ONLINE IMPLEMENTATION OF IMC BASED PID CONTROLLER IN BATCH ESTERIFICATION REACTOR

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ABSTRACT

Esterification is one of important process that operates in a batch reactor. Since the inherent nonlinear properties of this batch reactor, the control of such reactor to ensure an efficient operation remains a great challenge. In this work, an Internal Model Control based Proportional Integral Derivative (IMC-PID) is designed and implemented on-line to control the reactor temperature in a bench scale of batch esterification reactor. The reactor temperature was maintained at its desired value by manipulating the coolant flowrate. The controller design is based on the Internal Model Control (IMC), which end up with a single tuning parameter. The performances of the IMC-PID through set-point tracking and disturbance rejection are evaluated and then compared with the simulation results [Zulkeflee and Aziz, 2009]. The results achieved indicated that the on-line IMC-PID controller strategy was able to control the batch esterification reactor and in agreement with the results obtained using simulation study.

Keywords: Internal model control; Batch reactor; PID control; Esterification; IMC based PID

1. INTRODUCTION

Esterification is an important reaction in chemical industry. From this reaction, various types of esters are produced for commercial usage primarily as flavors and fragrances in food and pharmaceutical industry. Esterification is typically nonlinear process due to the nature of the process behavior such as reaction temperature, reaction time, pressure and in most cases, is caused by the complexity of the process kinetics [Le Lann *et al.*, 1999]. In order to increase the reaction rate and conversion of reactants beyond the thermodynamic equilibrium, enzymatic esterification process is used since the early production of esters by extraction from natural sources was too expensive for commercial use [Longo and Sanroman, 2006]. However, this kind of process has some limitations due to the sensitivity of the enzymatic process behavior to the reactor temperature [Serri *et al.*, 2006; Yadav and Lathi, 2003]. Thus, it is important to determine and control the optimal temperature of the reactor. However, controlling the operational of batch reactor to ensure maximum ester production is remains the challenge for control engineer because of the nonlinearity behavior of such process. Hence, advanced control methodologies need to be designed to improve the control performance.

There are many types of advanced control techniques using either specific algorithms for particular systems or very general methods with a wide application area and a well-developed

Proc. of the 5^{th} International Symposium on Design, Operation and Control of Chemical Processes

ISBN: 978-981-08-6395-1

theory. Recently, model-based control techniques have been largely extended and have gained prominence during the past decades. The increase of mathematical models in the chemical engineering field was a major driving force behind the development of the model-based control strategy [Agachi *et al.*, 2006]. A better model can replace laboratory or field tests that are difficult or costly to perform or to identify crucial experiments that should be carried out. There are many types of model based control strategies such as Model Predictive Control (MPC) [Garcia *et al.*, 1989], Generic Model Control (GMC) [Cott and Macchietto, 1989] and Internal Model Control (IMC) [Garcia and Morari, 1982]. However, the IMC strategy is found to be relatively easy to implement when compared to other model-based control methods.

The IMC controller has a simple structure and fewer parameters to be tuned. Moreover, it has significant effectiveness in improving the robustness and control performance of the system with a long time delay [Li *et al.*, 2009]. Because of these advantages, the IMC has received a lot of attention from many researchers for the process control system. IMC control technique was proposed by Smith in 1959 [Garcia and Morari, 1982]. Subsequently, there are many techniques were developed based on this IMC such as the multiloop-IMC structure [Economou *et al.*, 1986], the IMC based PID (IMC-PID) control [Rivera *et al.*, 1986], the adaptive IMC [Narayanan *et al.*, 1997], Neural Network based IMC [Aziz *et al*., 2000; Mujtaba *et al.*, 2006], and Support Vector Machine approximate based IMC (SVM-IMC) [Wang and Yuan, 2008]. Among of these IMC control strategies techniques, IMC-PID have a great potential since more than 95% of the control loops are still using the Proportional Integral Derivative (PID) controllers. It is because it's relatively simple structure, which can be easily understood and implemented [Lee *et al.*, 2006]. The IMC-PID tuning rules have the advantage of only one tuning parameter is needed to achieve good closed-loop performance. Since then, various modifications and enhancement to this technique have been reported [Yang *et al.*, 2002; Lee *et al.*, 2006; Shamsuzzoha and Lee, 2008].

