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PI AND PID CONTROL OF A FUEL ADDITIVE REACTIVE DISTILLATION PROCESS

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ABSTRACT

This research work has been carried out to investigate the performances of proportional-integral (PI) and proportional-integral-derivative (PID) controllers tuned with Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols techniques on a reactive distillation process used for the production of a fuel additive. The fuel additive considered was isopropyl alcohol that was obtained from the top section of a prototype reactive distillation column plant developed with the aid of Aspen HYSYS. The model used for the process control was estimated using the data generated from Parametric Utility of the Aspen HYSYS prototype plant and *pem* command of System Identification Toolbox of MATLAB. Furthermore, the open-loop and the closed-loop Simulink models of the system were developed and simulated appropriately. The results obtained from the open-loop simulations carried out revealed that the system was a stable one because it was able to attain steady-states within the simulation times considered. Also observed from the closed-loop simulations was that the best tuning method for both PI and PID controllers in suppressing large and small errors was Tyreus-Luyben technique. However, in suppressing any error persisting for a long period of time, Ziegler-Nichols method was found to be the best for PI controller while for PID controller, it was Cohen-Coon tuning technique. Further comparing the performance values of the controllers, it was discovered that the PID controllers tuned with the different techniques were better than the PI controllers because the corresponding integral of square error (ISE), integral of absolute value of the error (IAE) and integral of time-weighted absolute error (ITAE) values of the PID controllers were found to be less than those of the PI controllers considered for the process.

Keywords: fuel additive, reactive distillation, aspen HYSYS, parametric utility, proportional-integral (PI), proportional-integral-derivative (PID), Cohen-Coon, Tyreus-Luyben, Ziegler-Nichols.

INTRODUCTION

Fuel additives are compounds that are formulated, through treatments, for the enhancement of the quality and the efficiency of the fuels used in motor vehicles (Shekhawat and Padwa, 2015; Giwa and Giwa, 2016). Generally, treatment of fuels with additives occurs for various reasons. For instance, in the past, the production of high octane grades was achieved by the addition of octane enhancers to gasoline. These days, the use of cetane improvers offers the possibility of upgrading a base fuel very economically in comparison with refinery measures (Dabelstein *et al.*, 2007; Giwa and Giwa, 2016).

On the other hand, performance additives, which are added to modern high quality fuels, improve the behaviour of a base fuel in operation, and offer technical advantages that often cannot be achieved by measures taken in the refinery (Dabelstein *et al.*, 2007; Giwa and Giwa, 2016). In many cases, these types of additives offer the only possibility of guaranteeing trouble-free engine performance over a longer running period. Also, treatment of fuels with additives is a major route to achieve product differentiation and trademarked quality. As such, it is not surprising that further increase in the use of additives, especially in the aspect of treating gasoline, is anticipated (Dabelstein *et al.*, 2007; Giwa and Giwa, 2016).

The treatment of gasoline with additives is almost as old as the fuel itself. At first, the search for the so-called brisance increasing additives was predominant. Later on, treatment with certain additives was recognized to allow an increase of compression ratio without dangerous knocking. Also, an increase in the octane number became the major aim in additive technology for decades. Systematic research into additives that could positively influence many aspects of engine behaviour began around 1950 on a wider scale. Since about 1970, conventional, ash-forming antiknock additives became increasingly less important for environmental reasons. Nowadays, additive development is driven by environmental specifications as well as demanding new technologies like direct injected gasoline cars (Dabelstein *et al.*, 2007; