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DECOUPLING CONTROL OF A REACTIVE DISTILLATION PROCESS USING TYREUS-LUYBEN TECHNIQUE

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ABSTRACT

This work has been carried out to demonstrate the application of Tyreus-Luyben PI and PID methods in the decoupling temperature control of a reactive distillation process using the production of ethyl acetate and water (by-product) from the esterification reaction between acetic acid and ethanol as the case study. For comparison purposes, Ziegler-Nichols PI control method was also simulated. The process model, from which the decoupling matrix was estimated, was developed with the aid of System Identification Toolbox of MATLAB using the experimental data generated from the reactive packed distillation column set up. The developed decoupling control was simulated for set-point tracking using MATLAB/Simulink. The top segment temperature, the reaction segment temperature and the bottom segment temperature were selected as the controlled variables while the reflux ratio, the feed ratio and the reboiler duty were respectively chosen as the manipulated variables. The good responses with low oscillations obtained from the simulations of the decoupling control of the process using Tyreus-Luyben PI and PID control methods have shown that the control of the reactive distillation process has been achieved successfully with each of these methods and that the developed control system using these methods can thus be applied to the real process. In addition, due to its lowest values of IAE and ISE, Tyreus-Luyben PID method has been found to be the best one among the methods that were studied.

Keywords: reactive distillation, decoupling control, MATLAB/Simulink, tyreus-luyben technique, ethyl acetate.

INTRODUCTION

Reactive distillation is a process that combines both separation and chemical reaction in a single unit. It combines the benefits of equilibrium reaction with distillation to enhance conversion provided that the product of interest has the largest or the lowest boiling point (Giwa and Karacan, 2012c). It has a lot of advantages especially for those reactions occurring at temperatures and pressures suitable for the distillation of the resulting components (Giwa and Karacan, 2012b) which include shift of chemical equilibrium and increase of reaction conversion by simultaneous reaction and separation of products, suppression of side reactions and utilization of heat of reaction for mass transfer operation. It has been used in a small number of industrial applications for many years, but the last decade has shown an increase in both research and applications (Al-Arfaj and Luyben, 2002). By carrying out chemical reaction and separation in one process step, the operating and investment costs can be minimized. However, reactive distillation is not extensively used in industry since it is perceived that its operation will always be more difficult and will pose higher requirements on the quality of the design and control system than the conventional flow sheet. This behaviour can be mainly attributed to the complex interactions between the underlying phenomena taking place in the reactive columns.

The control of reactive distillation has received some attention only recently. Bock *et al.* (1997) developed a control structure for a reactive column with a recovery column by analyzing the reaction column's steady state and dynamic sensitivity of possible disturbances and manipulated variables. Sneesby *et al.* (1999) used an ethyl tert-butyl ether reactive distillation column as a case study to show how a two-point control configuration, which recognized the importance of both composition and conversion, can be developed and implemented for a reactive distillation process. Kumar and Daoutidis (1999) studied the dynamic behaviour and control of an ethylene glycol reactive distillation column by deriving a detailed tray-by-tray model that explicitly included the vapor-phase balances. Monroy-Loperena *et al.* (2000) also studied the control problem of an ethylene glycol reactive distillation column with the control objective of regulating the ethylene glycol composition in the product by manipulating the reboiler boil-up ratio. They proposed a new idea for robust stabilization based on an analysis of the underlying input/output bifurcation diagram and on modelling error compensation techniques. Al-Arfaj and Luyben (2000) explored the closed-loop control of a reactive distillation column with two products and discovered that single-end temperature control could keep both products at or above specified purity values, even for large disturbances, if reactive-zone holdup was sufficiently large. Vora and Daoutidis (2001) studied the dynamics and control of an ethyl acetate reactive distillation system and designed model-based linear and nonlinear state feedback controllers, along with conventional SISO PI controllers. They demonstrated the superior performance of the nonlinear controller over both the linear controller and the conventional PI controller. Khaledi and Young (2005) investigated the nonlinearity of an ethyl tert-butyl ether reactive distillation column and developed a 2 x 2 unconstrained model predictive control scheme for product purity and reactant conversion control by using the process dynamics approximated by a first-order plus dead time model to estimate the process model for the model predictive controller. They found that the controller

was very efficient for disturbance rejection and set-point tracking. Giwa and Karacan (2012e) used the decoupling technique to accomplish the model predictive control of a reactive packed distillation column that was used for the production of ethyl acetate. In their work, they used neural network and transfer function models as the controller models and discovered that the performance of the neural network model predictive controller was better than that of the transfer function model predictive controller.

Therefore, this work has been carried out to implement the control of a reactive distillation process with the aid of Proportional-Integral-Derivative Controller using Tyreus-Luyben as the tuning technique. The production of ethyl acetate from the esterification reaction between acetic and ethanol was used as the case study process.

