Dynamics and Tyreus-Luyben Tuned Control of a Fatty Acid Methyl Ester Reactive Distillation Process

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Abstract – This research work has been carried out to apply Tyreus-Luyben technique in tuning proportional-integral (PI) and proportional-integral-derivative (PID) controllers to the control of a reactive distillation process used for the production of methyl palmitate, a fatty acid methyl ester, from the esterification reaction between palmitic acid and methanol. The model used to represent the process was obtained from the work of Giwa et al. (2015c), and the open loop dynamics was first studied before carrying out its closed loop simulations with the aid of the model of the process developed in Simulink that was run via MATLAB Simulink. The results obtained from the open loop dynamic simulation of the process revealed that the developed Simulink model of the process was correct because the responses were discovered to compare very well with those obtained in the work of Giwa et al. (2015b and c). The results of the servo closed loop simulation carried out using the Tyreus-Luyben tuned PI and PID controllers showed that the system was able to get stabilized within the simulation time considered for the two control systems. However, the performance of the PID controller was found to be better because its estimated integral absolute error and integral squared error were lower. Furthermore, when the system was simulated for regulatory problem, the responses given by the two control systems were found to be very satisfactory. Moreover, from the values obtained when the integral absolute error and the integral squared error of the controllers were calculated for the regulatory problem, the PID controlled system was found to be better for this process. The comparison of the results obtained in the servo control of this work with that of Giwa et al. (2015b) revealed that Tyreus-Luyben tuning technique was the best for estimating the parameters for PI and PID controllers for the process considered because the number of oscillations observed in this case was found to be low. Also, the comparison made between the results of the regulatory control of this work to that of Giwa et al. (2015c) showed that the tuning technique (Tyreus-Luyben) investigated in this work was able to make the system maintain the desired state with lesser oscillations.

Keywords: Fatty acid methyl ester, reactive distillation, MATLAB/Simulink, servo control, regulatory control.

INTRODUCTION

Owing to the limited availability of conventional petroleum diesel and, also, as a result of environmental concerns, fatty acid methyl ester, otherwise known as biodiesel, which is an alternative fuel, is currently receiving attention in both academic and industrial research. This material can be used to replace petroleum diesel without any modification because their properties are similar (Simasatitkul et al., 2011; Giwa et al., 2014; Giwa et al., 2015a; Giwa et al., 2015c). A number of advantages are associated with this fuel as it can be derived from a renewable domestic resource as well as its reducing emission of carbon dioxide. Apart from that, it is nontoxic and biodegradable (Wang et al., 2004; Jaya and Ethirajulu, 2011; Giwa et al., 2014; Giwa et al., 2015a; Giwa et al., 2015c).

One of the ways of obtaining fatty acid methyl ester, especially in high purity, is through an esterification reaction of a fatty acid and an alcohol in a reactive distillation column (Giwa et al., 2014; Giwa et al., 2015c). Actually, the use of reactive distillation process is preferred for the production of fatty acid methyl ester so as to overcome the problems associated with the use of conventional batch reactor such as low conversion, heavy capital investments and high energy costs (Kusmiyati and Sugiharto, 2010; Giwa et al., 2014; Giwa et al., 2015a; Giwa et al., 2015b; Giwa et al., 2015c).

Reactive distillation is known to be a process that combines both separation and chemical reaction in a single unit (Giwa and Giwa, 2012; Giwa et al., 2015c). It is more advantageous than a conventional process with separate reaction and separation sections (Al-Arfaj and Luyben, 2002a; Giwa and Karacan, 2012b; Giwa and Karacan, 2012d; Giwa and Karacan, 2012e; Giwa and Karacan, 2012f; Giwa and Karacan, 2012g; Giwa, 2012; Giwa and Giwa, 2013a; Giwa, 2013a; Giwa et al., 2013; Giwa and Giwa, 2013b; Giwa, 2014). A small number of industrial applications have witnessed the application of this process for many years, but the last decade has shown an increase in both its research and applications (Al-Arfaj and Luyben, 2002b; Giwa et al., 2015a).

