Design of IMC-PI controller for nonlinear model of continuous stirred tank reactor

Trinh Luong Mien
University of transport and communications, No.3 Caugiay, Langhuong, Dongda, Hanoi, Vietnam
Email: mientl@utc.edu.vn

Abstract: The control problem of the continuous stirred tank reactor in the chemical industry in general and in the production of transport construction materials in particular are very important in order to create chemical additives that meet the user's technical requirements. The article presents the two-input-two-output nonlinear model of the continuous stirred tank reactor that are the temperature process and concentration process of output product. Then two PI controllers for the CSTR temperature and concentration processes are designed in this article. Continuously, the article presents two PI controllers based on internal model control (IMC-PI) for these CSTR nonlinear processes model and two IMC controllers combined with the CSTR temperature and concentration processes identification (IMC-Ident). The simulation results on Matlab show that IMC-PI and IMC-Ident have good CSTR control quality while designing and deploying applications in practice is not difficult.

Keywords: CSTR, IMC, PID, IMC-PI, nonlinear model, identification, reactor tank, MATLAB.

1. INTRODUCTION

In the trend of industrial revolution 4.0, the production equipment has been constantly improved and more modern. Among them, continuous stirred tank reactor (CSTR) is used to create new chemicals for variety of industries (construction materials, biofuels, pharmaceuticals, ...), are very interested in researching and applying modern control techniques to increase equipment performance, improve product quality and reduce product costs.

Nowadays, there are many ways to control CSTR equipment such as using PID control, fuzzy control, neural network, optimal control, internal control principle ... each controller has certain advantages and disadvantages. Traditional PID controller are still commonly used for CSTR equipment because of simplicity, stability, and low cost.

Recently, the design trend of controllers according to the internal model control principle is being applied quite popular in many production processes because this controller is quite easy to implement, especially when linking with the well-developed object identification methods such as ARX, ARMA ... has promoted the application of internal model controller for a number of typical industrial processes, which are typical here the process of controlling the concentration and temperature of the CSTR equipment.

Researches on CSTR are often based on approximation models with ideal conditions. In perfect CSTR, the compound at the output is uniformly composed of chemical compounds at the input, operating with time and stable reaction speed. If the mixing time is stable from 5 to 10 cycles, then it is considered as a technical requirement. CSTR equipments, when used, are often simplified with technical calculation formulas and can be used to describe reaction researches [1,2,3].

Research [2] has designed the PID controller for the CSTR linear model and obtained good result. Research [3] presents a nonlinear mathematical model of the CSTR, which allows studying the effects of parameters such as dynamics and hydrodynamics on reactor performance. The studies [4,5,13] also mentioned the design of the PID controller for the CSTR nonlinear model or PID adjustment with the CSTR unstable model [6], controlling the interference resistance of the CSTR [7], using genetic algorithms [8,12,15] or using the S-function [9] generally the studies have obtained certain results and enriched the CSTR control. Research on CSTR [14] provide the predictive controller. However these researches mainly mentioning the one in one out CSTR model. Moreover, the design and implementation of controllers in practice is difficult.

This article presents the two-input-two-output CSTR nonlinear model. Two typical processes of the CSTR are mentioned in this paper: temperature and concentration of output product. Then, two traditional PI controllers and PI controllers based on the internal model control (IMC-PI), IMC controller combined with CSTR process model indenfication (IMC-Ident) are designed for these two processes. Finally, the article presents simulation and evaluation the control quality of the CSTR temperature and concentration control processes on Matlab. The article organization included section 1–Introduction, 2–Problem statement, 3–Nonlinear model, 4–Design PI controllers, 5–Design IMC-PI controllers, 6–Design IMC-Ident controllers, 7–Conclusion.

