Model Predictive Control for pH Control of Cephradine Purification Process.

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ABSTRACT

This paper illustrates a new control technique for the process of pH control of the Cephradine purification process in Continuous Stirrer Tank Reactor (CSTR) using the Model Predictive Control (MPC) technique. The results show that the response of MPC is accurate and nearer to the ideal response when compared to Proportional Integral Derivative (PID). The operation of proposed model is also shown.

(Keywords: model predictive control, PID, controller, Cephradine, LabView, process control)

INTRODUCTION

Pharmaceutical products are produced under carefully controlled conditions to ensure product quality. Each process is different and requires close attention to details. Here we consider the process of purification of an impure compound, Cephradine. The purified form of Cephradine is an antibiotic, which is used to treat many bacterial infections. To obtain impure Cephradine in its purified form, one needs to adjust and maintain its pH at a desired level. Hence in this process, pH control is a critical factor.

The performance of the use of Model Predictive Controller (MPC) in the reactor is investigated in this study. "MPC is the family of controllers in which there is a direct use of an explicit and separately identifiable model" (Prett and Garcia, 1988). MPC algorithms can be described shortly by a model that must be obtained off-line, an objective function, a reference trajectory to follow, and the constraints (input/output) to apply. MPC is a user friendly and applicable technique for different industrial needs, where, the objective function, the model and optimization method are flexible. The advantages of MBPC compared with many other control techniques can be listed as follows (Li et al., 1989):

- It can use step and impulse response data which can easily be obtained,
- It can handle input/output constraints directly,
- It gives satisfactory performance even with time delays and high nonlinearities,
- It can be used in multivariable format,
- It is robust in most cases,
- Implementation of the technique is simple,
- It can optimize over a trajectory,
- It can be used to control various processes, whether simple or complex ones.

In this study, a Cephradine reaction system is considered. In the Cephradine system, a CSTR is used. The system is simple to model theoretically. The aim of this study is to investigate the MPC performance for a system, which can easily be modeled theoretically. Thus, a dynamic theoretical model is checked with dynamic experiments. As a result of a good match between experimental and model results, the developed model is used for the designing MPC.

An Auto Regressive Exogeneous Model is used for the control of pH variations of impure Cephradine being prepared in the glass lined CSTR thereby obtaining purified Cephradine. The influent liquid (impure Cephradine), obtained from the previous stage, flows into the tank where it is mixed with the reagent (ammonia solution) to alter its pH. The effluent (pure Cephradine) is acidic with a desired pH of 4.8 the reagent (NH_3 solution) is basic with a pH of 9.

The pH is controlled in a glass lined continuous stirrer tank reactor. The reactor is glass lined in order to reduce corrosion of the tank and the tank is well stirred so that the pH is uniform throughout the tank. In the simulation study, LabVIEW

Software® is adopted for the control of pH in the glass lined Continuous stirrer tank reactor. Later sections of this paper provide a description of the work, experimental results, and a comparison with proportional integral derivative (PID) results. Conclusions are presented in the final section of this paper.

DESCRIPTION OF THE WORK

This work concentrates on pH control during the purification stage of Cephradine. The final pH of 4.8 is obtained under carefully controlled conditions. In the purification stage, we get Cephradine from the previous stage, which has a pH of 1.8. The solution is clear with Cephradine of pH 1.8. Ammonia is then added which increases the pH slowly in the range of from 1.9 to 2.8. When the pH is 2.8, the color changes and the solution takes on a a slurry look. At this stage, ammonia addition and the rotation of the stirrer in the CSTR is stopped. The stirrer then starts to rotate after 20 min., the setup is stirred continuously, and the ammonia is again added and the pH increases slowly from pH 2.8 to pH 4.8. The condition is maintained until the set point 4.8 is reached.

