

CONTROL OF A PH NEUTRALIZATION PROCESS VIA THE BIG BANG BIG CRUNCH OPTIMIZATION

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ABSTRACT

The control of pH is common in the chemical process and biotechnological industries. The main complexity consists of the nonlinearity reflected in the S-shaped gain curve of the system. However, a model-based controller will inherit all the nonlinearities of pH system. Therefore using the inverse model as a controller in an open loop fashion will produce perfect control if there does not exist any disturbance or parameter variations. In this paper, a new model inversion technique that is based on an evolutionary search algorithm called Big Bang Big Crunch optimization is introduced. Moreover, a hybrid control scheme is proposed where a parallel PI controller, which will be only activated in a model mismatch, is implemented. The beneficial sides of the hybrid control approach based on the proposed model inversion technique are illustrated in a simulation study. This control scheme is applied to control the pH variable in a neutralization process.

Keywords: Inverse model control, Big Bang- Big Crunch optimization, pH neutralization process

1. INTRODUCTION

The control of the neutralization process has been studied for several years but still remains a challenging problem. The control of pH is not just a control problem, but also a chemical equilibrium problem (Wright and Kravaris 1991). It is challenging problem since the pH process inherits nonlinearity, high sensitivity at and near the neutralization point (Pishvaie and Shahrokh 2006). Control of pH process plays an important task in chemical plants like biological, wastewater treatment and electrochemistry (Fuente et al. 2006). However, modeling of a complex pH process is a difficult. It has been verified that high nonlinear behavior of pH system is caused by titration curve of process stream. Therefore it can be concluded that, the most nonlinear term of process is described by the relationship which describes the neutrality condition.

Several control techniques have been proposed lately. They range from linear controller to nonlinear controllers through fuzzy controllers. Most of the

successful linear controllers are based on using multiple linear models (Nystrom et al. 1998). In this technique, the controller design is based linear quadratic (LQ) technique, and then the controllers are combined with two gain scheduling methods. Beside the fact that linear controllers are easy to implement, the best performances are given by nonlinear controllers since the neutralization process inherits highly nonlinear terms. In Loh et al. (2001), an adaptive control strategy is proposed where the control and parameter estimation laws are derived based on a reference model. Moreover, Henson et al. (1994) proposed and implementable version of the indirect adaptive nonlinear control strategy. And Babuska et al. (2002) have proposed a fuzzy self-tuning PI controller for a pH control in a fermentation system, where PI parameters are tuned on-line. Another fuzzy control methodology is proposed by Fuente et al. (2006), in this strategy the pH process is divided in several sub fuzzy regions, so that the operating the process region is determined and according to this information a fuzzy PI controller is designed.

Recently, a new evolutionary computation algorithm named as Big Bang Big Crunch (BB-BC) is presented by Erol and Eksin (2006). The leading advantage of BB-BC is the high convergence speed and the low computation time. The working principle of this method can be explained as the transformation of a convergent solution to a chaotic state and then back to a single tentative solution point. This evolutionary search algorithm was first used as an online adaptation of the fuzzy model by updating the consequent parameters of the model (Kumbasar et al 2008a); moreover this optimization method is used as an inverse fuzzy model control structure (Kumbasar et al 2008b).

In this paper, a model based inversion technique is introduced. It is known fact that inverting the system is an effective way to control nonlinear systems. Therefore a model based open loop control structure is proposed in which the inverse model is used as the controller. In this structure, the output of the inverse model which would be the control signal for the system is generated via an optimization problem. The optimization problem can be defined as to decrease the error between the

process model output and the reference signal. Since the BB-BC optimization algorithm has a high convergence speed and low computational time, the optimal inverse process model control signal is generated within each sampling time. As the process model output converges to the set point; the process output will converge to the set point; unless there does not exist any disturbance or parameter variation in the system. In the case of disturbances of parameter perturbations, a hybrid control structure is proposed in which a PI controller is implemented in order to avoid steady state errors.

In the next chapter, brief information about the BB-BC optimization technique is given. In the third chapter, the BB-BC optimization based inverse model controller is introduced. Moreover the hybrid control structure is presented. Later, the highly nonlinear pH model described. Finally, the performance of this control structure is illustrated.

