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Temperature Control in Polyvinyl Chloride Production: Internal Model Control (IMC) and Proportional, Integral and Derivative (PID) controller Implementation

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Abstract

The Polyvinyl Chloride (PVC) suspension polymerization process is an exothermic reaction which is carried out in a batch reactor. In batch polymerization, there may occur unexpected thermal reactive runaway. Therefore, there is a difficulty in controlling the behavior of the system in order to keep the product in good and fine quality in each batch job. In polymerization process, the temperature of the reactor plays an important role because the molecular structure of the polymer is very sensitive to temperature. In this study, two type of controllers i.e. Proportional Integral & Derivative Control (PID) and Internal Model Control (IMC) are designed and implemented to track the temperature profile in batch reactor. The dynamic model of the batch polymerization reactor is solved using $4^{th}/5^{th}$ order Runge Kutta method (MATLAB ODE45) and the effect of temperature on the performance of polymerization reactor control is investigated using simulation. Both controllers performance of IMC and PID controllers are evaluated and compared. Finally robustness tests are conducted by changing some operating parameters process model. It has been observed that IMC is more effective in controlling the batch polymerization system at its optimal trajectory compared to PID control strategy.

Keyword: Temperature control, Polyvinyl Cloride, Internal Model Control, PID controller

1. Introduction

Batch reactors are used to produce a wide variety of expensive products. This process normally involves several competing reactions which may cause undesired product or waste. As a result, there is a great deal of interest to enhance batch operation to achieve high quality and purity products while minimizing the conversion of undesired by-products. However, control operation of batch reactor is quite difficult, and still provides challenging and the interesting problems. This is mainly due to the inherent complexity of the batch reactors. Only a few physical quantities such as temperature and pressure are available for direct on-line measurement. That makes direct control of product properties difficult [1]. In this work, a batch polymerization reactor of PVC is studied. The PVC suspension polymerization process is an exothermic reaction. There may occur unexpected thermal reactive runaway that cause a difficulty in controlling the behavior of the system in order to keep the product in good and fine quality in each batch job. In polymerization process, the temperature of the reactor plays an important part because the molecular structure of the polymer is very sensitive to temperature. The batch reactor temperature is controlled at its optimum value by manipulating the heat input to the batch reactor. The flow rate of the coolant in the reactor's jacket is made as the potential disturbance of the process. The process kinetic modeling and parameter estimation is obtained from work done by Lewin [2]. The effects of temperature to the conversion achieved in the polymerization process are studied and the optimal process condition is determined.

2. Modeling of batch reactor

The batch reactor models are based on the assumptions of perfect mixing and ideal liquid mixture behavior.

2.1 Mass Balance Equations

The mathematical modeling of PVC used in this work are taken from Kiparissides and Shah [3]:

$$\frac{dx}{dt} = K_1 \sqrt{I}\left(1 + Qx\right) \tag{1}$$

Equation 1 is the conversion of monomer to polymer. The following equations are the mass balance equations for the initiators

$$\frac{dI_A}{dt} = -K_A e^{-Ea_A/R(T+273.16)} \tag{2}$$

$$\frac{dI_B}{dt} = -K_B e^{-Ea_B/R(T+273.16)} \tag{3}$$

The local initiator concentration decays according to first order kinetics. The overall rate constant, K_1, can be expressed in the Arrhenius form:

$$K_1 = K e^{\frac{E_e}{R(T+273.16)}} \tag{4}$$

The coefficients Q and P depend on the state variable

$$Q = \frac{\left(P\left(1 - x_c\right) - 1\right)}{x_c} \tag{5}$$

$$P = 27.0 - 0.14T \tag{6}$$

I is actually the sum of the two initiator species used

$$I = I_A + I_B \tag{7}$$

2.2 Energy Balance Equations

$$\frac{dT}{dt} = \frac{\left(-\Delta H_R\right)m_o \frac{dx}{dt} - a - b - c}{\left(m_M C_{PM} + m_P C_{PP} + m_{Wtot} C_{PW}\right)} \tag{8}$$