When the desired pH of 4.8 is obtained, the setup is left ideal for 20 min (timed). Cooling is applied to lower the temperature by 10 degrees. This 10 degree temperature decrease is attained within two and a half hours. Once the desired temperature is reached, the set up is left for 1 hour. Thus, the Cephradine is purified at pH 4.8. Table 1 shows the positions of stirrer and valve. At present, pH is controlled by PID in the plant. PID controller does not produce quality in its output and it can do only a single mode of operation. Hence, to overcome these problems, a new controller (MPC) was tried which can overcome the above drawbacks.

Table 1: Positions of Stirrer and Valve.

pH	Stirrer	Solenoid Valve
1.8 – 2.8	Rotates	Open
2.8- 4.7	Rotates	Open
4.8	Rotates	Closed

ARX MODEL ESTIMATION

The general form is:

$$y(k) = -a_1 y(k-1) - a_2 y(k-2) \cdots - a_n y(k-n) + b_0 u(k) + b_1 u(k-1) \cdots + b_m u(k-m) \quad (1)$$

Z transform:

$$y(z) = Z[y(k)] \quad (2)$$

backward shift operator (z^{-1})

$$Z[y(k-1)] = z^{-1} y(z) \quad (3)$$

$$Z[y(k-2)] = z^{-2} y(z) \quad (4)$$

$$(1 + a_1 z^{-1} + \cdots + a_{n-1} z^{-n+1} + a_n z^{-n}) y(z) = (b_0 + b_1 z^{-1} + \cdots + b_m z^{-m}) u(z) \quad (5)$$

$$y(z) = \frac{(b_0 + b_1 z^{-1} + \cdots + b_m z^{-m}) u(z)}{(1 + a_1 z^{-1} + \cdots + a_{n-1} z^{-n+1} + a_n z^{-n})}$$
$$\therefore g(z) = \frac{b_0 + b_1 z^{-1} + \cdots + b_m z^{-m}}{1 + a_1 z^{-1} + \cdots + a_{n-1} z^{-n+1} + a_n z^{-n}} \quad (6)$$

for most process systems there is not an immediate effect of the input on the output so b_0 =0; for four parameters

$$y(k) = -a_1 y(k-1) - a_2 y(k-2) + b_1 u(k-1) + b_2 u(k-2)$$
$$\text{for } k = 1 \cdots N \quad (7)$$

$$y(1) = -a_1 y(0) - a_2 y(-1) + b_1 u(0) + b_2 u(-1)$$
$$y(2) = -a_1 y(1) - a_2 y(0) + b_1 u(1) + b_2 u(0)$$
$$y(N) = -a_1 y(N-1) - a_2 y(N-2) + b_1 u(N-1) + b_2 u(N-2) \quad (8)$$

EXPERIMENTAL RESULTS

The pH control using MPC is modeled and simulated using LabVIEW Software® as shown in Figure 1.

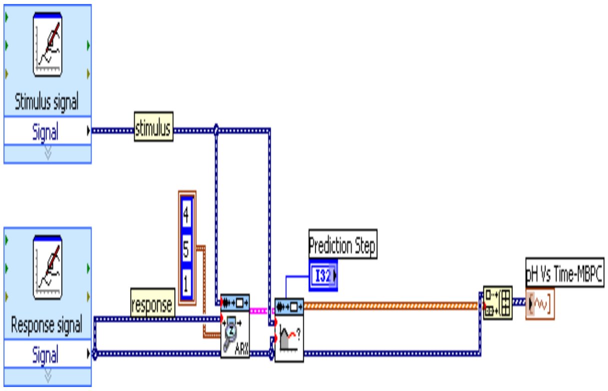

Figure1: Block Diagram of ARX Model in LabVIEW® Environment.

The block diagram contains this graphical source code. Front panel objects appear as terminals on the block diagram. Additionally, the block diagram contains functions and structures from built-in LabVIEW® VI libraries. Wires connect each of the nodes on the block diagram, including control and indicator terminals, functions, and structures. For each of the components created in the front panel, there appears an indicator automatically in the block diagram. For the variation of process value, selecting it from the structure icons in the function palette creates a flat sequence. The flat sequence is created in order to integrate the various stages of the program. Next a while loop is created from the numeric data type of the functions palette, obtain the addition block.