2. BIG BANG–BIG CRUNCH OPTIMIZATION

The Big Bang-Big Crunch (BB-BC) optimization method is built on two main steps: The first step is the Big Bang phase where candidate solutions are randomly distributed over the search space and the next step is the Big Crunch where a contraction procedure calculates a center of mass for the population. The initial Big Bang population is randomly generated over the entire search space just like the other evolutionary search algorithms. All subsequent Big Bang phases are randomly distributed about the center of mass or the best fit individual in a similar fashion. In (Erol and Eksin 2006), the working principle of this evolutionary method is explained as to transform a convergent solution to a chaotic state which is a new set of solutions. The procedure of the BB-BC optimization is given in the table below:

Table 1: BB-BC Optimization Algorithm

Step 1 (Big Bang Phase)

An initial generation of N candidates is generated randomly in the search space.

Step 2

The cost function values of all the candidate solutions are computed.

Step 3 (Big Crunch Phase)

The center of mass is calculated. Either the best fit individual or the center of mass is chosen as the point of Big Bang Phase.

Step 4

New candidates are calculated around the new point calculated in Step 3 by adding or subtracting a random number whose value decreases as the iterations elapse.

Step 5

Return to Step 2 until stopping criteria has been met.

After the Big Bang, a contraction procedure is applied during the Big Crunch. In this phase, the contraction operator takes the current positions of each candidate solution in the population and its associated

cost function value and computes a center of mass. The center of mass can be computed as:

$$x_c = \frac{\sum_{i=1}^N \frac{1}{f^i} x_i}{\sum_{i=1}^N \frac{1}{f^i}} \quad (1)$$

where x_c = position of the center of mass; x_i = position of candidate; f^i = cost function value of candidate i ; and N = population size. Instead of the position of the center of mass, the best fit individual can also be chosen as the starting point in the Big Bang phase.

The new generation for the next iteration Big Bang phase is normally distributed around x_c

$$x_i^{new} = x_c + \sigma \quad (2)$$

where x_i^{new} = the new candidate solution i ; and σ standard deviation of a standard normal distribution. The standard deviation decreases as the iterations elapse according to the following formula

$$\sigma = \frac{r\alpha(x_{max} - x_{min})}{k} \quad (3)$$

where r is random number; α is a parameter limiting the size of the search space, x_{max} and x_{min} are the upper and lower limits; and k is the number of the iterations. Therefore, the new point is generated as follows:

$$x_i^{new} = x_c + \frac{r\alpha(x_{max} - x_{min})}{k} \quad (4)$$

Since normally distributed numbers can be exceeding ± 1 , it is necessary to limit population to the prescribed search space boundaries. This narrowing down restricts the candidate solutions into the search space boundaries (Erol and Eksin 2006).

3. CONTROLLER STRUCTURE

In the first part of this section the proposed BB-BC based Inverse Model controller will be introduced. This controller structure assumes that there is neither disturbance nor model mismatch. It is common known fact it is almost impossible to perfectly model industrial process. Since this proposed control structure is based on the obtained model, the controller will not be able to reject parameter perturbations or disturbances. Therefore, in the second part of this section, a hybrid control structure will be proposed where a parallel PI controller is proposed to force the system output to the desired set point. The PI controller will only be activated if there is model mismatch.

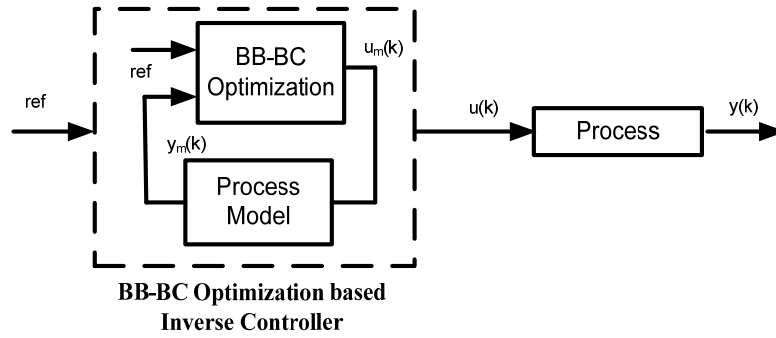


Figure 1: BB-BC based Inverse Open Loop Control Scheme

3.1. BB-BC based Inverse Model Controller

In this proposed control structure, the control signal generation is handled as an optimization problem. The problem can be defined as to decrease the error between the process model output and the reference signal.

Assuming that the process model matches the process perfectly, as the process model output converges to the set point; the process output will converge to the set point, too. Since an online implementation of this evolutionary algorithm is feasible, at each sampling the optimal control signal can be generated. Then the optimal control signal is then applied to the process. The scheme is illustrated in Figure 1.