2. PROBLEM STATEMENT

This article focused on CSTR equipped with heat source as shown in Figure 1. The pure liquid A flows into the CSTR with \( c_{A0} \) [mol/lit] concentration, the input temperature is \( T_0 \) [°C] and the flow rate is \( q \) [lit/min]. In the CSTR equipment, there is a one-way reaction process \( A \rightarrow B \), producing the output product is a mixture of A and B, with a concentration of \( c_A \) [mol/lit], temperature is \( T \) [°C] and the output flow is \( q \) [lit/min]. The volume of mixture in the tank is \( V \) [lit]. The temperature in the reaction tank is ensured by the flow of cooling liquid flowing around the tank with the inlet flowrate of \( q_c \) [millilit/min] with the input temperature of \( T_{a0} \) [°C], the output flowrate is \( q_c \) [millilit/min], the output temperature is \( T_c \) [°C].
Requirements: Design to control system for the processes of $c_d$ concentration and $T_d$ temperature of the CSTR following on the reference input.

We add the following assumptions:

+ The CSTR equipment is ideal for mixing: the temperature and concentration at every position in the equipment are the same and the same as the temperature and concentration of the output product flow.
+ The overall reaction rate is directly first proportional to the concentration of substance $A$ in the equipment.
+ The heat exchange process takes place in the equipment is ideal, considering the heat loss to the surrounding environment is zero.
+ The volume of the reaction equipment is constant.

3. CSTR NONLINEAR MATHEMATICAL MODEL

Analysis of this system shows that there are eight process variables: $q_i, T_i, c_{a0}, T_{a0}, c_{d}, T_{d0}$, $T_c$, $C$, there are two output variables and also are the controlled variables $c_d$, $T_d$ six input variables including two manipulated variables are $q$ and $c$ and four disturbance variables $c_{a0}, T_{a0}, T_{c0}, T_c$.

The reaction rate of the chemical equation A $\rightarrow$ B, dependent on temperature and is determined by Arrhenius as follows:

$$k = k_0 e^{-E/(RT)}$$

Where $k_0$ is the reaction constant (collision coefficient); $E$ is the activation energy depending on the temperature; $R$ is the ideal gas constant.

The reaction rate of the chemical equation A $\rightarrow$ B depends on the specific reaction rate and the concentration of the reaction substances $c_a, c_b$ (with $a, b \in \mathbb{R}$ is the exponent-order of the chemical reaction), and when it is guaranteed to be redundant. Substance $B$, consider the reaction $1^{st}$ grade:

$$r = k(T)c_a = k_0c_a e^{-E/(RT)}$$

Applying the equation that is equal to the mass of the component for pure A (lost when participating in the reaction):

$$\frac{d(c_a)}{dt} = q(c_{a0} - c_a) - Ve c_d$$

This equation change is obtained:

$$\frac{dc_d}{dt} = q(c_{a0} - c_a) - k_0c_a c_b e^{-E/(RT)}$$

Applying the energy balance equation for CSTR when there is no loss of external environment:

$$\frac{d(\rho V)}{dt} = \rho q C_p T_c - \rho q C_p T_i + Q_r - Q_o$$

Where $Q_r$ is the radiant heat (generated) of the reaction process; $Q_r$ is the return heat of the cooling flow (heat is lost in the reaction equipment); $\rho$, $C_p$ is the specific heat capacity of substance $A$.

The heat (output) of the reaction is proportional to the reaction rate:

$$Q_r = (-\Delta H)\bar{r} = (-\Delta H)\bar{V}c_k = (-\Delta H)\bar{V} c_k e^{-E/(RT)}$$

Where $(-\Delta H)$ (cal/mol) is the thermal coefficient of a chemical reaction $(-\Delta H) > 0$.

The internal heat of the reaction equipment, released less by the cooling fluid flow through the flask, is determined as follows:

$$Q_r = UA(T_i - T_c)$$
Where $U$ is the heat transfer coefficient; $A[m^2]$ is the heat transfer surface area.