In this paper, an IMC-PID control strategy is designed to control batch esterification process and then be implemented in bench scale of 1 liter batch reactor. The reactor temperature, coolant flow rate and inlet coolant temperature have been chosen as control, manipulated and disturbance variables respectively. As a case study, Citronellyl laurate esterification has been chosen. The performance of IMC- PID controller in tracking the desired reactor temperature profiles and rejecting disturbance is evaluated. The results achieved are then being compared with the simulation results [Zulkeflee and Aziz, 2009].

2. MATERIALS AND METHODS

2.1 Chemicals and Enzymes

Lauric acid was supplied by Fluka (Swizerland) with the purities of 98 % and DL-Citronellol (95 % pure) by Sigma-Aldrich (Japan), support Amberlite MB-1 by Sigma-Aldrich (USA), iso-octane (99.84 % assay) by Fisher Chemicals (UK) and *Candida rugosa* lipase L1754-5G (Type VII, 901 units per mg solids) by Sigma-Aldrich (Japan). All the chemicals were analytical grade and were used without further purification.

2.2 Enzyme Immobilisation

20 mg of enzyme was dissolved in 5mL of sodium phosphate buffer (pH 7.5) mixed with 2 g of dried support and was gently stirred at 200 rpm for 24 hours at room temperature. The immobilized lipase preparation was filtered and washed thoroughly with deionized water and rinsed with sodium phosphate buffer solution.

2.3 Citronellyl Laurate Synthesis

All the experiments were performed in a batch reactor with 1 L iso-octane as a solvent. In the experiments, 30 mM of DL-Citronellol and 20 mM lauric acid were used as reactants. The stirring rate was adjusted to 100 to 300 rpm. The system was operated to reach the desired conversion of ester while samples were taken every five minutes. The samples of 1 mL were taken from the outlet to analyze the concentrations. The concentration analysis was done by adding 1 mL quenching agent (Ethanol-Acetone) to 1 mL sample immediately. The samples were later titrated with 20 mM NaOH in order to obtain an un-reacted amount of lauric acid where phenolphthalein was used as an indicator.

2.4 Temperature Control System

A system was developed to control the temperature in a litre-scale batch esterification reactor; a schematic schedule of the system is shown in Figure 1. The reactor is a jacketed glass reactor with a propeller stirrer and water as cooling medium. Temperature was measured by thermocouples (pt100:SEM203P) and connected to a PC for monitoring. The software simulink in MATLAB R2008a was used for the PID controller algorithm to manipulate the inflow of cooling water to maintain the temperature of reactor at the desired set-point. The measured temperature of the reactor was compared with the set-point and the cooling water flow into the jacket was manipulated via a proportional valve (Burkert 2835).

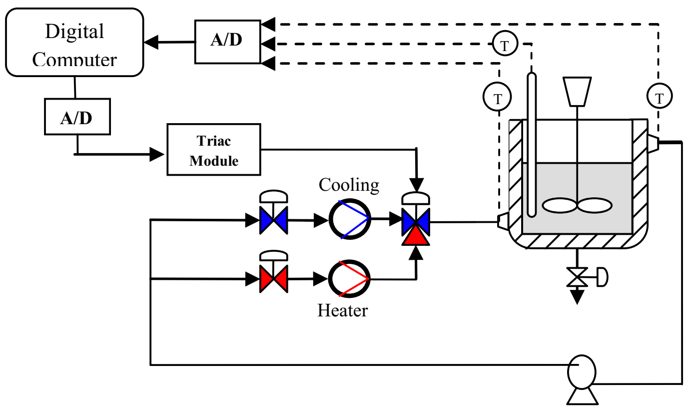

Figure 1: Schematic diagram of the batch esterification reactor system.