The cost function J_1 which is minimized at every sampling time is chosen as:

$$J_1 = (ref - y_m)^2 \quad (5)$$

Since BB-BC is a stochastic evolutionary algorithm, the performance of the controller will vary for each trial.

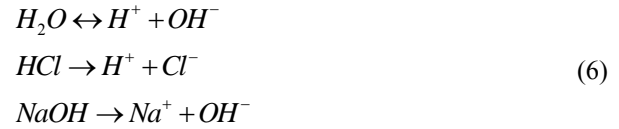
3.2. Hybrid Controller Structure

As it has been mentioned before, the BBBC inverse control structure will not be able to reject disturbances or parameter perturbations. Therefore a hybrid control structure is proposed. This structure is similar to the well known Internal Model Scheme; however the error is only used to activate the PI controller. The PI controller will be activated in the case of a model mismatch or disturbance. So it will be guaranteed that the system output will converge to the set point. The scheme is illustrated in Figure 2.

4. PH PROCESS MODELING

4.1. Process chemistry

The pH process is characterized by the presence of acid/base reactions. In this study the reaction of strong acid (HCl) and strong base (NaOH) reaction will be considered. It is a known fact that this type of reactions occur quickly. In the reaction tank the decomposition of HCl, NaOH and H_2O is represented with the following equations (McAvoy et al. 1972).



The electro neutrality principle indicates that the concentration of positive and negative ions in a solution has to be neutral in the equilibrium. So, the following must be satisfied;

$$[H^+] + [Na^+] = [OH^-] + [Cl^-] \quad (7)$$

Beside this equation, the equilibrium of the pure water must also be satisfied which is given as:

$$k_w = [H^+][OH^-] = 10^{-14} \text{ mol}^2 / L^2 \quad (8)$$

where k_w is the dissociation constant of the water.

Defining,

$$\begin{aligned} w_a &= [Cl^-] \\ w_b &= [Na^+] \end{aligned} \quad (9)$$

Replacing in the equation (7),

$$w_b + [H^+] = w_a + \frac{k_w}{[H^+]} \quad (10)$$

After rearranging the equation, the following second-order polynomial is found

$$[H^+]^2 + [H^+](w_b - w_a) - k_w = 0 \quad (11)$$

So the morality of H^+ is found as:

$$[H^+] = \frac{(w_a - w_b) + \sqrt{(w_a - w_b)^2 + 4k_w}}{2} \quad (12)$$

The morality of H^+ is directly related with pH value which indicates the acidic value of the process.

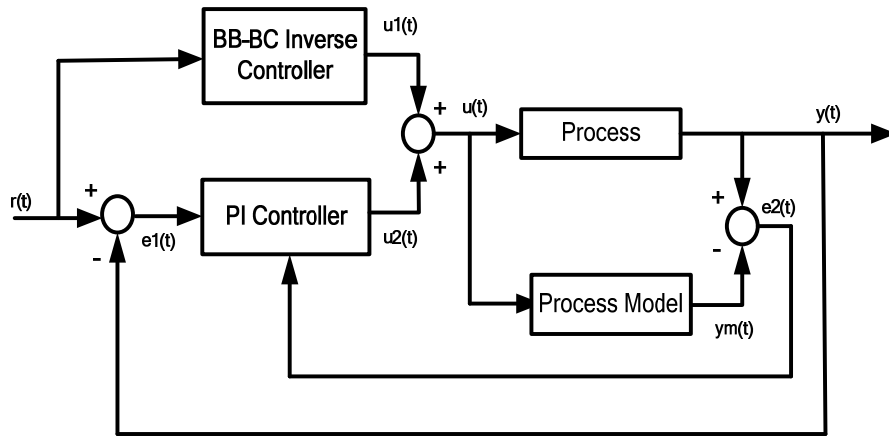


Figure 2: Proposed Hybrid Control Scheme

The relationship is defined as:

$$pH = -\log([H^+]) \quad (13)$$

Replacing the solution from equation (12), we obtain

$$pH = -\log\left(\frac{(w_a - w_b) + \sqrt{(w_a - w_b)^2 + 4k_w}}{2}\right) \quad (14)$$

Via this equation the pH value of the mixture of strong acid and base can be calculated. It can be clearly seen from Figure 3 that there is static nonlinear relationship between pH and $[H^+]$.