Energy balance equation for reactive equipment inside the enclosure:

$$\frac{dT_A}{dt} = \frac{q}{V}(T_0 - T_A) + \frac{(-\Delta H)k_0}{\rho C_p}C A e^{-E/(RT_A)} - \frac{UA}{\rho C_p}(T_A - T_c)$$  \hspace{1cm} (11)

Similarly, we obtain the thermal equilibrium equation for the cooling shell of the reaction device, as follows:

$$\frac{d(\rho C_p V T_c)}{dt} = \rho C_p q_c(T_c - T_A) + UA(T_A - T_c)$$  \hspace{1cm} (12)

Where $\rho_c$, $C_{pc}$ is relative density, the specific heat capacity of the coolant.

Combining (11) and (12), according to Ruiyao Gao, we obtain the energy balance equation in the reaction device in the following form:

$$\frac{dT_A}{dt} = \frac{q}{V}(T_0 - T_A) + \frac{(-\Delta H)k_0}{\rho C_p}C A e^{-E/(RT_A)} - \frac{\rho C_p q_c}{\rho C_p V}(1 - e^{-h_a(\rho C_p q_c)}) (T_A - T_c)$$  \hspace{1cm} (13)

Here $h_a[\text{cal/min.K}]$ is heat transfer coefficient.

Finally, we obtain the mathematical equations describing the kinetics (concentration, temperature) of the CSTR equipment, in the form of differential equations, as follows:

$$\frac{dc_A}{dt} = \frac{q}{V}(C_{A0} - C_A) - a_0 C_A e^{-a_1 T_A}$$  \hspace{1cm} (14)

$$\frac{dT_A}{dt} = \frac{q}{V}(T_0 - T_A) + a_0 C_A e^{-a_1 T_A} + a_2 C_A(1 - e^{-a_3/T_A}) (T_A - T_c)$$  \hspace{1cm} (15)

With $a_0 = k_0$; $a_1 = \frac{(-\Delta H)k_0}{\rho C_p}$; $a_2 = \frac{\rho C_p q_c}{\rho C_p V}$; $a_3 = \frac{h_a}{R}$

Thus, the mathematical model of the CSTR equipment is the differential equation system (14), (15) with two output variables that need to be controlled $T_A$, $c_A$, nonlinear, coupled. Two input variables, acting as manipulated/controlled variables: $q$, $q_c$.

Table 1. Parameter of continuous stirring reaction device [5]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{A0}$</td>
<td>Molar concentration of pure A is included in the reaction</td>
<td>1 (mol/lit)</td>
</tr>
<tr>
<td>$T_0$</td>
<td>Temperature of substance A is included in the reaction</td>
<td>350 (K)</td>
</tr>
<tr>
<td>$T_c$</td>
<td>Cooling liquid temperature at the inlet</td>
<td>350 (K)</td>
</tr>
<tr>
<td>$V$</td>
<td>Tank volume, equal to volume of reaction mixture</td>
<td>100 (lit)</td>
</tr>
<tr>
<td>$h_a$</td>
<td>Heat transfer coefficient</td>
<td>$7x10^{-9}$ (cal/min.K)</td>
</tr>
<tr>
<td>$k_0$</td>
<td>Impact coefficient</td>
<td>$7.2x10^{-8}$ (1/min)</td>
</tr>
<tr>
<td>$E/R$</td>
<td>Activated energy (R is the ideal gas constant)</td>
<td>$1x10^5$ (K)</td>
</tr>
<tr>
<td>$(-\Delta H)$</td>
<td>Thermal coefficient of reaction (heat emission)</td>
<td>$2x10^5$ (cal/mol)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of reactants</td>
<td>$1x10^3$ (g/lit)</td>
</tr>
<tr>
<td>$\rho_c$</td>
<td>Density of cooling liquid</td>
<td>$1x10^3$ (g/lit)</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific heat of reactant</td>
<td>1 (cal/g.K)</td>
</tr>
<tr>
<td>$C_{pc}$</td>
<td>Specific heat of cooling liquid</td>
<td>1 (cal/g.K)</td>
</tr>
</tbody>
</table>

Develop a nonlinear model of CSTR temperature and concentration process in Matlab as shown in Figure 3.