where;

$$a = \dot{m}_J \, C_{PW} \left(T_J - T_{J0}\right) \tag{9}$$

$$b = \dot{m}_B \, C_{PW} \left(T_B - T_{J0}\right) \tag{10}$$

$$c = \dot{m}_W \, C_{PW} \left(T - T_W\right) \tag{11}$$

As a result of the assumptions made regarding the negligible thermal accumulation in the jacket and baffle coolants, the effluent temperatures of these coolant streams can be computed based on pseudo steady state energy balances:

$$T_J = \frac{T + \alpha_J T_{J0}}{1 + \alpha_J} \tag{12}$$

$$\alpha_J = \frac{m_J C_{PW}}{(UA)_J} \tag{13}$$

$$T_B = \frac{T + \alpha_B T_{J0}}{1 + \alpha_B} \tag{14}$$

$$\alpha_B = \frac{m_B C_{PW}}{(UA)_B} \tag{15}$$

For this study, the optimal conditions are shown in Table 1:

Table 1: Operating conditions

T_r (ºC)	60.0
Initiator A, I_A (kg)	20.0
Initiator B, I_B (kg)	16.3
m_0 (kg/minute)	6000.0
m_J (kg/minute)	60.0
m_B (kg/minute)	20.0
m_W (kg/minute)	30.0
T_W (ºC)	10

3. Controller Design & Implementation

Two types of controllers are applied using the Proportional Integral Derivative (PID) controller and Internal Model Control (IMC) controller.

3.1 Proportional, Integral & Derivative (PID) control

In this work, the PID control was developed using the Ziegler-Nichols method [4]. Ziegler-Nichols published a classic paper that introduced the continuous cycling for controller tuning. Using the controller relations stated, the parameters for the PID were calculated. After fine tuning, the parameters found to be as followed:

Table 2: Controller settings

PID Controller Settings	
Proportional Gain, K_c	167.8
Integral Time, τ_I	2.5
Derivative Time, τ_D	0.625

Where $f(s)$ is a filter. A filter is added to make the controller proper. The transfer function is proper if the order of the denominator polynomial is at least as high as the numerator polynomial. The filter transfer function is;
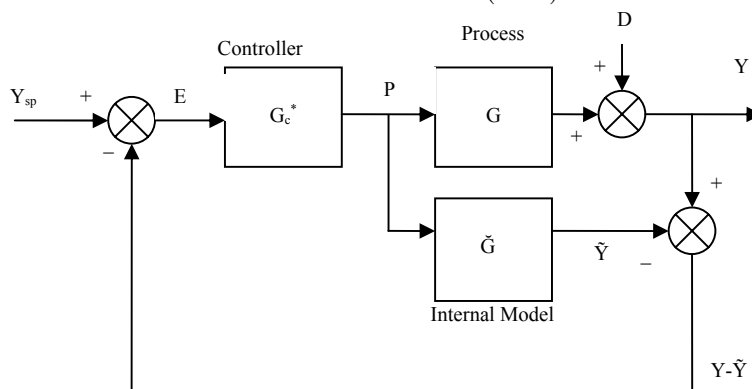
$$f(s) = \frac{1}{(\lambda s + 1)} \qquad (20)$$

Figure 1: Internal Model Control

3.2 Internal model control (IMC)

The Internal Model Control was developed by Morari and coworkers [4]. The IMC controller is based on an assumed process model and leads to analytical expressions for the controller settings. The schematic block diagram of the IMC system is depicted in Figure 1, where $G(s)$ is the given stable process to be controlled, $\breve{G}(s)$ a model of the process and $G_c^*(s)$ the IMC primary controller. The transfer function for the process was obtained by performing the Laplace Transform on the process equations given in section 2.0. The transfer function is;

$$\widetilde{G}(s) = \frac{-4.02 \times 10^{-6}}{s + 5.42} \qquad (17)$$

The IMC is the inverse of the invertible portion of $\widetilde{G}(s)$, therefore;

$$\widetilde{q}(s) = \widetilde{G}^{-1}(s) = \frac{s + 5.42}{-4.02 \times 10^{-6}} \qquad (18)$$