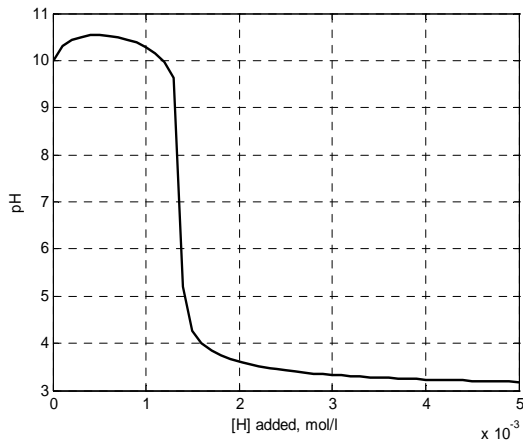


Figure 3: pH Variation

4.2. Process dynamics

The dynamic model of the pH process is proposed by (McAvoy et al. 1972) and is shown in Figure 4. Assumption of perfect mixing is general in the modelling of pH processes. Balances in the reactor can be given by

$$\left. \begin{aligned} V \frac{dw_a}{dt} &= F_a C_a - (F_a + F_b) w_a \\ V \frac{dw_b}{dt} &= F_b C_b - (F_a + F_b) w_b \end{aligned} \right\} \quad (15)$$

where V is the volume of the mixture tank, C_a and C_b are the acidic and basic concentration, F_a and F_b are the acidic and basic flow rates respectively.

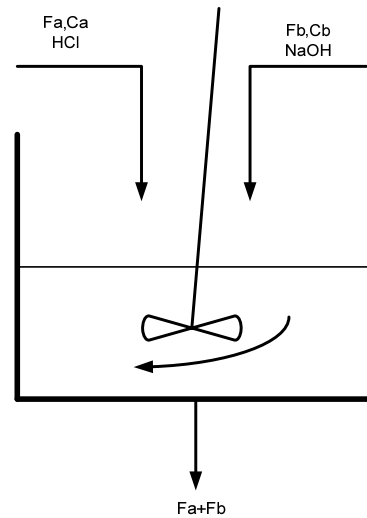


Figure 4: Schematic of CSTR

5. SIMULATION STUDY

In this section a simulation study will be performed in order to show the effectiveness of the proposed control structure. As it has been explained briefly in the previous section, the pH neutralization process inherits not only a static nonlinear gain but also the dynamics of CSTR are also nonlinear. Simulations are performed on MATLAB®/Simulink toolbox.

The description of the pH process used in this simulation study is given in Table 2.

The initial condition of the CSTR is assumed to be that the morality of H^+ and OH^- are equal, therefore the initial pH value is 7.

Table 2: Description of the pH process

Symbols	Description	Value
V	Volume of the CSTR	0.8L
F _a	Flow rate of the influent stream	1 l/h
F _b	Flow rate of the titrating stream	0-2.1 l/h
C _a	Concentration of the influent stream	0.001 mol/l
C _b	Concentration of the titrating stream	0.001 mol/l

