control of CSTR is always a challenging task for control systems engineer. Usually the industrial reactors are controlled using linear PID control configurations and the tuning of controller parameters is based on the linearization of the reactor models in a small neighborhood around the stationary operating points. If the process is subjected to larger disturbance and/or it operates at conditions of higher state sensitivity, the state trajectory can considerably deviate from the aforementioned neighborhood and consequently deteriorates the performance of the controller. They are inherently nonlinear. In spite of the knowledge that one of the characteristic is inherent nonlinearity of the process, it is traditionally controlled using linear control design techniques the ability of PID controllers is to compensate most practical industrial processes has led to their wide acceptance in industrial applications.

In this paper, CSTR has been considered in which concentration of two chemicals is controlled for better results, the chemical X and Y and the by product is Z. Ethylene oxide (X) is reacted with water (Y) in a continuously stirred tank reactor (CSTR) to form ethylene glycol (Z).Assume that the CSTR is manipulated at a constant temperature and that the water is in large excess.

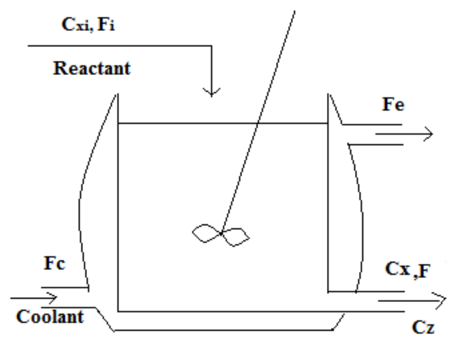

Fig. 1 CSTR with cooling jacket

The stoichiometric equation is

$$X + Y = Z \tag{1}$$

The reactant conversion in a chemical reactor is a function of residence time or its inverse, the space velocity. For an isothermal CSTR, the product concentration can be controlled by manipulated the feed flow rate, which change the residence time (for a constant volume reactor). It is convenient to work in molar units when writing components balances, particularly if chemical reaction is involved. Let CX and CZ represent the molar concentration of X and Z (mol/volume).

$$\frac{dC_X}{dt} = \frac{Fi}{V}(C_{Xi} - C_X) + r_X \tag{2}$$

$$\frac{dC_Z}{dt} = -\frac{F}{V}C_Z + r_Z \tag{3}$$

Where r_x and r_z represent rate of generation of species X and Z per unit volume, and C_{xi} represents the inlet concentration of species X . If the concentration of the water change than the reaction rate is second order with respect to the concentration of Ethylene oxide,

$$r_X = -k_1 C_X - k_3 C_X{}^2 \quad , \tag{4}$$

where k_1, k_2, and k_3 are the reaction rate constants and the minus sign indicate that X is consumed in the reaction. Each mole X reacts with a mole of Y and produces one mole of Z. Therefore, the rate of generation of Z is,

$$r_Z = -k_1 C_X - k_2 C_Z \tag{5}$$

Equation (2) and (3) can be written as,

$$\frac{dC_X}{dt} = \frac{F}{V}(C_{Xi} - C_X) - k_1 C_X - k_3 C_X{}^2 \tag{6}$$

$$\frac{dC_Z}{dt} = -\frac{F}{V} C_Z + k_1 C_X - k_3 C_Z \tag{7}$$

The manipulated input in this system is dilution rate. By solving the equation (6) and (7) the Steady state concentration of X and Z is defined as

$$C_{Xs} = \frac{-(k_1 + \frac{F_S}{V})}{2k_3} + \frac{\sqrt{(k_1 + \frac{F_S}{V})^2 + 4k_3 \frac{F_S}{V} C_{Xis}}}{2k_3} \tag{8}$$

$$C_{Zs} = \frac{k_1 C_{Xs}}{\frac{F_s}{V} + k_2} \tag{9}$$

3. Problem Formulation

The linear space model or case study of CSTR is given by

$$x = Ax + Bu \tag{10}$$
$$y = Cx + Du \tag{11}$$

Where the states, inputs and output are in deviation variable form. The first input (dilution rate) is manipulated and the second (feed concentration of A) is a disturbance input. Linearization of the two modeling equations (from equation (6) &(7)) at steady state solution to find the following state space matrices is done:

$$A = \begin{bmatrix} \frac{-F_i}{V} - k_1 - 2k_3 C_X & 0 \\ k_1 & \frac{F_s}{V} \end{bmatrix}$$

$$B = \begin{bmatrix} C_{Xfs} - C_{Xs} & \frac{F_s}{V} \\ -Cz & 0 \end{bmatrix}$$

$$c = \begin{bmatrix} 0 & 1 \end{bmatrix} \; D = \begin{bmatrix} 0 & 0 \end{bmatrix}$$