4. DESIGN PI CONTROLLER FOR CSTR

The PI controller has a simple and easy-to-use structure, so it is widely used in industry. The PI controller is responsible for bringing the system's deviation $e(t)$ to 0 so that the transition process satisfies the basic control quality requirements. PI controller has the form:

$$u(t) = k_p e(t) + \frac{1}{T_i} \int_0^t e(\tau) d\tau$$  \hspace{1cm} (16)

Here $e(t)$ is the input signal; $u(t)$ is the output signal; $k_p$ is the proportional coefficient; $T_i$ is the integral time constant.

Among many methods of determining PID parameters (Ziegler-Nichols, Chien-Hrones-Reswick; T-Kuhn, Skogestad, modular optimization and symmetry optimization), Ziegler-Nochols method is simple and easy to apply.

Ziegler-Nichols method is an experimental method to determine PI controller parameters by relying on the step response of the control object that has an S-shaped step response form (when the input signal is signal 1(t)).

Table 2. Parameters of PI controller by step signal 1(t)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_p$</td>
<td>$0.9T_i$ / $(kT_i)T_i = T_i / 0.3$</td>
</tr>
</tbody>
</table>

Performing two-input excitation $q$, $q_c$ of the CSTR by step signal 1(t), we obtain two step response of the CSTR equipment as shown below: step response of concentration $c_A$ (Figure 5), step response of temperature $T_A$ (Figure 6).
In the ideal case, suppose the input $q$ only affects the output $c_A$ and the input $q_C$ only affects the output $T_A$, then according to Ziegler-Nichols 1 (ZN1) parameters of the PI controller for the object control with input and output signal pairs ($q$, $c_A$):

$$k_p = \frac{0.9}{k \theta} = \frac{0.9 \times 110}{1 \times 0.3} = 99 \text{, } T_i = \frac{T}{0.3} = \frac{110}{0.3} = 366.667$$

The parameters of PI controller for control object with input and output signal pairs ($q_C$, $T_A$) are determined as:

$$k_p = \frac{0.9T}{k \theta} = \frac{0.9 \times 56}{350 \times 2} = 0.072 \text{, } T_i = \frac{T}{0.3} = \frac{110}{0.3} = 366.667$$

Response to the CSTR device control system with PI/PI controller according to ZN1 as shown below:

Performing to adjust these PI parameters, we get better system quality as shown in Figure 8, with the following new PI parameters:

- $k_p = 99$, $T_i = 15$
- $k_p = 0.072$, $T_i = 88.1$

The system responses in Figure 7-8 indicate that the PI controllers according to ZN1 provides quality control for the concentration and temperature of CSTR equipment to meet the requirements. However, the quality of control is not good: $c_A$ concentration response has swing 2 times, overshoot (~11%), steady-state error (<3%), acceleration long time (~4.5s), steady long time (~22s); $T_A$ response is overshoot (~12.5%), steady-state error (<1%), good acceleration time (~2s) & good steady time (~3s).

5. DESIGN IMC-PI CONTROLLER FOR CSTR

The block diagram of the CSTR control system structure according to internal model control as Figure 9.

The process model is written in the form as:

$$G_p(s) = \frac{k e^{-\theta s}}{Ts + 1}$$

Here: $k$ is the gain, $T$ is the inertial time, $\theta$ is the time delay

General algorithm for design IMC-PI controller as below:

- Step 1. Identify process model $\hat{G}_p(s)$
- Step 2. Implement process models following form

$$\hat{G}_p(s) = \hat{G}_p(s)\hat{G}_M(s)$$
Where $\hat{G}_d$ includes delay component and zero point component on the right of the virtual axis with $\hat{G}_d(0) = 1$; $\hat{G}_M$ is the portion of the process model inverted by the controller.