Furthermore, the operating and investment costs of a plant can be minimized by carrying out chemical reaction and separation in one process. Also, increased yield, because of its overcoming chemical and thermodynamic equilibrium limitations, improved selectivity via suppression of side reactions (Giwa and Karacan, 2012c), reduced energy consumption, due to effective utilization of reaction heat, in the case of exothermic reactions, avoidance of hot spots by simultaneous liquid evaporation, ability to separate close boiling components (Prakash et al., 2011; Giwa et al., 2015a) and ability to avoid azeotropes (Giwa and Karacan, 2012a) are some other benefits resulting from the application of reactive distillation technology. As a result of these advantages and with growing process understanding, an increasing number of processes based on reactive distillation have been developed by chemical process industries.
In an attempt to address those issues raised about the dynamics and control of the process, different researches have been carried out on the subject matter. To start with, Sneesby et al. (1997) worked on the dynamic simulation and control of reactive distillation process that was used for ethyl tert-butyl ether synthesis and presented some recommendations required for the control of the reactive distillation column studied. The recommendations included the need for early addressing of the control issues in the design process. Bock et al. (1997) developed a structure for the control of a reactive column with recovery by analysing the steady state and dynamic sensitivity of the column with respect to possible disturbance and manipulated variables. Sneesby et al. (1999) used an ethyl tert-butyl ether reactive distillation column to demonstrate how a two-point control configuration recognizing the importance of both composition and conversion could be developed and implemented for a reactive distillation process. Kumar and Daoutidis (1999) studied the dynamic behaviour and control of a reactive distillation column used for the production of ethylene glycol. A detailed tray-by-tray model that explicitly included the vapour-phase balances was derived in their work. Also developed in the work was a nonlinear controller that yielded good performance with stability in the high-purity region; through simulations carried out, the superior performance of the developed controller over linear PI controllers was demonstrated. In order to regulate ethylene glycol composition in the product, Monroy-Loperena et al. (2000) studied the control problem of a reactive distillation column taking the reboiler boil-up ratio as the manipulated variable. In their work, a new idea for robust stabilization based on an analysis of the underlying input/output bifurcation diagram and on modelling error compensation techniques was proposed. Al-Arfaj and Luyben (2000) worked on the closed loop control of a reactive distillation column and discovered that, even in the presence of large disturbances, single end temperature control could be used to keep the products at or above the specified purity values provided that the reaction zone holdup was sufficiently large. Vora and Daoutidis (2001) studied the dynamics and control of an ethyl acetate reactive distillation process and designed model-based linear and nonlinear state feedback controllers with classical single-input single-output (SISO) proportional-integral (PI) controllers. They demonstrated the superior performance of the nonlinear controller over both the linear and the classical PI controllers in the work. Grüner et al. (2003) carried out the simulation of an industrial reactive distillation column unto which asymptotically exact input/output-linearization was applied and discovered that the designed controller in the work showed a superior performance with respect to set-point changes and disturbances, in comparison to a well-tuned linear controller, even in the presence of unknown input delays. Khaledi and Young (2005) studied the nonlinearity of a reactive distillation column used for the production of ethyl tert-butyl ether and developed a 2 x 2 unconstrained model predictive control scheme for product purity and reactant conversion control using a first-order-plus-dead-time model estimated as the process model of the controller. They found from the study carried out that the controller was very efficient for disturbance rejection and set-point tracking. Völker et al. (2007) designed a multivariable controller for a medium-scale semi-batch reactive distillation column and demonstrated that the controller performed well for large set-point changes and in the face of disturbances. Also, Giwa and Karacan (2012a) used AutoRegressive with eXogenous Inputs (ARX) and AutoRegressive Moving Average with eXogenous Inputs (ARMAX) models they developed from some generated experimental data to study the dynamics of an ethyl acetate reactive distillation column. They discovered from the work carried out that the performance of the ARMAX model was better because it had higher calculated fit value. It was also discovered from the studies of the work that the ARX model was faster in getting to steady state upon the application of a step input to the two models. However, the models they developed were not utilized to study the control of the process. Giwa and Karacan (2012c) started from first principles and developed dynamic models for a reactive packed distillation column. They solved the developed models with the aid of MATLAB and compared the experimental and the theoretical results obtained. It was revealed from their results that there were good agreements between them (the experimental and the theoretical results) because the calculated percentage residuals were small. Similarly, the models they developed were not used for the control of the column in the work. Giwa and Karacan (2012d) studied the application of decouplers in the design of model predictive controllers for a reactive distillation process used for ethyl acetate production by taking the top segment temperature, the reaction segment temperature and the bottom segment temperature as the controlled variables while the reflux ratio, the feed ratio and the reboiler duty of the process were the manipulated variables of the control system. The results they obtained from the work showed that neural network decoupling model predictive controller (NNDMPC) was able to perform better than that transfer function decoupling model predictive controller (TFDMPC) because the calculated integral squared error values for the top segment and the reaction segment temperatures obtained from the control simulation carried out with the NNDMPC were found to be less than those of the TFDMPC. Moreover, Giwa and Karacan (2012e) applied decoupling proportional-integral-derivative control to a reactive distillation column for set-point tracking and disturbance rejection using tuning parameters calculated with Ziegler-Nichols and Cohen-Coon techniques. The results obtained from the simulations of the work revealed that, for the process considered in the work, decoupling PID control with Cohen-Coon tuning technique was better than that of Ziegler-Nichols. Giwa et al. (2015b) studied the dynamics and, also, performed the set-point tracking control of a reactive distillation process used for biodiesel production taking the biodiesel purity obtained from the bottom section of the column as the controlled variable and the reboiler duty as the manipulated variable. They used Cohen-Coon and Ziegler-Nichols tuning techniques to calculate the controller parameters, and from the comparisons made among the controllers considered, it was discovered that the best one for the system was PID controller tuned with Ziegler-Nichols method because its calculated integral absolute error (IAE) and integral squared error (ISE) were the lowest. Giwa et al., 2015c also carried out the control of a reactive distillation process used for biodiesel production from an esterification reaction between palmitic acid and methanol for regulatory
problem using P, PI and PID controllers tuned with Ziegler-Nichols and Cohen-Coon techniques and discovered that the best controller for the disturbance rejection control of this process was PID controller tuned with Cohen-Coon technique.