The primary controller takes the form of;

$$G_C^*(s) = \widetilde{q}(s)f(s) = \widetilde{G}^{-1}(s)f(s) \qquad (19)$$

Where λ is the filter-tuning parameter. A few tuning variables were tried on λ, and was found that the best λ value was 200. Therefore the primary controller is:

$$G_C^*(s) = \frac{s + 5.42}{(-4.02 \times 10^{-6})(200s + 1)} \qquad (21)$$

4. Results and discussion

4.1 The effect of the temperature on the performance of polymerization reactor

In the first part of this study, MATLAB 7.0 software was used to simulate the process modeling and controlling parts. The model equations which were used are the reactor temperature, initiator and the conversion of the PVC. All these model equations are all in the form of ordinary differential equations and solved using $3^{rd}/4^{th}$ order Runge Kutta method (MATLAB ODE45) to observe the polymerization of PVC profile. Figure 2 showed the time-activity curves of different reactor temperature from 57ºC to 62ºC. The results showed that the conversion was increased with increases of reactor temperature. The optimal range of temperature is in between 57ºC to 62ºC. Below that range the conversion is very little and takes a long time to reach optimum conversion. Above that

range, a run-away polymerization could result. The temperature 60ºC was chosen as the optimal temperature value because it is the minimum temperature that can achieved the optimal conversion faster than other temperatures value except for 61ºC and 62ºC. However in the industry, temperatures of 61ºC and 62ºC cannot be used because the initiators are decomposed faster at these temperatures. When the initiators decompose faster, the chances of initiating a chain reaction for polymerization will deter. From Kiparissedes [3], the reaction time is 450 minutes (about 7 hours).
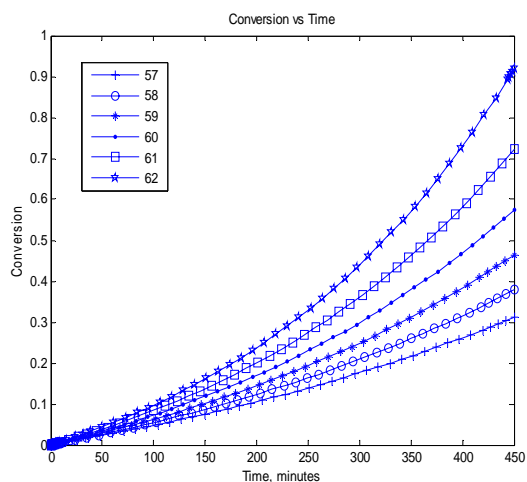
Figure 2: The change of conversion to time
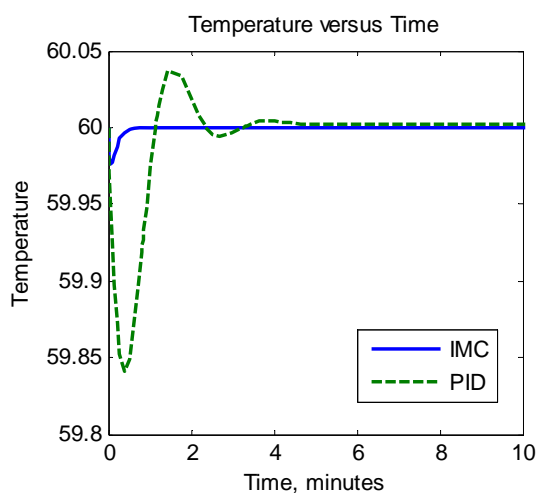
Figure 3: Comparison of set-point responses for PID and IMC Control Systems

4.2 Comparison of the IMC and PID control

In this work, the batch reactor temperature is controlled at its optimum value by manipulating the heat input to the batch reactor. Here, the potential disturbance of the process is the temperature of the coolant.