IMC controller is designed following formula as:

$$Q(s) = \hat{G}_m^{-1}(s)G_j(s)$$  \hspace{1cm} (20)

IMC's optimal filter structure for CSTR has the form [10,11]:

$$G_j(s) = \frac{(\beta s + 1)^2}{(T_j s + 1)^2}$$  \hspace{1cm} (21)

Here: $T_f$ is the adjustable parameter which controls the tradeoff between the performance and robustness: as selecting smaller than the object's inertial time constant, the response speed is fast. $\beta$ is the additional degree of freedom of the filter, chosen so that removing the pole $s=-1/T$ slows the response to the load disturbance.

Controller according to IMC principle becomes

$$G_c(s) = \frac{(Ts + 1)(\beta s + 1)^2}{k\left[(Ts + 1)^2 - e^{-\alpha u}(\beta s + 1)^2\right]}$$  \hspace{1cm} (22)

From there, we can get PI parameters as follows:

$$k_p = \frac{T_j}{k(3T_j - 2\beta + \theta)}$$

$$T_i = (T + 2\beta) - \frac{3T_j^2 - \theta^2 / 2 + 2\beta\theta - \beta^2}{3T_j - 2\beta + \theta}$$  \hspace{1cm} (23)

When the value $\beta$ is chosen to remove the pole point $s=-1/T$ because it slows the response to the load disturbance, then we determine $\beta$ as follows:

$$\beta = T(1 - \sqrt{(1-T_j/T)^2 e^{-\alpha T}})$$  \hspace{1cm} (24)

Based on the step response of CSTR, we can determine the function of approximating the input signal pair object $(q, c_A)$ and $(q_C, T_A)$ of CSTR when ignoring the cross-impact as follows.

$(q, c_A)$: $G_{p_{-cA}}(s) = \frac{e^{-s}}{110s + 1}$

$(q_C, T_A)$: $G_{p_{-TA}}(s) = \frac{350e^{-2s}}{56s + 1}$

Using the above formulas, we can identify the IMC-PI controllers for input and output pair $(q, c_A)$ as below

$$k_p = 4.6528, T_i = 105.5122$$

$$f_{sd}(s) = \frac{(4.16s + 1)^2}{(10s + 1)^2}$$

and IMC-PI controller for input and output pair $(q_C, T_A)$

$$k_p = 0.006, T_i = 50.894$$

$$f_{sd}(s) = \frac{(3.4s + 1)^2}{(10s + 1)^2}$$

Performing simulations on Matlab, we obtained the response of the IMC-PI control system as shown Figure 10.

Adjusting IMC-PI controller’s parameters is as below, the CSTR control system response show as Figure 11.

$(q, c_A)$: $k_p = 2500, k_i = 0.04$

$(q_C, T_A)$: $k_p = 0.006, k_i = 60$

Thus PI-IMC controllers follow the internal model control to provide good quality control of concentration & temperature: $c_A$ concentration response has no oscillation, no overshoot, eliminates steady-state error, fast acceleration time (~0.3s) and short transition time (~0.8s); $T_A$ temperature response has no oscillation, small overshoot, eliminates steady-state error, fast acceleration time (~0.4s) & short transition time (~0.8s).

6. DESIGN IMC CONTROLLER COMBINED WITH THE CSTR CONTROL OBJECT IDENTIFICATION

The CSTR control object identification by measuring the input and output value of each signal pairs $(q, c_A)$ and $(q_C, T_A)$ and using ARX/ARMA algorithm to identify the control object –
process model $\tilde{G}_{p}(s)$. The output of the identifier is the entire parameter of the control object, which will be used to redefine and redesign the object model and the IMC controller.

Figure 12. IMC controller combined with identification for CSTR

The control object is identified and performed by the process model transfer function $\tilde{G}_{p}(s)$ by suitable ARX/ARMA algorithm; $G_{IMC}(s)$ is an IMC controller designed with inverse process model

$$G_{IMC}(s) = \tilde{G}_{p}^{-1}(s)$$  (25)

The object control is always changed by the impact external noise. By measuring the input and output values and using the suitable indentification algorithm, the parameters of the process model can be determined. These parameters will be fed to the controller $G_{IMC}(s)$ to stabilize the output object.