For the particular reaction under consideration, the rate constants are k1=5/6 /min k2 =5/3 /min k3=1/6 mol/litre.min Based on the steady state operating point of C = 3 gmol/liter, C_{Zs} = 1.117 gmol/liter and Fs /V = 0.5714 min-1. The state model is

$$A = \begin{bmatrix} -2.4 & 0 \\ 0.83 & -2.23 \end{bmatrix} \; B = \begin{bmatrix} 7 & 0.57 \\ -1.17 & 0 \end{bmatrix}$$

$$C = \begin{bmatrix} 0 & 1 \end{bmatrix} \; D = \begin{bmatrix} 0 & 0 \end{bmatrix}$$

Converting state space model to transfer function

$$G(s) = C(SI - A)^{-1} B \tag{12}$$

$$G_p(s) = \frac{-1.117S + 3.1472}{S^2 + 4.6429S + 5.3821} \tag{13}$$

It is desired to produce 100 million pounds per day of ethylene glycol. The feed stream concentration is 1.0 lbmol/ft3 and an 80% conversion of ethylene oxide has been to be determined reasonable. Since 80% of ethylene oxide is converted to ethylene glycol, the ethylene glycol concentration is 0.8 lbmol /ft3. It is seen that the output has inverse response with overshoot while tuning in conventional tuning method, to overcome this soft computing based optimization method is used.

4. Particle Swarm Optimization

The PSO method is based on swarm intelligence. The research on it is just at the beginning. Far from the Genetic algorithm (GA) and the simulated annealing (SA) approach, the POS has no systematical calculation method and it has no definite mathematic foundation. At present, the method can only be used successfully in the aspect of Evolutionary neural network, and its other applications are still being explored [6]. The algorithm proposed by Eberhart and kennedy uses a 1-D approach for searching within the solution space. For this study the PSO algorithm will be applied to a 2-D or 3-D solution space in search of optimal tuning parameters for PI, PD and PID control. The flowchart of the PSO – PID control system [11] is shown in fig 5. Consider position $X_{i,m}$ of the i^{th} particle as it traverses a $n-$dimensional search space: The previous best position for this i^{th} particle is recorded and represented as $Pbest_{I,n}$. The best performing particle among the swarm population is denoted as $gbest_{I,n}$ and the velocity of each particle within the $n-$dimension is represented as $V_{i,n}$. The new velocity and position for each particle can be calculated from its current velocity and distance respectively [11.In the PSO algorithm, instead of using evolutionary operators such as mutation and crossover, to manipulate algorithms, for a d-variable optimization problem, a flock of particles are put into the d-dimensional search space with randomly chosen velocities and positions knowing their best optimized values so far (Pbest) and the position in the d-dimensional space.

For example, the i^{th} particle is represented, as $x_i = \left(x_{i,1}, x_{i,2}, \ldots, x_{i,d}\right)$ in the $d-$dimensional space. The best previous position of the i^{th} particle is recorded as,

$$Pbest_i = (Pbest_{i,1}, Pbest_{i,2}, \ldots\ldots, Pbest_{i,d}) \qquad (14)$$

The index of best particle among all of the particles in the group in gbest d .The velocity for particle i is represented as

$$\mathrm{V}_{\mathrm{i}} = (\mathrm{V}_{\mathrm{i},1}, \mathrm{V}_{\mathrm{i},2}, \ldots\ldots\ldots, \mathrm{V}_{\mathrm{i,d}}) \qquad (15)$$