A shift register with initial value set to 1.8 is given as one of the inputs to the addition block while the other input is 0.1. The other end of the shift register is given to the output of the addition block. The output of the addition block is given to the less than or equal to block obtained from the comparison option in the functions palette. The other input to this block is the constant 2.8. For the stirrer operation, a divide block is created from the numeric option in the functions palette. The iteration is given as one of the inputs to this block and the other input is a constant 2 since there are 2 LEDs in the stirrer.

The division operation is performed and the remainder, so obtained, is compared with the value 1.The output of the equal to block is given to 2 Boolean indicators; to one directly and to the other through a NOT gate so that both the LEDs can glow alternately. For increasing the level of the tank gradually, a case structure block is created from the structures option in the functions palette. Next the fill color of the tank can be obtained by expanding the property node of the tank for fill color and to change the level of the ammonia solution in the tank, expand the property node by value.

All these are placed inside the case structure and the connections for the true and false conditions are given. The solenoid valve and the pipe indicators are given to the true condition while the relay is given to the false condition through the NOT gate. The V/I converter is given to a true condition through the Boolean data type. The waveforms of the PID and MPC are obtained through the waveform charts given to the pH indicator through the PID block from the control design and simulation tool kit and the ARX and model prediction block, respectively. In the next flat sequence when the setup is ideal, the waveform after the value 2.8 is obtained from the waveform chart by using for loop.

In the next flat sequence, the above steps are followed for the variation of pH from 2.8 to 4.8. In the next flat sequence, the condition for fluctuation of pH and finally the stabilizing of pH is obtained.

PERFORMANCE OF PROPOSED MODEL

The performance of the designed predictive controller for pH control of the Cephradine purification process was simulated using LabVIEW® and the graphical user interface (GUI) front panel is shown in Figure 2.

The front panel is used to interact with the user when the program is running. Users can control the program, change inputs, and see data updated in real time. The controls are used for inputs. Indicators are used as outputs.

When the program is run, the relay inside the MPC closes, the solenoid valve is opened, the ammonia solution flows into the tank, and the pH level of the solution inside the tank gradually increases.

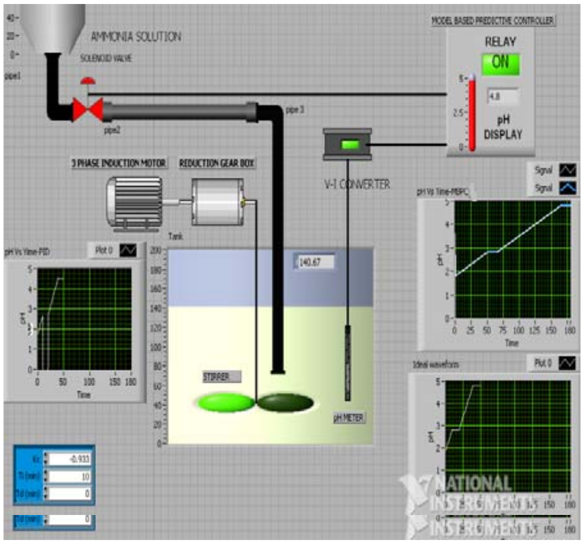

Figure 2 : Front Panel Diagram at pH 4.8.

Simultaneously the two-waveform charts show the variation of pH with respect to the time for PID and MPC. The display of the pH is shown inside the MPC.

Initially the value of pH increases linearly from 1.8 to 2.8. After reaching 2.8 the pH is maintained constant for a particular time and then again increases gradually from 2.8 to 4.8. At 4.8, the waveform chart shows some fluctuations for certain time and then settles to the value of 4.8. When comparing the waveform of the PID with MBPC, it is seen that the waveform of PID shows greater deviations.