Assuming that the cross-effects between $(q, T_A)$ and $(q_C, c_A)$ are negligible and the transfer function of the input and output pairs $(q, c_A)$ and $(q_C, T_A)$ as following.

$$G_{p}(s) = \frac{ke^{-\alpha}}{Ts + 1}$$  (26)

Measure the value of the input and output pairs $(q, c_A)$ and $(q_C, T_A)$ as shown in the diagram below.

![Diagram](image)

100 giá trị đầu vào $u(0), u(1), u(2), \ldots, u(997)$  
100 giá trị đầu ra $y(0), y(1), y(2), \ldots, y(99)$

Figure 13. Measured value of the input and output pairs $(q, c_A)$ and $(q_C, T_A)$ of the CSTR equipment

Suppose we obtain the measurement data as shown Table 2.

| Table 2. Measurement data of the pairs $(q, c_A)$ and $(q_C, T_A)$ |
|---|---|---|---|---|
| $q$ | $c_A$ | $q_C$ | $T_A$ | $y$ |
| 1  | 2  | 3  | 4  | 5  |
| 6  | 7  | 8  | 9  | 10 |
| 11 | 12 | 13 | 14 | 15 |

Based on this data table, we proceed to identify the CSTR process model. Here assume the use Matlab's Identification Toolbox, we get the following result

$$\tilde{G}_{p,q_A}(s) = \frac{e^{-\alpha}T_{q_A}^1}{(1+110s)(1+s)}$$  (27)

Similarly, we can identify the transfer function with the input and output pair $(q_C, T_A)$

$$\tilde{G}_{p,T_A}(s) = \frac{350e^{-2\alpha}}{(1+56s)(1+2s)^2}$$  (28)

From which we can easily determine the IMC controller for each pair of input and output variables $(q, c_A)$ and $(q_C, T_A)$ as:

$$G_{IMC,q_A}(s) = \frac{(1+110s)(1+s)}{(1+T_{q_A}c_A)^2}$$  (29)

$$G_{IMC,T_A}(s) = \frac{(1+56s)(1+2s)^2}{350(1+T_{q_A}T_A)^2}$$  (30)

Here $T_{q_A}$, $T_{T_A}$ is the time constant of the low-pass filter, selected to satisfy $T_{q_A}$, $T_{T_A}$<1. We choose $T_{q_A}=0.15$; $T_{T_A}=0.85$

Figure 14. Simulation IMC controller with CSTR identification

Implementing the simulation of the CSTR control system with IMC controller combined with CSTR process identification, we obtained the results as shown Figure 15.

Figure 15. The IMC controller combined with CSTR identification
Simulation results show that IMC controller combined with the CSTR identification for good quality control. Here do not need to adjust controller parameters but the control system quality is still very good, as follows: \(c_A\) concentration response has not oscillation, not overshoot, not steady-state error, fast acceleration time (~1s) & short transition time (~2.5s); \(T_A\) temperature response has not oscillation, not overshoot, eliminates steady-state error, fast acceleration time (~0.4s) & short transition time (~0.8s).

7. CONCLUSION

The article proposes the two-input-two-output nonlinear model of the continuous stirred tank reactor, that are the temperature process and concentration process of output product. This is close to the typical actual physical process commonly used in chemical industry. Based on this nonlinear model, the article presented the simple PI controller, which effectively controls the process of temperature and concentration of output product. Then based on internal model control, the article introduced the effective IMC-PI controller and IMC-Ident controller for the CSTR temperature and concentration control processes. Simulation results, when compared to using PI controllers, show that the CSTR control system quality when using IMC-Ident is better when using IMC-PI. These controllers are designed based on internal model control: simple, reliable, easily applicable to industrial production.

REFERENCES