The modified velocity and position of each particle can be calculated using the current velocity and distance from $Pbest_{i,d}$ to $gbest_d$ as shown in the following equations:

$$V_{i,m}^{(t+1)} = W.V_{i,m}^{(t)} + c_1 * rand() * (Pbest_{i,m} - x_{i,m}^{(t)}) + c_2 * Rand() * (gbest_m - x_{i,m}^{(t)}) \qquad (16)$$

$$x_{i,m}^{(t+1)} = x_{i,m}^{(t)} + v_{i,m}^{(t+1)} \quad i = 1, 2, \ldots, n \ \ and \ \ m = 1, 2, \ldots\ldots, d \qquad (17)$$

Where n is the number of particles in the group, t = Pointer of iterations (generations), $V_{i,m}^{(t)}$ = Velocity of particle *i* at iteration *t*, W is the inertia weight factor, c_1, c_2 are the acceleration constant srand ()= Random number between 0 and 1, $x_{i,m}^{(t)}$ is the current position of particle i at iteration t, $Pbest_{i,}$ is the best previous position of the i^{th} particle and $gbest_m$ is the best particle among all the particles in the population. In the proposed PSO method each particle contains three members P, I and D. It means that the search space has three dimension and particles must 'fly' in a three dimensional space [11]. Figure 2 shows the flow chart of PSO algorithm. Optimized PSO algorithm generate the values of Proportional gain, Integral time and Derivative time in accordance with minimum setting time. PSO parameters used in this paper are given below.

Size of the Swarm or no of particles	= 100
No of iterations	= 50
Dimension of the problem space	= 3
Velocity constants C1 and C2	= 1.5
Inertia factor	= 1

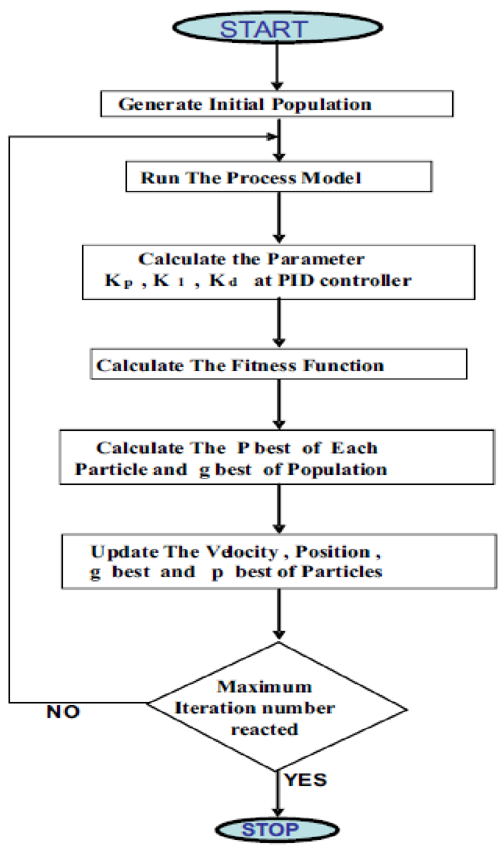

Figure 2. Flow chart of Particle Swarm Optimization

5. Controller design

Industrial PID controllers usually available as a form and to perform well with the industrial process problems, the PID controllers structures requires modifications[13]. The structures are given below

$$G_{PID} = K_P e(t) + K_i \int_0^T e(t)dt + K_d \frac{de(t)}{d(t)} \tag{18}$$

$$G_{I-PD}(s) = K_i \int_0^T e(t)dt - [K_p y(t) + K_d \frac{dy(t)}{dt}] \tag{19}$$

Where $e(t)$ is the error signal between the setpoint and actual output, $u(t)$ is the controller output and K_p, K_i, K_d are the PID controller gains. A basic PID controller directly operates on the error signal and this may produce a large overshoot in the process response due to the proportional and derivative kick. The process is unstable and to overcome the effect of proportional and derivative kick, a modified PID structure known as I-PD is considered . In I- PD structure, the integral term responds based on the error and the P+D terms works based on the measured process output [16] .