4.2.1 Set point tracking

Figure 3 shows the performance of IMC and PID in tracking the temperature profile at 60°. It indicates that the IMC controller has a shorter settling time compared to the PID controller. The IMC controller also gives less oscillatory response compared to the PID controller response. Both controllers do not show an overshoot.

A step set-point change was introduced at time equal to 30 minutes. From the result shown in Figure 4, the IMC controller as usual has a faster settling time than the PID controller. The PID controller shows greater overshoot and has a longer settling time.
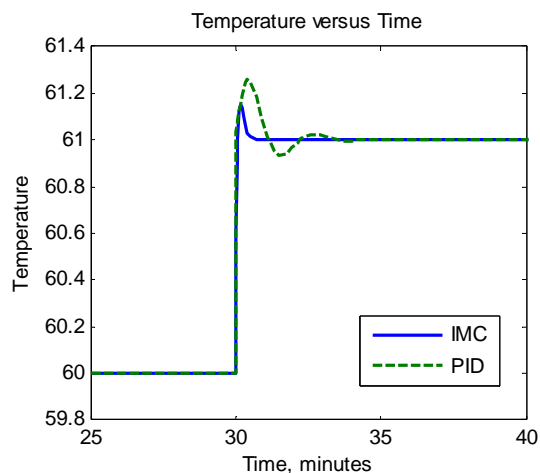

Figure 4: Comparison of set-point change responses for PID and IMC Control Systems

4.2.2 Disturbance rejection

At 26 minutes, a step change disturbance is introduced. From the graph shown in Figure 5, the PID controller produces a slower disturbance response compared to the IMC controller. The PID controller has a settling time of 4 minutes whereas the IMC controller has a settling time of less than a minute. The IMC provides much better disturbance rejection in view of their smaller settling time.
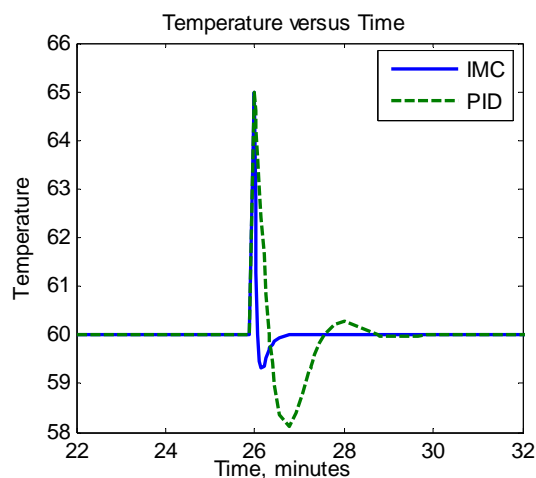
Temperature versus Time

Figure 4: Comparison of disturbance responses for PID and IMC Control Systems

4.2.3 Robustness tests

Previously, the process model was assumed to be an ideal model. However, practically most models are non-ideal. Thus, for a control system to function efficiently, it should be unduly sensitive to small changes in the process or inaccuracies in the process model. A control system that satisfies this requirement is said to be robust or insensitive. Robustness test were carried out for both PID and IMC controllers. The robustness tests are carried out by:

Test 1: Increase the heat of reaction from 1540.0 kJ/kg to 1925 kJ/kg, a 25% increase. It represents a change in operating conditions that could be cause by the behavior of the phase of the system.

Test 2: Reduction of heat transfer coefficient from 40.842 kJ/(minutes.m^2.°C) to 30.63 kJ/(minutes.m^2.°C), a 25% decrease. This test simulates a change in heat transfer that could be expected due to fouling of the heat transfer surfaces.