3. IMC BASED PID TUNING

In this section, the basic framework for the IMC-PID algorithm and the implementation of the algorithm in the batch esterification reactor is detailed out. Based on Rivera *et al.* [1986], the goal of control system design is to achieve a fast and accurate set-point tracking;

$$y \cong y_s \ \forall t, \ \forall d \tag{1}$$

This implies that the effect of external disturbances should be corrected as efficiently as possible and also being assured of insensitivity to modeling error

$$y' \cong y_s - d \quad \forall t, \ \forall d \tag{2}$$

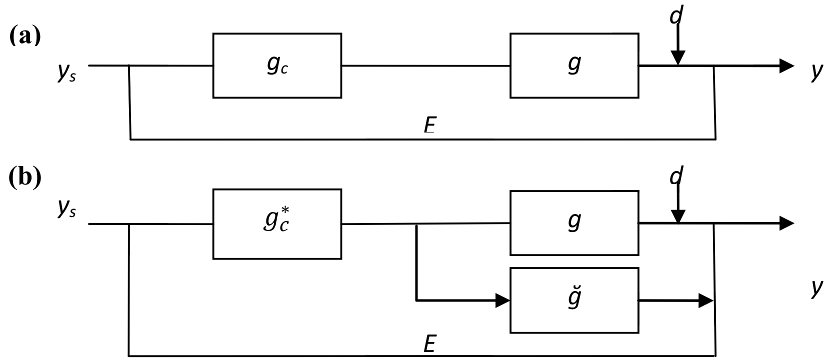

Figure 2: (a) conventional configuration and (b) Internal Model Control configuration

The PID parameter tuning law based on the relationship of the IMC and the PID controller has been proposed by Rivera *et al*. [1986]. PID control structure is shown in Fig. 2(a), where $\boldsymbol{g_c}$ and $\boldsymbol{g}$ are the PID controller and the controlled process, respectively. They are given by:

$$\boldsymbol{g_c} = K_c(1 + \frac{1}{T_I s} + T_D s) \tag{3}$$

$$\boldsymbol{g} = \frac{K}{1 + Ts} e^{-\theta s} \tag{4}$$

Where k_c, T_I and T_D are the proportional gain, the reset time and the derivative time, respectively. Meanwhile, the structures of the IMC is shown in Fig. 2(b), where $\boldsymbol{g_c^*}$ and $\boldsymbol{\breve{g}}$ are the IMC controller and the internal model respectively. The IMC controller $\boldsymbol{g_c^*}$ is given by

$$\boldsymbol{g_c^*} = \frac{1 + Ts}{K} X \frac{1}{1 + \lambda s} \tag{5}$$

By comparing Fig. 2(a) with Fig. 2(b), the following relation is given:

$$\boldsymbol{g_c} = \frac{\boldsymbol{g_c^*}}{1 - \breve{g}\boldsymbol{g_c^*}} \tag{6}$$

The IMC-PID tuning parameters design for First-Order plus Time delay (FOPTD) process shown in Appendix A has resulted in a PID control law. After the derivation, the IMC-PID setting for FOPTD process is shown in Table 1.

Table 1- PID Controller settings for IMC-PID

PID parameters	**IMC-PID** [Rivera et al., 1986]
Proportional Gain (K_c)	$K_c = \frac{T + 0.5\theta}{K(\lambda + 0.5\theta)}$
Integral Time (T_I)	$T_I = T + 0.5\theta$
Derivative Time (T_D)	$T_D = \frac{T\theta}{2T + \theta}$

4. RESULT

4.1 Process Model

In the first part of the study, the process reaction curve was build by performing the open-loop step-test by both experiment and simulation. In simulation, the FOPTD was obtained using first principle model that developed by Zulkeflee and Aziz [2009]. For all control works, flowrate of coolant was selected as a manipulated variable. The ranges of input signals for jacket flowrate was varying between 0 to 0.15L/min and a ±0.002L/min step change is given to the inlet flowrate of coolant. Worst case of model parameters of the process (largest process gain, smallest time constant and largest time delay) was chosen to develop FOPTD [Bhaba *et al.*, 2005]. The FOPTD model obtained to represent the system behaviour was:

$$\boldsymbol{g} = \frac{15540}{1+11.1s}e^{-6.573s} \tag{7}$$

The temperature response to the step change is presented in Fig. 3. It is observed that the reactor temperature profiles obtained from simulation and experiment of the batch esterification reactor is in good agreement with R^2=0.947.