In conventional PID controller (Fig. 3), the changes in set point cause an impulse signal or sudden change in the controller output as well as in output response [2]. This spike in the controller output is called proportional or derivative kick. The controller output is given to the final control elements like control valve, motor or electronic circuit in which the spikes create serious problem. But in I-PD controller (Fig. 4) , the proportional and derivative terms are acting only to the change in process variable not on the error as these terms are given in the feedback path. This structure may eliminate the proportional and derivative kick during any set point change [5]. Minimizing the ISE criterion generates the controller parameters. The values of the controller parameters are continuously adjusted, until the ISE of the closed loop system is minimum [7]. The equation is given as,

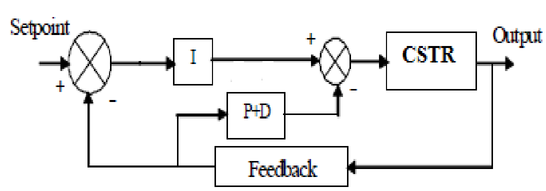

Figure 3. Tuning of I-PD controllers

$$ISE = \int_0^T e(t)^2 d(t) = \int_0^T [r(t) - y(t)]^2 d(t) \ , \tag{20}$$

where $e(t) = error$ e, $r(t) = reference\ input$, and $y(t) =$ measured variable.

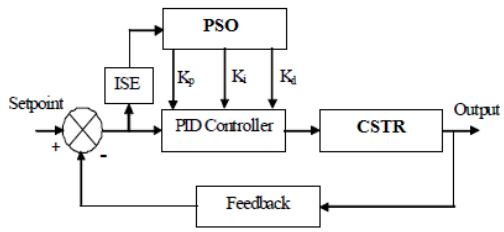

Figure 4. Tuning of PID controllers

The minimization of ISE provides optimal controller parameters using PSO[13]. Performance of PID depends upon gain parameters, so adjusting the parameter is needed. Different methods are used for tuning that are open loop method and closed loop method[16]. In open loop applying a step to the process and get the response like as shown in the Figure5 and get the dead time ,reaction rate and process gain. Using Ziegler-Nichols Open loop Method the controller Parameters are calculated. Another tuning method is formally known as the Ziegler Nichols method, by John G. Ziegler and Nathaniel B. Nichols in the 1944. As in the method above, the *Ki* and *Kd* gains are first set to zero. The *P* gain is increased until it reaches the ultimate gain, *Ku*, at which the output of the loop starts to oscillate finally get the Ultimate period Pu.With that help of Ultimate period and Ultimate gain, closed loop method of PID controller parameters are calculated[16].

6. Result and discussion

PID controller is placed in a unity feedback loop with the system transfer function. Initially open loop test has been done.

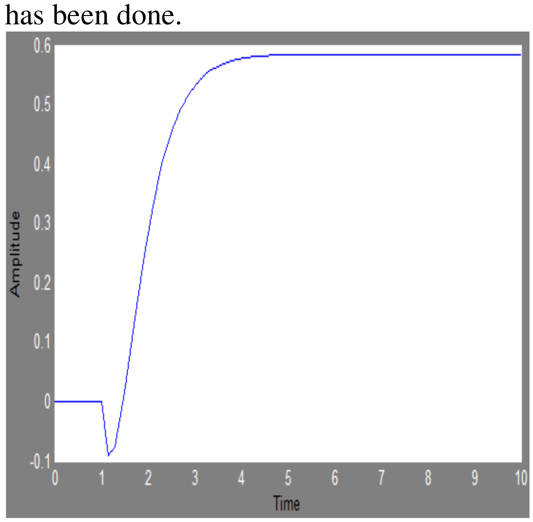

Figure 5. Response of Open loop step response method

The K_i and K_d gains are first set to zero. The P gain is increased until it reaches the ultimate gain Ku, at which the output of the loop starts to oscillate. From the sustained oscillation Ku (ultimate) gain and Pu (ultimate period) is calculated. Using the Ziegler Nichols tuning formulae K_p, K_i, K_d controller parameters are calculated.

Table1.Controller Parameters

Tuning methods	PID parameters		
	K_p	K_i	K_d
ZN	1.2	5.85	0.73
PSO	0.5686	0.5090	0.0131

All the drawback of the conventional PID can be eliminated while using the PSO optimization method. To eliminate the derivative kick I-PD controller is used

Table 2. Comparison Result of ZN and PSO based PID and I-PD methods

Tuning method		Dynamic performance specifications			Performance Index
		$T_r(s)$	$T_s(s)$	$M_p(\%)$	ISE
ZN	PID	1.95	41	74.5	2.186
	I-PD	1.78	35	85	2.324
PSO	PID	6.86	23	0	1.802
	I-PD	6.50	20	0	2.759

From the figure 6 it is shown that the PSO based PID tuning give the better response, the response of the ZN tuning gives the more oscillation compare to the PSO tuning an also inverse response is presented.