Test 3: Increase the reaction rate constant from 7.761 × 10^{13} minute^{-1} to 9.7 × 10^{13} minute^{-1}, a 25% increase. This test is important to study the sensitivity of a given control strategy to variations in reaction chemistry.

Test 4: Combined all three cases at the same time to model the imperfectness of the process.

Figure 5 gives the responses of both controllers in response to a changed heat of reaction. The responses showed that the PID control system took 5 minutes to reach the desired temperature while the IMC controller took 1 minute to reach the set point. The time required

for both PID and IMC controllers to track the setpoint was similar to the time required in controller setting before. However, there were overshoot for both controllers, but for IMC controller the overshoot is smaller compared to PID controller. This situation represents a much more dangerous operation than the previous one, because an overshoot in temperature brings the system much closer to instability.
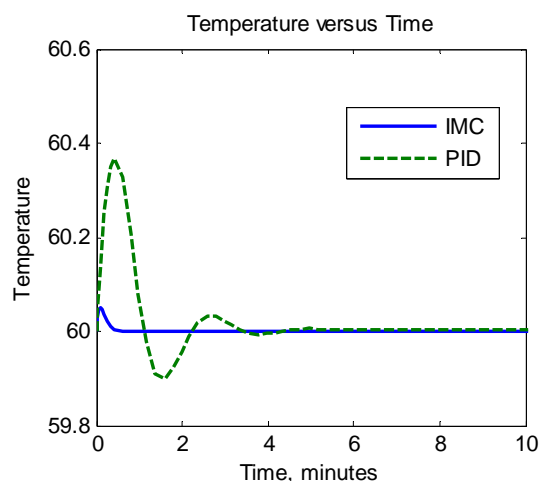
Temperature versus Time

Figure 5: Temperature Response of Robustness Test 1 for PID and IMC Control Systems

Meanwhile for robustness Test 2, when heat transfer coefficient was decreased, figure 6 shows that the time to reach the set point for the PID and IMC controllers are 5 minutes and 1 minute respectively. The time required for the both PID and IMC controller to tracking the setpoint was similar to the time required in controller setting before.

The results of the third test are given in Figure 7. Once again, it can be seen that the PID controller's performance has again deteriorated by changing the reaction rate. On the other hand, the IMC controller's performance has changed very little when compared with the nominal response.
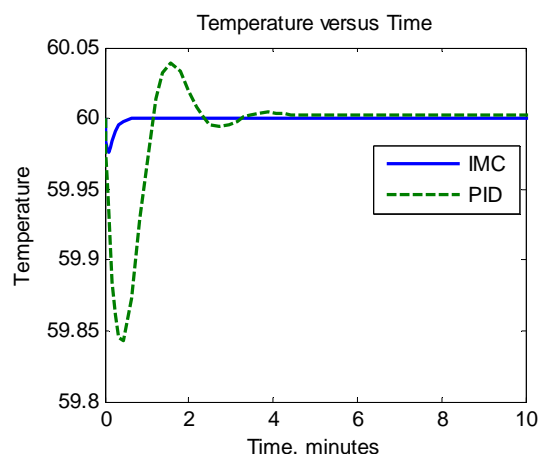
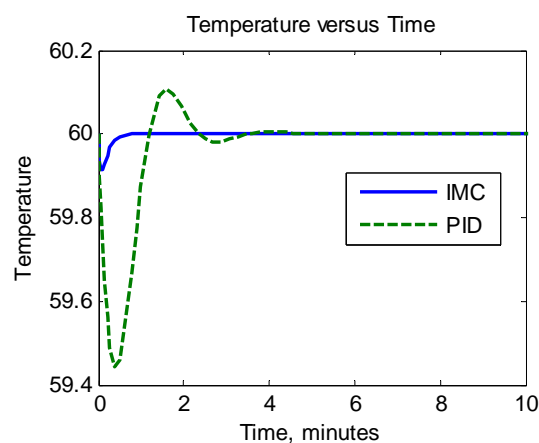**Figure 6: Temperature Responses of Robustness Test 2 for PID and IMC Control Systems**