As can be seen from the literature review carried out, most of the researches carried out on the control of reactive distillation process for biodiesel (fatty acid methyl ester) production has been based on using Ziegler-Nichols and Cohen-Coon methods as the tuning techniques. It was, therefore, deemed necessary to investigate how the process would behave to a controller tuned with another technique. As a result of that, this work has been carried out to apply Tyreus-Luyben tuning technique to proportional-integral (PI) and proportional-integral-derivative (PID) controllers used for the control of a reactive distillation process producing palmitic acid methyl ester (fatty acid methyl ester).

**METHODOLOGY**

**Process Modelling**

The model used in this work to study the dynamics and the control of the palmitic acid methyl ester (methyl palmitate) reactive distillation process was a transfer function obtained from the work of Giwa et al. (2015c), and it is given in Equation (1).

\[
x_{\text{fame}}(s) = \frac{0.3382 e^{-0.9993s}}{248.43s + 1} Q(s) + \frac{0.283 e^{-0.9912s}}{151.87s + 1} R(s)
\]

The input variable of the model was taken as the reboiler duty while the reflux ratio was chosen as the disturbance variable, and the output variable was the mole fraction of palmitic acid methyl ester obtained from the bottom section of the reactive distillation column used.

**Open Loop Simulation**

To carry out the open loop simulation of the process, the transfer function model taken from the work of Giwa et al. (2015c) was first represented as a Simulink (MathWorks, 2015) model of the process as shown in Figure 1. The process Simulink model composed of two parts, viz. the main fatty acid methyl ester reactive distillation system and the disturbance system, as can be seen from the Figure 1. As can be seen from the figure, the blocks (transfer function and delay Simulink blocks) for the two parts of the model have been inserted inside a subsystem of the Simulink to make the appearance of the model look tidy.

Figure 1. Open loop Simulink model of the palmitic acid methyl ester reactive distillation process
After the Simulink modelling of the process, it was run by applying steps to both the input and the disturbance variables of the process via codes written in *m*-file of MATLAB.

**Closed Loop Simulation**

Upon the completion of the open loop simulation of the process, its closed loop dynamics were also investigated by simulating the closed loop dynamic model developed, also, with the aid of Simulink and shown in Figures 2 and 3, respectively, for PI and PID controllers tuned with Tyreus-Luyben technique. The closed loop models of the process developed were simulated for both servo (set-point tracking) and regulatory (disturbance rejection) with the controllers (PI and PID) by applying step changes to the steady state value of the output (controlled) and the disturbance variables, accordingly. For the control system of this work, as mentioned earlier, the controlled, the manipulated and disturbance variables of the process were selected to be the palmitic acid methyl ester bottom mole fraction, the reboiler duty and the reflux ratio, respectively.