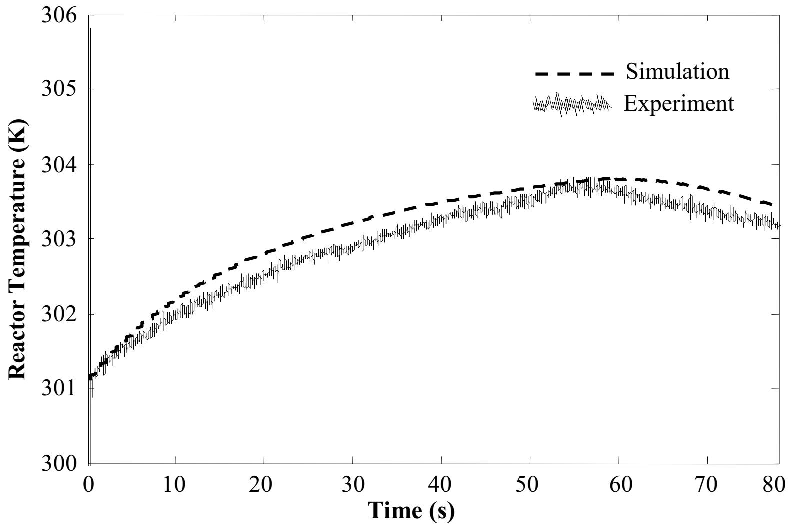

Figure 3: Process reaction curve (ΔF_j=±0.002L/min)

4.2 PID Controller Settings for IMC-PID and Conventional PID Controller

As can be seen in the IMC-PID parameter equations, there is no need to tune integral time, T_I and derivative time, T_D since they are function of time delay, θ, only. Only the proportional gain, K_c needs to be adjusted and it is inversely related to filter constant, λ. The value for λ recommended by Rivera et al. [1986] should be greater than 0.8θ because of the model uncertainty due to the Padé approximation. Hence, in this study, the lowest value of λ allowed is 6. The effects of λ have been studied since the performance of a closed-loop system designed based on the IMC design method is determined solely by the filter dynamic [Kaya, 2004]. Using simulation, the value of λ have been varied from 6 to 20 and it is noticed from Fig. 4 that the reactor temperature response gets faster as λ is decreased. However, decreasing the λ value leads to the overshoot response for reactor temperature. In the upper plot of Fig. 4, it is shown that the reactor temperature response for λ=6 and λ=10 achieved the set-point at the same time. However, the response for λ=6 gave faster rising time. In the lower plot of Fig. 4, the jacket flowrate profiles for both λ are acceptable. As a result, λ value equal to 6 is chosen as a best tuning since it give the best response.