A. Simulation Results

Figure 3 shows the pH responses for our application. In the ideal response H initially varies from 1.8 to 2.8 linearly and remains constant at 2.8 for some time and again varies from 2.8 to 4.8 linearly and maintained constant at 4.8.

Fig 4and 5 shows the responses of pH Vs time for MPC and PID. The response of MPC coincides with the idea response, which can be well observed in the above figure. This is the main advantage of MPC since the delay periods are well shown without any disturbance.

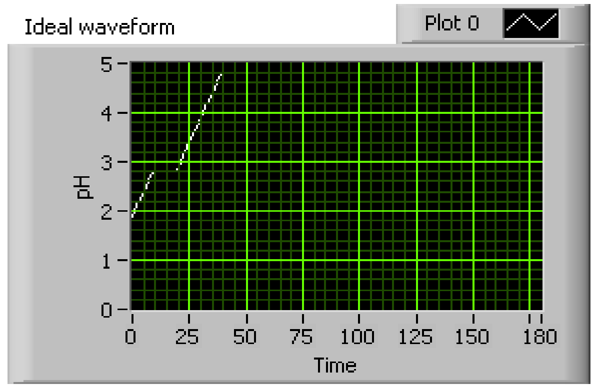

Figure 3: Ideal Response.

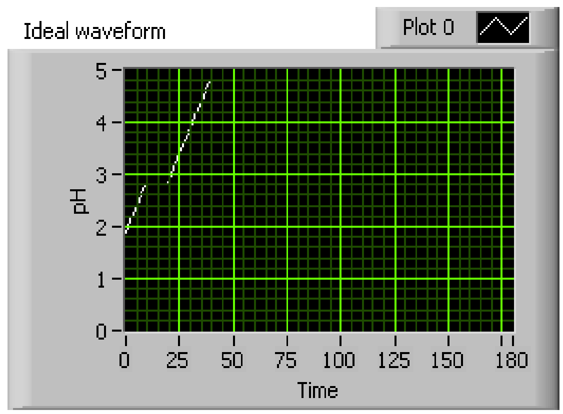

Figure 4: PID Response.

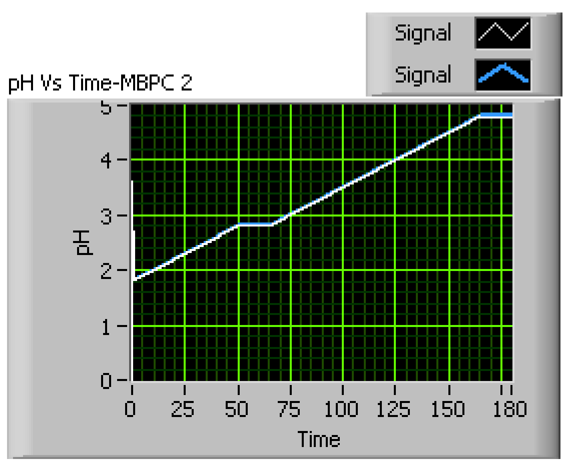

Figure 5: MPC Response.

In the response of PID, the graph shows a large deviation for the time at which 2.8 is constant and small amount of deviations for the rest of the part of the graph. Hence, the obtained response of MPC is better than that of PID.

CONCLUSION

A control strategy is applied for the process of pH control in CSTR using Model Predictive Control technique in order to improve the control performance on the reactor that could not be controlled satisfactorily using proportional integral derivative controls. The MPC technique not only controls the status of the valve but is also used to control the stirrer whereas PID could be used only to control the status of the valve. The automatic control of the pH now enables the plant to reduce the batch cycle time and to increase the plant productivity. Using LabVIEW® software the output response of our application with MPC and PID controller was compared. From this, the results showed that the response of MPC is accurate and nearer to the ideal response, when compared to PID.

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