![Figure 2. Closed loop Simulink model of the process with PI controller tuned with Tyreus-Luyben technique](image2.png)

![Figure 3. Closed-loop Simulink model of the process with PID controller tuned with Tyreus-Luyben technique](image3.png)
In order to use the expressions of the Tyreus-Luyben tuning technique (shown in Table 1) to calculate the required parameters of the controllers, their (the controller’s) transfer function was taken to be as given in Equation (2).

\[ G_c(s) = K_c \left( 1 + \frac{1}{\tau_I s} + \tau_D s \right) \]  

(2)

Table 1: Tyreus-Luyben tuning parameter expressions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proportional-Integral (PI)</th>
<th>Proportional-Integral-Derivative (PID)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K_c )</td>
<td>0.31( K_u )</td>
<td>0.45( K_u )</td>
</tr>
<tr>
<td>( \tau_I )</td>
<td>2.2( P_u )</td>
<td>2.2( P_u )</td>
</tr>
<tr>
<td>( \tau_D )</td>
<td>0</td>
<td>( \frac{P_u}{6.3} )</td>
</tr>
</tbody>
</table>

Source: Seborg et al. (2004)

RESULT AND DISCUSSION

Shown in Figure 4 is the closed loop dynamic response of the fatty acid methyl ester reactive distillation process studied in this work to a unit step change in the reboiler duty, which was the input variable, of the process. As can be seen from the figure, even though the time was a little bit long, the system was able to get to a steady state value that was found to compare very well with the one obtained in the work of Giwa et al. (2015b). That was an indication that the open loop Simulink model of the reactive distillation process developed in this work was very correct.

After carrying out the open loop simulation, Tyreus-Luyben tuning technique was used to obtain the tuning parameters of the controller for set point tracking, and the results obtained from the control of the process accomplished by applying a step change of 0.1 to the steady-state value of the mole fraction of palmitic acid methyl ester, which was the controlled variable of the closed loop system, were as given in Figures 5 and 6.

Figure 5 shows the response of the system to a 0.1 step change in the set point when it was controlled with a PI controller. From the figure, it was discovered that the system was able to attain its desired steady state within 300 min of the simulation time used. Comparing the response obtained in this work for the PI controller tuned with Tyreus-Luyben to that tuned with Ziegler-Nichols and Cohen-Coon techniques (see Giwa et al., 2015b), it was found that the response obtained in this work for the control was less oscillatory. In addition, the time required by the system to get to a value higher than that of the open loop simulation has been found to reduce, meaning that the control carried out on the process with the PI controller tuned with Tyreus-Luyben technique was effective.
Figure 5. Closed loop response of Tyreus-Luyben tuned PI controlled process to a 0.1 step change in the controlled variable

Shown in Figure 6 is the dynamic response of the closed loop system to a step change of 0.1 in the set point of the output variable controlled with PID controller tuned with Tyreus-Luyben technique. According to the figure, the response of the PID controlled system tuned with Tyreus-Luyben technique was also found to get to its desired set point within 300 min, but it was found to be more oscillatory than that of the PI controller system tuned with the same technique. This observation can be clearly seen by comparing Figures 5 and 6.

Table 2. Performance values of PI and PID controllers tuned with Tyreus-Luyben technique for servo problem

<table>
<thead>
<tr>
<th>Controller</th>
<th>IAE</th>
<th>ISE</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI</td>
<td>13.28</td>
<td>3.09</td>
</tr>
<tr>
<td>PID</td>
<td>8.36</td>
<td>1.94</td>
</tr>
</tbody>
</table>

In order to be able to compare the two controllers, their performance values were calculated. The performance criteria used in this work were integral absolute error (IAE) and integral squared error (ISE) and their calculated values for the controllers considered are given in Table 2. Comparing the two (PI and PID) controllers based on the values of the performance criteria given in Table 2, it was...
discovered numerically that the PID controller tuned with Tyreus-Luyben technique was better than the PI controller in controlling the process because its IAE and ISE were lesser.

Also considered in this work was the behaviour of the system with the controllers tuned with Tyreus-Luyben technique after a unit step change was applied to the reflux ratio (disturbance variable) of the process; that is, the disturbance rejection control. However, before doing that, the open loop simulation involving a unit step change in the disturbance variable (reflux ratio) of the process was first carried out.

Shown in Figure 7 is the open loop dynamic response given by the system when a unit step change was applied to the reflux ratio. The response obtained was observed to compare very well with that obtained in the work of Giwa et al. (2015c), and this was found to be another indication of the fact that the developed Simulink model of the process was a good representation of the palmitic acid methyl ester reactive distillation system and that the disturbance variable was actually having effects on the system because the response was, then, supposed to be zero, but was not.