2. PROCEDURES

(a) Process description

The process involved in this work was an esterification reaction occurring simultaneously with distillation operation that was carried out in the reactive packed distillation column (RPDC) set up as shown pictorially in Figure-1 (also described in the work of Giwa and Karacan (2012a, 2012b, 2012c, 2012d and 2012e). The column, excluding the condenser and the reboiler, had a height of 1.5 m and a diameter of 0.05 m. It consisted of a cylindrical condenser with a diameter and a height of 5 and 22.5 cm, respectively. The main column section of the plant was divided into three subsections of 0.5 m each. The upper, middle and lower sections were the rectifying, the reaction and the stripping sections respectively. The rectifying and the stripping sections were packed with raschig rings while the reaction section was filled with Amberlyst 15 solid catalyst that had a surface area of 5300 m^2/kg, a total pore volume of 0.4 cc/g and a density of 610 kg/m^3. The reboiler was spherical in shape with a volume of 3 Litre. The column was fed with acetic acid at the top (between the rectifying and the reaction sections) while ethanol was fed at the bottom (between the reaction and the stripping sections) with the aid of peristaltic pumps which were operated with the aid of a computer via MATLAB/Simulink program. All the signal inputs (reflux ratio (R), feed ratio (F) and reboiler duty (Q)) to the column and the measured outputs (top segment temperature (T_{top}), reaction segment temperature (T_{rxn}) and bottom segment temperature (T_{bot})) from the column were sent and recorded respectively on-line with the aid of MATLAB/Simulink computer program and electronic input-output (I/O) modules that were connected to the equipment and the computer system. The esterification reaction occurring in the column was an equilibrium type that is given as:

$$CH_3COOH + C_2H_5OH \xleftrightarrow{K_{eq}} CH_3COOC_2H_5 + H_2O \quad (1)$$

Figure-1. Reactive packed distillation column.

(b) Process identification

The data generated by operating the reactive distillation column described above and shown in Figure-1 below were used for the development of the transfer function models of the process using Process Identification Technique. The forms of the transfer functions developed for this process are given as shown in Equations (2) - (4).

The process model parameters were estimated with the aid of System Identification Toolbox of MATLAB.

$$T_{top}(s)=\frac{k_{p_{1,1}}e^{(-T_{d_{1,1}}s)}}{\tau_{1,1}s+1}R(s)+\frac{k_{p_{1,2}}e^{(-T_{d_{1,2}}s)}}{\tau_{1,2}s+1}F(s)+\frac{k_{p_{1,3}}e^{(-T_{d_{1,3}}s)}}{\tau_{1,3}s+1}Q(s) \quad (2)$$

$$T_{rxn}(s)=\frac{k_{p_{2,1}}e^{(-T_{d_{2,1}}s)}}{\tau_{2,1}s+1}R(s)+\frac{k_{p_{2,2}}e^{(-T_{d_{2,2}}s)}}{\tau_{2,2}s+1}F(s)+\frac{k_{p_{2,3}}e^{(-T_{d_{2,3}}s)}}{\tau_{2,3}s+1}Q(s) \quad (3)$$

$$T_{bot}(s)=\frac{k_{p_{3,1}}e^{(-T_{d_{3,1}}s)}}{\tau_{3,1}s+1}R(s)+\frac{k_{p_{3,2}}e^{(-T_{d_{3,2}}s)}}{\tau_{3,2}s+1}F(s)+\frac{k_{p_{3,3}}e^{(-T_{d_{3,3}}s)}}{\tau_{3,3}s+1}Q(s) \quad (4)$$

(c) Tuning of controllers

The controllers designed for the reactive distillation process were tuned using Tyreus-Luyben technique by considering its PI and PID. In addition, for comparison purposes, the PI version of Ziegler-Nichols technique was also designed and simulated. Given the transfer function of the controller as (Equation (5),

$$G_c(s)=K_c\left(1+\frac{1}{\tau_I s}+\tau_D s\right) \quad (5)$$

the relationships used for the calculation of the tuning parameters of the techniques for the PI and PID versions are as shown in Table-1 below.

Table-1. Relationships for the calculations of the tuning parameters.

Parameter	Tyreus-Luyben PI Tuning	Tyreus-Luyben PID Tuning	Ziegler-Nichols PI Tuning
K_c	$0.31K_{cu}$	$0.45K_{cu}$	$0.45K_{cu}$
τ_I	$2.2P_u$	$2.2P_u$	$\frac{P_u}{1.2}$
τ_D	0	$\frac{P_u}{6.3}$	0

Source: Seborg *et al.* (2004).