Figure 7: Temperature Responses of Robustness Test 3 for PID and IMC Control Systems
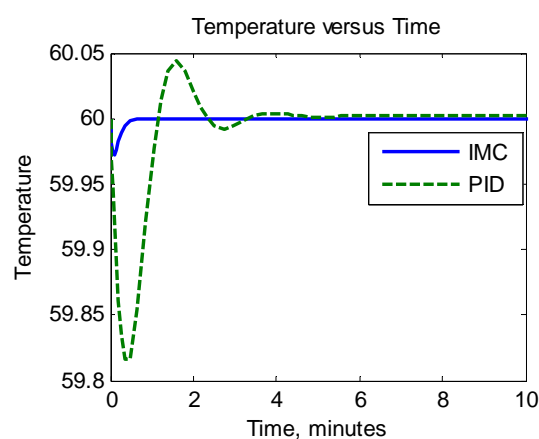

Figure 8: Temperature Responses of Robustness Test 4 for PID and IMC Control Systems

Finally for robustness Test 4, when the heat of reaction, and reaction rate constant was increased as well as the heat transfer coefficient at the same time, figures 8 shows that, the PID and IMC controller's response observed time to reach the set point are 5 minutes and 1 minute respectively. For the both controllers, the responses seem to be the same as in robustness Test 2. Therefore, this case confirms the result that the IMC controller is much more robust than PID controller and provides not only better controller performance but also increase the safety of operation.

5. Conclusions

The effect of temperature on the performance of polymerization reactor control had been studied and from the study it was found that the conversion of the monomer to polymer depends on the reactor temperature. The conversion was increased with increases of reactor temperature and both the initiators decomposed but at a slower pace. Two different types of controller namely PID and IMC controllers were designed and implemented to track optimal reactor temperature profiles using simulations of process model obtained from literature. Open-loop transient was induced by a step change in set-point tracking. Extensive simulations had been performed to show that the proposed IMC method was generally applicable regardless process involved. For IMC control, if a set-point change occurs, the controller acted very quickly to reach its latest set point. Compared with the PID controller, the IMC controller also provided improved performance if a disturbance occurs; the controller acted very quickly to hold the reaction temperature at its set point. Robustness (sensitivity) of both controllers had been conducted by changing process parameters like the heat of reaction, heat transfer coefficient and the reaction rate constant. Overall, the IMC controller had be found to be more effective and robust in tracking the optimal reactor temperature compared to PID control strategy.

6. Nomenclature

x = fractional polymerization of the monomer
T = reaction temperature (ºC)
I = local initiator concentration (moles/m^3)
T = time (sec)
ΔH_R = heat of reaction (kJ/mole)
m_o = initial concentration of monomer(kmoles/m^3)
m_j = flow rates of coolant in jacket (kg/s)

m_H = flow rates of coolant in baffles (kg/s)
T_J = effluent temperature of jacket (ºC)
T_B = effluent temperature of baffles (ºC)
m_w = flow rate of "cold-shot" (kg/s)
T_W = feed temperature of "cold-shot" (ºC)
T_{J0} = feed temperature of coolant (ºC)
m_M = local mass of monomer in the reactor (kg)
m_P = local mass of polymer in the reactor (kg)
m_{Wtot} = accumulated water in the reactor fluid (kg)
C_{PM} = specific heats of monomer (kJ/kg. ºC)
C_{PP} = specific heats of polymer (kJ/kg. ºC)
C_{PW} = specific heats of water (kJ/kg. ºC)
x_c = critical conversion (conversion)
R = gas constant (kJ/mol. ºC)

7. Acknowledgment

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