Figure 7. Open loop response of the process to 1 unit step change in the reflux ratio of the process

Figure 8. Closed loop response of Tyreus-Luyben tuned PI controlled process
Consequently, Tyreus-Luyben tuning technique was applied to obtain the controller parameters used with the control system to maintain the response of the controlled variable at the desired value (in this case of the regulatory control, zero). Given in Figures 8 and 9 are the responses obtained from that.

As can be seen from Figure 8, which is showing the dynamic response of the system to a Tyreus-Luyben tuned PI controller, the response was able to get settled with very few oscillations at the desired set point. In fact, the oscillations found in this response obtained with the Tyreus-Luyben tuned PI controller were found to be less than that given by the same PI controller tuned with Ziegler-Nichols and Cohen-Coon methods, as can be seen in the work of Giwa et al. (2015c). It should be recalled that similar observations were made in the case of the servo control of the system. This is, actually, showing the superiority of Tyreus-Luyben tuning technique over Ziegler-Nichols and Cohen-Coon techniques, at least, for this reactive distillation process studied.

Moreover, Figure 9 shows the response of the process when it was controlled using a PID controller that was tuned with Tyreus-Luyben technique. From the figure, it was discovered that the number of oscillations displayed by the closed loop system of the palmitic acid methyl ester reactive distillation process was not up to that of the ones given by a similar (PID) controlled system tuned with Ziegler-Nichols and Cohen-Coon techniques (cf. Giwa et al., 2015c).

The two controllers tuned with Tyreus-Luyben technique that were considered in this work for regulatory problem were also compared by estimating their IAEs and ISEs, and the results obtained were as given in Table 3. Looking at the values of the IAEs and ISEs given in the table, it was found that the performance of the PID controller tuned with Tyreus-Luyben technique was better than that of the PI controller tuned with the same technique because it had lower IAE and ISE values, and the lower the values of the IAE and ISE of a controller, the better the performance of that controller.

**CONCLUSION**

From the results given by the open loop dynamic simulation of the reactive distillation process used for the production of palmitic acid methyl ester, it was revealed that the developed model of the process was correct because the responses compared very well with those
obtained in the work of Giwa et al. (2015b and c). The results of the servo closed loop simulation carried out with the Tyreus-Luyben tuned PI and PID controllers showed that the system was able to get stabilized at the desired set point within 300 min of the simulation time considered with the two controllers. However, the performance of the PID controller was found to be better because its estimated integral absolute error and integral squared error were lower. Furthermore, when the system was simulated for regulatory problem, the responses given by the two control systems were found to be very satisfactory. In addition, from the values obtained when the integral absolute error and the integral squared error were calculated, the performance of the PID controlled system was found to be better. The comparison of the results obtained in the servo control of this work with that of Giwa et al. (2015b) revealed that Tyreus-Luyben technique was the best in tuning the controllers for the process because the number of oscillations observed in this case was found to be low. Also, comparing the results of the regulatory control with that of Giwa et al. (2015c), it was discovered that the tuning technique (Tyreus-Luyben) investigated in this work was able to make the system remain at the desired steady state with fewer oscillations.

NOMENCLATURE

\( \tau_D \)  Derivative time of the controller (min)
\( \tau_d \)  Time constant of the disturbance process model (min)
\( \tau_I \)  Integral time of the controller (min)
\( \tau_p \)  Time constant of the main process model (min)
\( G_c(s) \)  Controller transfer function
\( G_p(s) \)  Process transfer function
\( \text{IAE} \)  Integral Absolute Error
\( \text{ISE} \)  Integral Squared Error
\( K_c \)  Proportional gain of the controller
\( K_d \)  Static gain of the disturbance process model
\( K_p \)  Static gain of the main process model
\( K_u \)  Ultimate gain
\( \text{NNDMPC} \)  Neural Network Decoupling Model Predictive Controller
\( P \)  Proportional
\( \text{PI} \)  Proportional-Integral
\( \text{PID} \)  Proportional-Integral-Derivative
\( P_u \)  Ultimate period (min/cycle)
\( Q \)  Reboiler duty (kJ/s)
\( R \)  Reflux ratio
\( \text{SISO} \)  Single-input single-output
\( T_{dd} \)  Dead time of the disturbance process model (min)
\( T_{dp} \)  Dead time of the main process model (min)
\( \text{TFDMPC} \)  Transfer Function Decoupling Model Predictive Controller
\( x_{f\text{ame}} \)  Bottom fatty acid methyl ester mole fraction

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