(d) Design of decouplers

In this study, the interaction decouplers applied to the control of the reactive distillation process were calculated in form of a matrix (decoupling matrix) with reference to Equations (2), (3) and (4) and using the mathematical relationship shown in Equation (6) below.

$$\boldsymbol{K}_I=\begin{bmatrix} k_{p_{1,1}} & k_{p_{1,2}} & k_{p_{1,3}} \\ k_{p_{2,1}} & k_{p_{2,2}} & k_{p_{2,3}} \\ k_{p_{3,1}} & k_{p_{3,2}} & k_{p_{3,3}} \end{bmatrix}^{-1} \quad (6)$$

The decouplers, after being applied to the process, were expected to be able to eliminate the effects of the interactions among the variables involved in the control of the 3 x 3 MIMO reactive distillation system. As such, the control of the MIMO system was expected to be accomplished easily like those of three different SISO systems.

(e) Control configuration and simulation

The reactive distillation process being controlled in this work was a Multi-Input Multi-Output (MIMO) type that had three controlled variables (top segment, reaction segment and bottom segment temperatures) and three manipulated variables (reflux ratio, feed ratio and reboiler duty). In order to facilitate easy control, the MIMO process was decoupled and thus controlled like three different SISO processes by the application of the decouplers that were estimated from the MIMO transfer function models of the system. After the decoupling, the reflux ratio, the feed ratio and the reboiler duty were used as the manipulated variables of the top segment, the reaction segment and the bottom segment temperatures respectively for the control studies. The control studies were achieved using codes written with MATLAB-mfile in combination with the control algorithm (Figure-2) developed in Simulink environment of MATLAB (Mathworks, 2011).

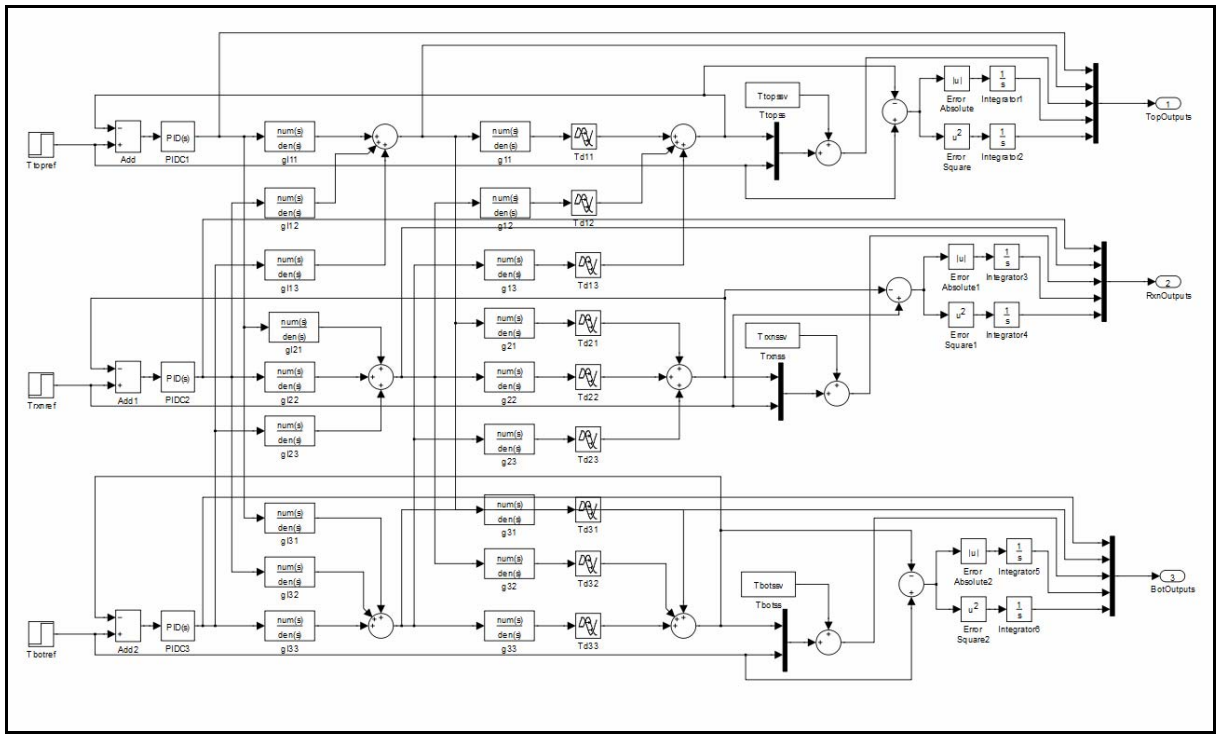

Figure-2. Simulink algorithm of decoupling control of reactive distillation process.

3. RESULTS AND DISCUSSIONS

(a) Experimental studies

Figures 3, 4 and 5 shows the responses of the segment temperatures obtained after the application of the inputs (R- reflux ratio, F - feed ratio and Q - reboiler duty) that were also shown as subfigures in the main figures. As can be seen from the figures, a step value from 3 to 5 was applied to the reflux ratio while a PRBS signal between 0.5 and 2 was applied to the feed ratio. Also applied to the reboiler duty was a PRBS signal between 0.595 and 0.63 kJ/s.