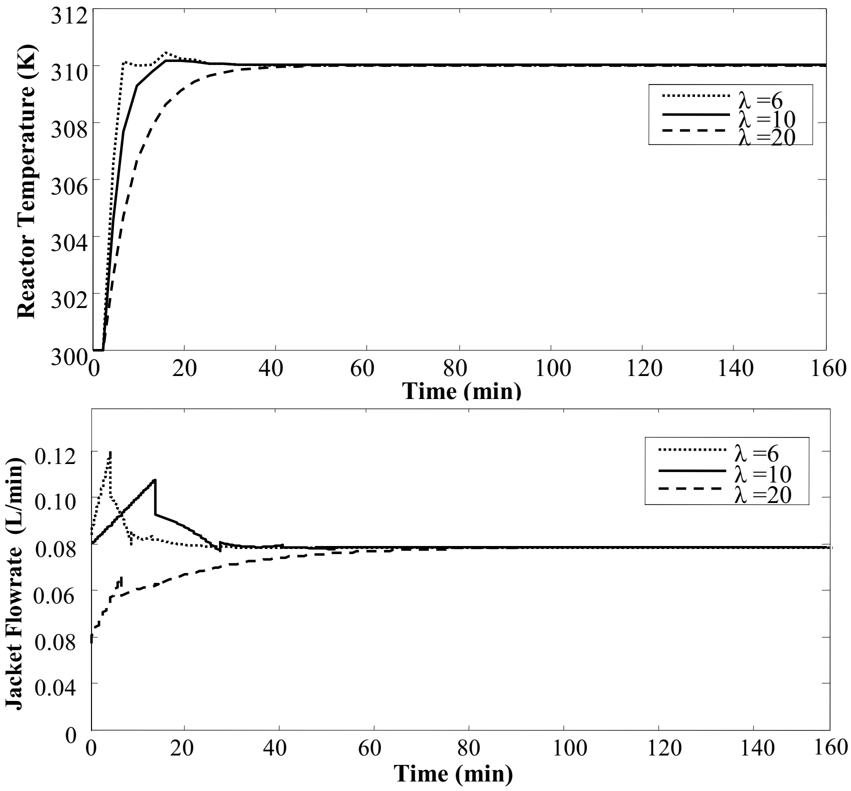

Figure 4: The reactor temperature and manipulated variable response by varying filter constant (λ).

The final tuning PID parameters of the IMC-PID controller are given in Table 2 and these parameters tuning were implemented in the PID controller which have been installed in the temperature control system of batch esterification reactor.

Table 2- PID pameters for IMC-PID and conventional PID controller

Controller	K_C	T_I	T_D
IMC-PID	0.000099	14.3865	2.535
PID	0.00016	13.17	0.328

4.3 Set-point Tracking and Disturbance Rejection

Set-point Tracking: The on-line and simulation responses of the IMC-PID system in tracking the constant set-point at 310K are shown in Fig. 5. As can be seen in the upper plot of Fig 5, the on-line response for IMC-PID controller (IAE=365.60) drives the process output to desired set-point with faster response time with no overshoot or oscillatory response. Meanwhile, the output response for simulation IMC-PID controller (IAE=137.99) was observed to have small overshoot response. The simulation and on-line IMC-PID controller action (the manipulated variable changes) in order to track the set-point is shown in lower plot of Fig. 5. As can be seen in the figure, the manipulated variables for the on-line response for IMC-PID controller were more fluctuated and slower if compared to the simulation response. This late response might due to factors such as heat loss while transfering coolant into the cooling jacket, time delay related to the process as well as intrumentations. In terms of ester conversion, after 80 minutes of the implementation of the on-line IMC-PID controller leads to a 93.22% conversion of Citronellyl laurate, while the simulation IMC-PID controller lead to 95.01% conversion.