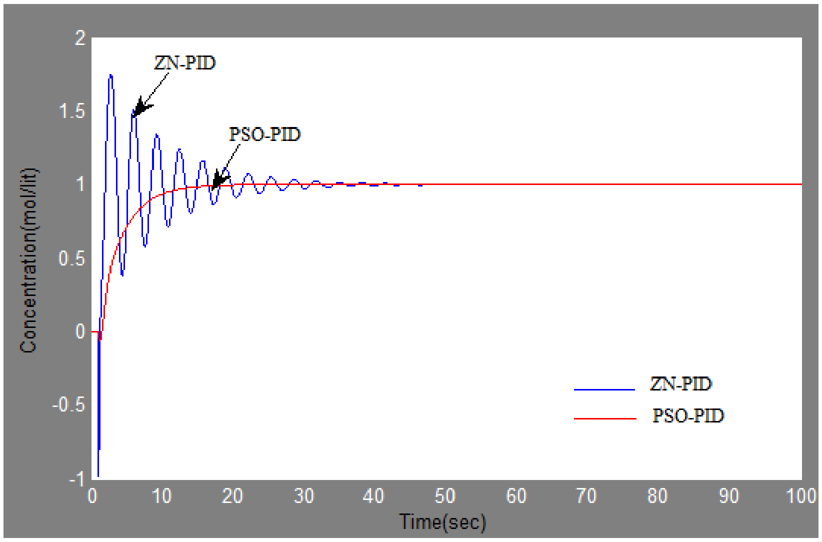

Figure 6. Tuned response of PID controller

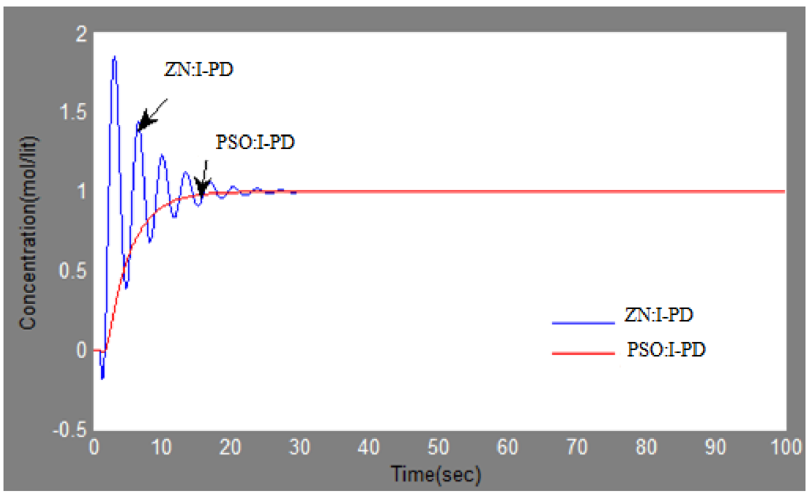

Figure 7. Tuned response of PID controller

The closed-loop response for the Z-N method yields higher overshoot and longer settling time. Figure 6 and 7 show that the PSO method delivers better control performance with improved dynamic performance specifications over the other tuning methods. Using the I-PD controller, the inverse response is reduced, that is derivative kick is eliminated.

7. Conclusion

The ZN and tuning methods have been implemented on flow control loop and a comparison of control performance using these methods has been completed. For the Z-N controller set point tracking performance is characterized by lack of smooth transition as well it has more oscillations. Also it takes much time to reach set point. The PSO based controller tracks the set point faster and maintains steady state. Also, the ISE is found to be very minimal compared to the Z-N. It was found for all control loops the performance of the PSO based controller was better compared to the Z-N control. PID controller tuning is a small-scale problem and thus computational complexity is not really an issue here. It took only a couple of seconds to solve the problem. Compared to conventionally tuned system, PSO tuned system has good steady state response and performance indices. This project can be extended using the Bacterial foraging optimization algorithms in order to overcome the drawbacks of the conventional controllers and PSO optimization.

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