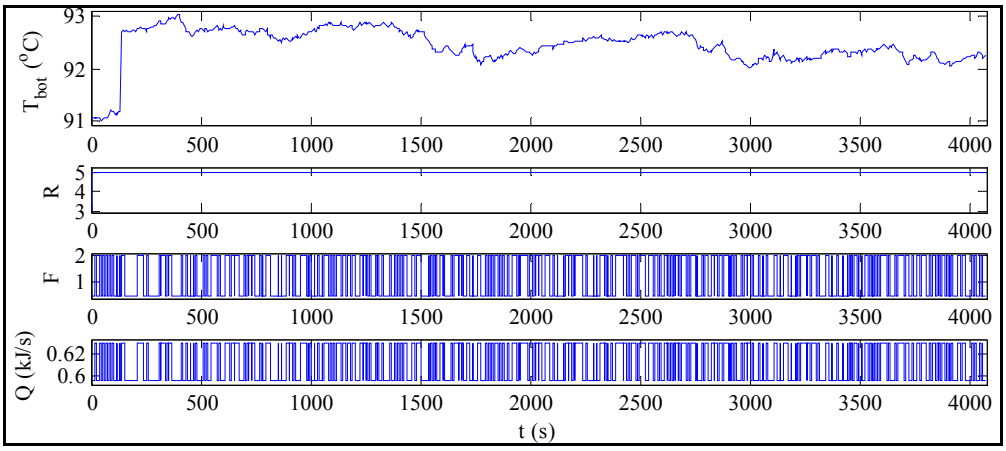

Figure-3. Experimental dynamic response and process inputs of top segment temperature.

Figure-3 shows the response of the top segment temperature (one of the process outputs) to the process inputs. As can be observed from the figure, the applications of the inputs resulted in a change in the top segment temperature profile of the process. That was an indication that this output variable was able to respond to the input variables and that the input variables could be used as the manipulated variables of the said output (controlled) variable.

In Figure-4, the experimental response of the reaction segment temperature is shown. As was observed in the case of the top segment temperature profile, the application of the inputs to the process also resulted in a change in the profile of the reaction segment temperature.

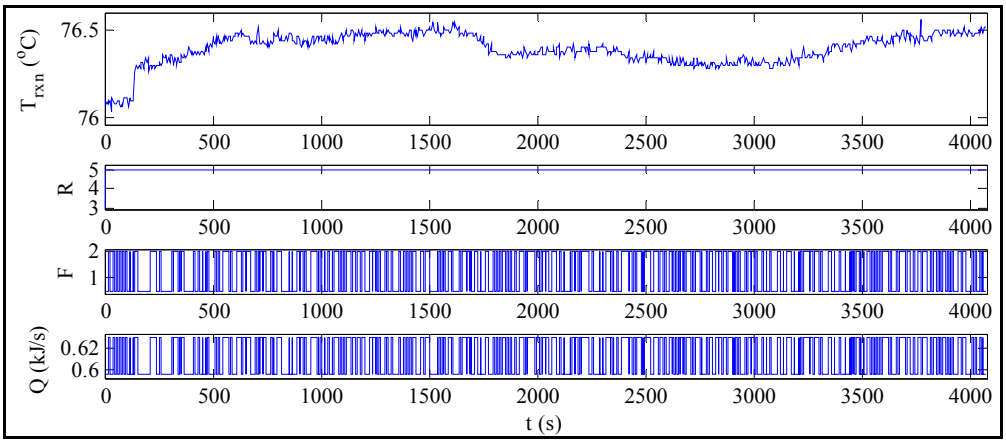

Figure-4. Experimental dynamic response and process inputs of reaction segment temperature.

Another profile obtained from the experimental work was that of the bottom segment temperature shown in Figure-5. From the figure, a change was noticed in the bottom segment temperature profile due to the applications of the inputs to the process. This change in the profile can be seen clearly from the figure by noticing the upward rise in the temperature profile of the bottom segment temperature from its steady-state.