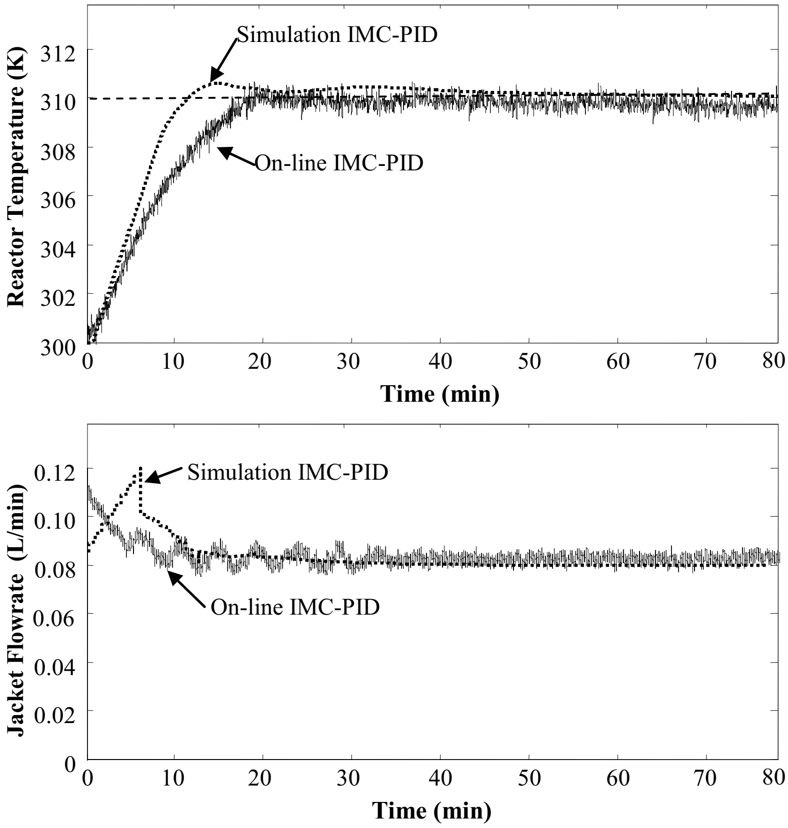

Figure 5: Reactor temperature response of on-line and simulation IMC-PID controller for set-point tracking and their respective manipulated variable profiles.

***Disturbance Rejection**:* Here, the initial jacket temperature was considered as the process disturbance. A step change (+5%) of the initial jacket temperature from 294K to 309K was implemented into the system. The temperature responses for on-line and simulation IMC-PID in rejecting the disturbance are presented in Fig. 6. The simulation response for IMC-PID controller (IAE=53.67) was found to drive the temperature response faster than the on-line IMC-PID controller (IAE=92.33) with no oscillation and less overshoot. From the results, it was observed that the IMC-PID controller was able to reject the effect of disturbances. It is also indicates that the variations of the jacket flowrate responses for the on-line IMC-PID controller is larger and more oscillated as compared to the simulation response of IMC-PID controller.

The results of both set-point tracking and disturbance rejection indicate that the on-line and simulation IMC-PID controller responses was in a good agreement. However, the speed of on-line implementation of IMC-PID controller in tracking the desired set-point was slower compared to the simulation implementation. Eventhough there were slightly difference in terms of time response between on-line and simulation implementation, the trend of reactor temperature profile are same for both simulation and on-line implementation. Thus it prove the suitability of the algorithm purposed to be implemented in the real-time application.