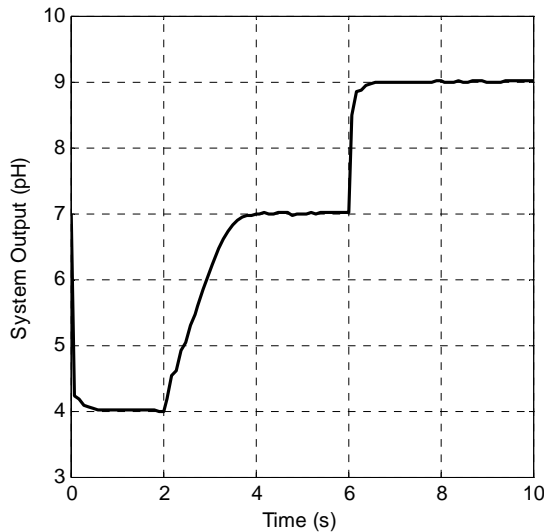


Figure 5: System Output for Varying Reference Signal

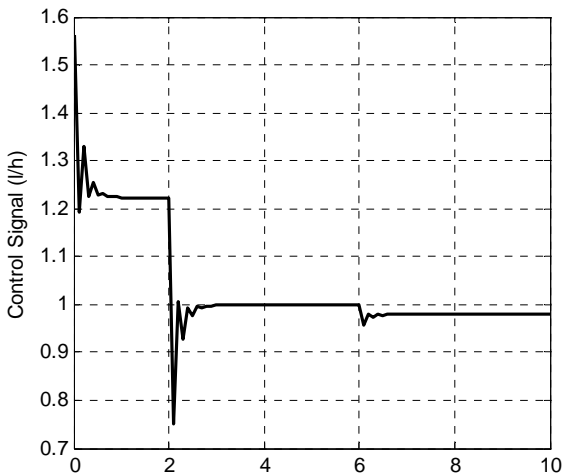


Figure 6: Control Signal for Varying Reference Signal

In the first part, since the dominant nonlinearity is related to the morality of H^+ , the controller has been tested under varying pH reference values. It can be seen from Figure 5 that the controller provides satisfactory performances for different pH reference signals. Especially, it is observed that, the process output has been the set point value 7 pH successfully. In this case, since there is nor parameter perturbation nor

disturbance, the PI controller is not activated. The process is forced the set value, only by BB-BC inverse controller. The control sign is also presented in Figure 6.

In the second part, at first the neutralization process has been forced to the set point reference signal 7 pH. Then in order to examine the disturbance case, the flow rate of the influent stream has been increased %10 percent in the 5th second. As soon as the disturbance affects the process, the PI controller is activated and disturbance has been compensated in a short period of time. The system output and the control signal are presented in Figure 7 and Figure 8, respectively.

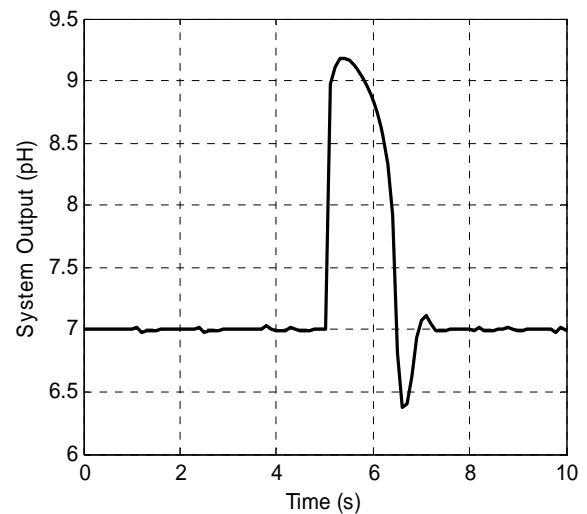


Figure 7: System Output Under Disturbance

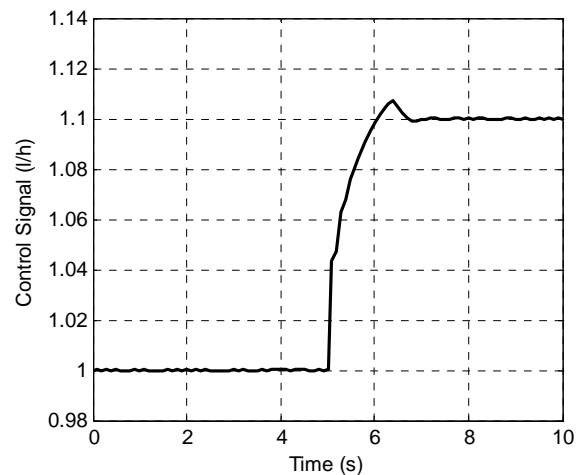


Figure 8: Control Signal Under Disturbance

6. CONCLUSIONS

In this study, a new iterative inversion technique based on the BB-BC optimization has been presented. In this new technique, the inverse model control signal generation is handled as an optimization problem. Since the BB-BC optimization algorithm has a high convergence speed and low computational time, the optimal inverse model control signal can be generated

within each sampling time in an on line fashion. In order to show performance of the new approach a simulation study has been performed. In this study, the pH process which has high sensitivity at and near the neutralization point has been controlled. It has been shown that pH process could have been controlled perfectly in an open loop control scheme. Since the proposed methodology is based on a stochastic global search algorithm, the generated inverse model control signals may vary at each trial and this is the only arguable point of this inversion technique. Moreover, a hybrid control structure is proposed where a parallel PI controller is implemented to the BBBC inverse model controller. In the case of various disturbances and parameter perturbations, PI controller will get activated so that the convergence of the system output to the reference signal is guaranteed. It has been demonstrated via simulation examples that the proposed controller scheme really provides quite satisfactory results.

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