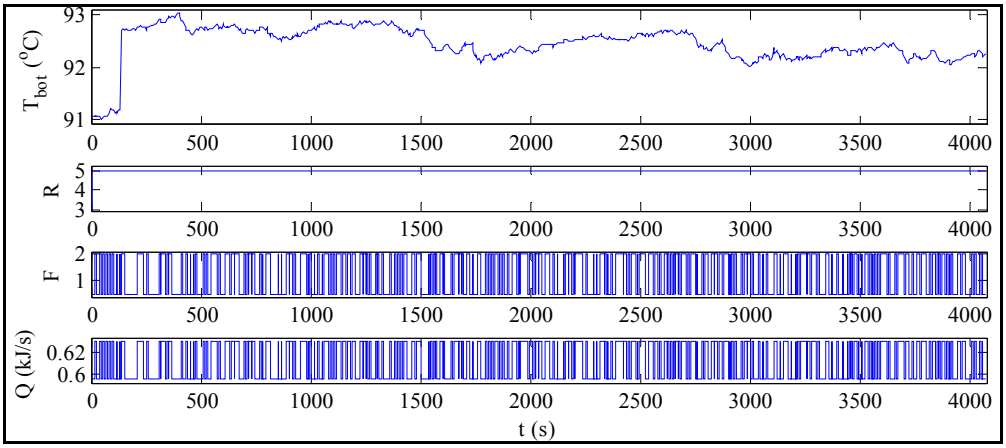

Figure-5. Experimental dynamic response and process inputs of bottom segment temperature.

Due to the fact that changes were noticed in the dynamic responses of the segment temperatures owing to the changes in the selected inputs of the process, it was concluded that the segment temperatures were functions of the selected process inputs. These verifications of the different segment temperatures to be functions of the selected inputs were very important before using the inputs as the manipulated variables of this process control.

(b) Process identification studies

Using the dynamic responses of the segment temperatures shown in Figures 3 - 5 above, the transfer function models of the process were developed between the process inputs and outputs with the aid of System Identification Toolbox of MATLAB. The transfer function models had three inputs variables (reflux ratio, feed ratio and reboiler duty) and three output variables (top segment temperature, reaction segment temperature and bottom segment temperature). The developed transfer function models are as given in Equations (7)-(9).

$$T_{top}(s) = \frac{-79.32e^{(-9.20E-04s)}}{5.50s+1}R(s) + \frac{-1.37e^{(-4.96E-01s)}}{5.18s+1}F(s) + \frac{-89.11e^{(-1.78E-03s)}}{5.17s+1}Q(s) \quad (7)$$

$$T_{rxn}(s) = \frac{31.95e^{(-4.89E-01s)}}{8.47s+1}R(s) + \frac{427.90e^{(-9.04E-03s)}}{5.27s+1}F(s) + \frac{-18434.90e^{(-9.02E-03s)}}{5.29s+1}Q(s) \quad (8)$$

$$T_{bot}(s) = \frac{-739.47e^{(-8.59E-06s)}}{35.64s+1}R(s) + \frac{6.79e^{(-4.99E-01s)}}{1.01s+1}F(s) + \frac{-231.19e^{(-5.00E-01s)}}{0.79s+1}Q(s) \quad (9)$$

As can be observed from the model parameters, while some static gains of the process (K_p) were positive, others were negative. That is, there were sign changes among the static gains of this reactive distillation process. This phenomenon of static-gain sign change has been found in the literature to be one of the peculiar characteristics of reactive distillation process. The sign changes were occurring as a result of the complex behavior of the process.

Observing the time constant (τ) of the process, the transfer function of the relationship between the reflux ratio and the bottom segment temperature was found to possess the highest value. This is indicating that if the same input unit is applied to the process, this part of the process is most likely to have the highest effect on the time required for the process to get to the steady state.

According to the values of the delay times (T_d) of the process, the maximum delay possessed by this process being 0.5 min implied that the output variables of the reactive distillation process studied in this work were responding fast to the changes in the selected input variables of the process.

Since the method used in this work for the estimation of the tuning parameters of the controllers required models, and since the control system was decoupled, there was the need to have as many controllers as there were controlled variables. Thus, having three controlled variables and three manipulated variables resulted in having three different controllers. In order to tune these controllers, three different tuning models were required. It was mentioned before that, after the decoupling, the MIMO process of this work would be controlled like three different SISO processes. Therefore, the models used for the estimation of the tuning parameters of the Tyreus-Luyben PI, Tyreus-Luyben PID and Ziegler-Nichols PI methods were estimated as SISO types and they are as shown in Equations (10), (11) and (12), respectively for the top segment temperature, the reaction segment temperature and the bottom segment temperature controllers.

$$T_{top}(s) = \frac{23.64e^{(-0.34s)}}{165.14s+1}R(s) \quad (10)$$

$$T_{rxn}(s) = \frac{47.80e^{(-0.13s)}}{18.94s+1}F(s) \quad (11)$$

$$T_{bot}(s) = \frac{173.01e^{(-0.21s)}}{579.53s+1}Q(s) \quad (12)$$

(c) Tuning parameters

Using the controller models given in Equations (10), (11) and (12), and with reference to the controller equation given in Equation (5), and also applying the equations contained in Table-1, the values obtained from the calculations of the tuning parameters of the controllers are as shown in Table-2 below. The table presents the tuning parameters of the Tyreus-Luyben PI, Tyreus-Luyben PID and Ziegler-Nichols PI controllers.

Table-2. Estimated tuning parameters of the controllers.