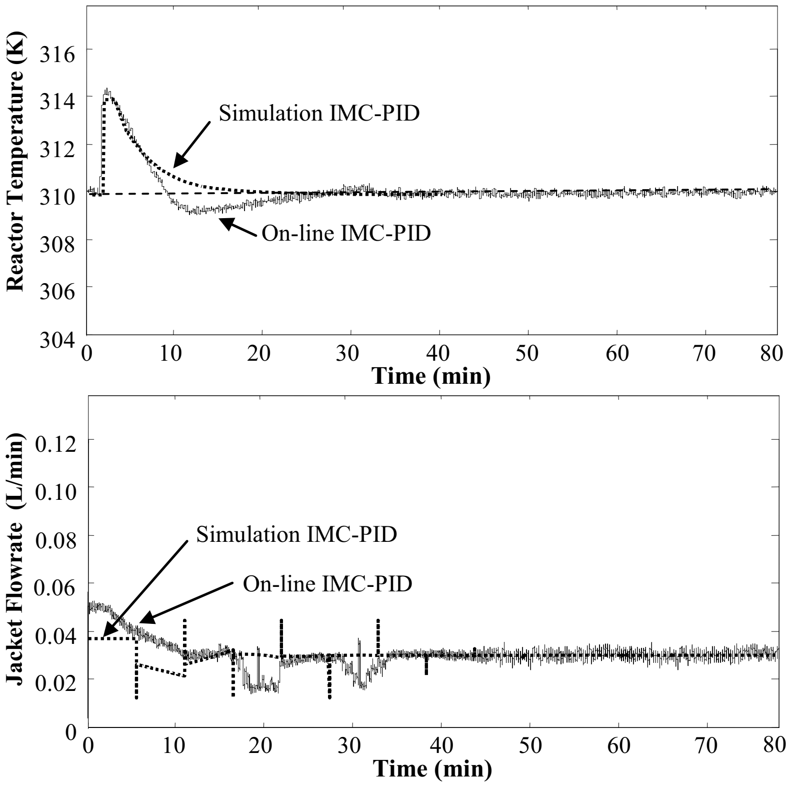

Figure 6: Reactor temperature response of on-line and simulation IMC-PID controller for load change and their respective manipulated variable action.

5. CONCLUSIONS

In this work, the on-line implementation of IMC-PID control strategy to control the temperature of batch esterification reactor has been proposed. Tuning relations for IMC-PID controller for FOPTD process model have been presented and only proportional gain, K_c needs to be adjusted to get the best control response for IMC-PID controller. The performance of on-line implementation of IMC-PID controller were evaluated for set-point tracking and disturbance rejection and then compared with simulation results. The results showed that the on-line IMC-PID controller have a satisfactory performance and were in good agreement with the simulation results. As a conclusion, the IMC-PID controller was found to be effective in tracking the desired reactor temperature profiles and rejecting the disturbance and thus can be applied in the batch esterification system.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the financial support by Ministry of Science, Technology and Innovation (MOSTI), Malaysia through the NSF scholarship for the first author and sciencefund project no 03-01-05-SF0090.

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Appendix

In this work, the process model is considered as FOPTD:

$$\boldsymbol{g} = \frac{K}{1+Ts}e^{-\theta s} \tag{A.1}$$

Use a first-order Padé approximation for deadtime

$$e^{-Ls} \approx \frac{-0.5\theta s+1}{0.5\theta s+1} \tag{A.2}$$

$$\breve{\boldsymbol{g}} = \frac{K(-0.5\theta s+1)}{1+Ts(0.5\theta s+1)} \tag{A.3}$$

Factor out the non-invertible elements, where $\breve{\mathbf{g}}_-$ is transfer function of minimum phase part and $\breve{\mathbf{g}}_+$ is non-minimum phase part containing time delay.

$$\breve{\boldsymbol{g}}_- = \frac{K}{1+Ts(0.5\theta s+1)} \tag{A.4}$$

$$\breve{\boldsymbol{g}}_+ = -0.5\theta s+1 \tag{A.5}$$

Form the idealized controller

$$\boldsymbol{g_c} = \frac{1+Ts(0.5\theta s+1)}{K} \tag{A.6}$$

The filter is added to make the numerator of $\boldsymbol{g_c}$ to be one order higher than the denominator.

$$\boldsymbol{g_c^*} = \frac{1+Ts(0.5\theta s+1)}{K}\frac{1}{\lambda s+1} \tag{A.7}$$

Now, find the PID equivalent. Recall that

$$\boldsymbol{g_c} = \frac{\boldsymbol{g_c^*}}{1-\breve{g}\boldsymbol{g_c^*}} \tag{A.8}$$

$$\boldsymbol{g_c} = (\frac{1}{K})\frac{1+T(0.5\theta s+1)}{(\lambda+0.5\theta)s} \tag{A.9}$$

We can expand the numerator term to find

$$\boldsymbol{g_c} = (\frac{1}{K})\frac{0.5T\theta s^2+(T+0.5\theta)s+1)}{(\lambda+0.5\theta)s} \tag{A.10}$$

We can multiply Eq. A.10 by $(T+0.5\theta/T+0.5\theta)$ to find the PID parameters as shown in Table 1.

Brief Biography of the Presenter

Miss Siti Asyura Zulkeflee received her bachelor degree from Universiti Sains Malaysia in 2006. She received her master degree in 2010 in the field of advanced process control. Currently, she is pursuing her doctorate degree in the same field and focus on the real-time implementation of advanced process control in batch system. Her current research areas also include process modeling, model based control strategy and optimization.