Controller	Tyreus-Luyben PI			Tyreus-Luyben PID			Ziegler-Nichols PI		
	K_c	τ_I	τ_D	K_c	τ_I	τ_D	K_c	τ_I	τ_D
PIDC1	10.02	2.99	0.00	14.55	2.99	0.22	19.39	0.68	0.00
PIDC2	1.52	1.12	0.00	2.20	1.12	0.08	2.94	0.25	0.00
PIDC3	7.70	1.86	0.00	11.18	1.86	0.13	14.91	0.42	0.00

As can be observed from Table-2, among the tuning parameters (controller gain, integral time and derivative time) of the controllers, the one with the highest value, for the three controllers (PIDC1, PIDC2 and PIDC3) and for the three methods (Tyreus-Luyben PI, Tyreus-Luyben PID and Ziegler-Nichols PI), was found to be the controller gain, which was the proportional aspect of the controllers.

(d) Decouplers

In this study, the decoupling matrix was estimated using the mathematical relationship given in Equation (6). The estimated and applied decoupling matrix of this control work is as given in Equation (13) below.

$$\boldsymbol{K}_I = \begin{bmatrix} -0.0005 & 0.0000 & -0.0013 \\ -0.2788 & 0.0010 & 0.0300 \\ -0.0065 & -0.0000 & 0.0007 \end{bmatrix} \quad (13)$$

(e) Control studies

Before going into the control aspect of this process, its steady values were investigated and found to be 69.89, 70.81 and 87.97°C, respectively for the top segment temperature, reaction segment temperature and bottom segment temperature. However, it was discovered

from the literature that very high composition of ethyl acetate (desired product) could be obtained when the top segment temperature was 70.75°C. As such, this work was purposely aimed at raising the top segment temperature to 70.75°C from 69.89°C. In addition to that, in order to test the performance of the controllers in the control of other segment temperatures, 0.5 and 2.5°C step units were applied to the steady state values of the reaction segment temperature and the bottom segment temperature respectively. The control system was simulated for 40 minutes and the results obtained from the simulation are as shown in Figures 6-8.

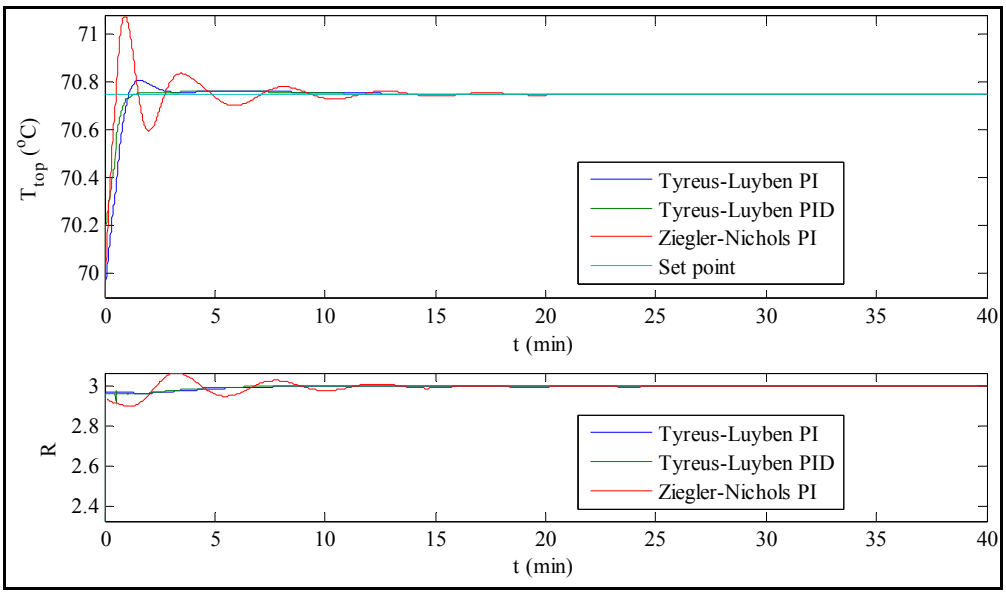

Figure-6. Dynamic responses of top segment temperature and reflux ratio to a set-point change from 69.89 to 70.75°C.

From Figure-6, the responses of the top segment temperatures obtained using the three tuning methods (Tyreus-Luyben PI, Tyreus-Luyben PID and Ziegler-Nichols PI) revealed that while the top segment temperature responses of the Tyreus-Luyben PI and PID methods were able to get to the desired steady-state value within 10 minutes, that of the Ziegler-Nichols PI method was only able to get there at approximately the 15th minute. This was showing that Tyreus-Luyben was faster than Ziegler-Nichols in taking the temperature to the desired steady-state for the process studies in this work. Also, it was noticed that the response of the Ziegler-Nichols PI method was more oscillatory than those of the Tyreus-Luyben PI and PID methods. Apart from that, the overshoot of the Ziegler-Nichols PI method was discovered to be very large compared to the other two methods used. These behaviors of the Ziegler-Nichols PI method were found to correspond to what are available in the literature because it has been discovered that among the characteristics of a PI controller was the production of oscillatory responses and large overshoots for set-point changes. According to Bequette (2003), the fact that the closed-loop behavior of Ziegler-Nichols technique tends to be oscillatory and sensitive to uncertainty is the reason why it is not widely used today. Among the three methods studied, for the responses of the top segment temperature, the method with the lowest overshoot was found to be the Tyreus-Luyben PID method. At the desired steady-state, each value of the input (reflux ratio) for each of the three methods was found to be approximately 3.

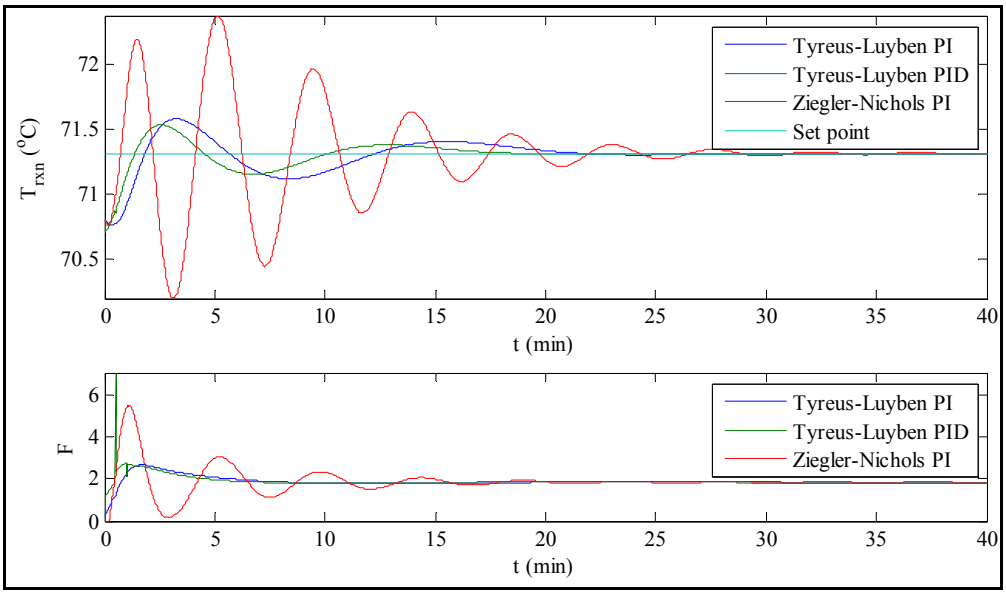

Figure-7. Dynamic responses of reaction segment temperature and feed ratio to a 0.5°C unit set-point change.

Considering the responses of the reaction segment temperatures shown in Figure-7, it was discovered that Tyreus-Luyben PID method was the fastest to take the reaction segment temperature of the process to the desired steady-state value within about 18 minutes; that of the Tyreus-Luyben PI was able to take the response of the reaction segment temperature to the desired steady-state after about 20 minutes while that of the Ziegler-Nichols PI method was only able to take the reaction segment temperature to the desired steady-state value after 29 minutes. At the steady state of each of the methods, the values of the manipulated variable (feed ratio) were found to be approximately 1.84 for both Tyreus-Luyben PI and PID methods, while that of the Ziegler-Nichols PI was approximately 1.83.

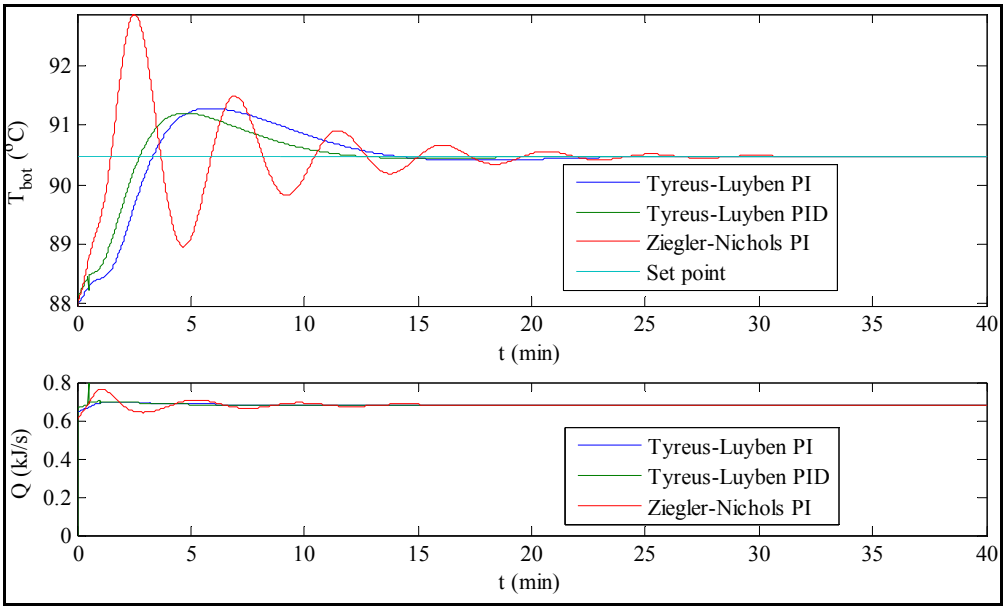

Figure-8. Dynamic responses of bottom segment temperature and reboiler duty to a 2.5°C unit set-point change.

Also simulated using the three tuning methods considered in this work was the control system involving the responses of the bottom segment temperatures. The results of this simulation are shown in Figure-8. As can be

seen from the figure, similar to what was obtained in the case of the top segment temperature; the responses of the Tyreus-Luyben PI and PID methods were found to have less oscillations and overshoots than that of the Ziegler-Nichols PI. However, the rise time of the bottom segment temperature response of Ziegler-Nichols PI method was found to be the lowest among the three methods, followed by that of the Tyreus-Luyben PID while that of the Tyreus-Luyben PI had the highest rise time. The first method to take the bottom segment temperature to the desired steady-state was Tyreus-Luyben PID method at about the 13th minute. The response obtained from the Tyreus-Luyben PI was able to get to the steady state after about 20 minutes while that of the Ziegler-Nichols PI method got there at approximately the 27th minute. At the steady state of each of the control methods, the value of the manipulated variable (in this case, the reboiler duty) for each of the methods was found to be 0.69 kJ/s.

Furthermore, in order to quantitatively determine the best one among the control methods that were studied in this work, their performance criteria were calculated. The performance criteria used in this work were Integral Absolute Error (IAE) and Integral Squared Error (ISE). The calculations of the performance criteria were carried out simultaneously with the control simulation in Simulink Environment of MATLAB and the results obtained from the calculations are as shown in Table-3 below. The concept of the criteria is that the lower the values of these performance criteria (IAE and ISE) for a particular control method or technique, the better the control method or technique because low values of the criteria generally imply that the controller is able to take the controlled variable to the desired steady-state (also known as the set point) within the shortest possible time.

Table-3. Performance criteria for the control methods.

Tuning method	**Integral absolute error** (IAE)			**Integral squared error** (ISE)		
	$\mathbf{T_{top}}$	$\mathbf{T_{rxn}}$	$\mathbf{T_{bot}}$	$\mathbf{T_{top}}$	$\mathbf{T_{rxn}}$	$\mathbf{T_{bot}}$
Tyreus-Luyben PI	0.57	2.67	10.22	0.22	0.60	12.21
Tyreus-Luyben PID	0.35	1.77	7.44	0.10	0.35	8.38
Ziegler-Nichols PI	0.84	8.06	11.74	0.19	4.79	14.08

From the Table-3 shown above, among all the three methods investigated, the one with the lowest IAE and ISE for all the three segment temperatures considered was found to be Tyreus-Luyben PID control method. These observations from the performance criteria of the segment temperatures (shown in Table-3) have been seen to be in agreement with what was observed from their graphical responses (Figures 6-8).

4. CONCLUSIONS

The good responses with low oscillations obtained from the simulations of the decoupling set-point tracking temperature control of the reactive distillation process used for the production of ethyl acetate using Tyreus-Luyben PI and PID control methods have shown that the control of the reactive distillation process has been achieved successfully with each of these methods. Therefore, the developed control system using these methods can be applied to the real process. In addition, Tyreus-Luyben PID method was found to have the lowest values of IAE and ISE and thus discovered to be the best one among the control methods that were investigated in this work.

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NOMENCLATURES

τ	Time constant of the process (min)
τ_D	Derivative time constant of the controller (min)
τ_I	Integral time constant of the controller (min)
F	Feed ratio (mL s^{-1} of acetic acid feed rate / mL s^{-1} of ethanol feed rate)
IAE	Integral Absolute Error
ISE	Integral Squared Error
K_c	Proportional gain of the controller
K_{cu}	Ultimate gain
K_p	Static gain of the process
MIMO	Multi-Input Multi-Output
PI	Proportional-Integral
PID	Proportional-Integral-Derivative
PRBS	Pseudo-Random Binary Sequence
P_u	Ultimate period
Q	Reboiler duty (kJ/s)
R	Reflux ratio
RPDC	Reactive Packed Distillation Column
SISO	Single-Input Single-Output
t	Time (min or s)
T_{bot}	Bottom segment temperature (^oC)
T_{rxn}	Reaction segment temperature (^oC)
T_{top}	Top segment temperature (^oC)

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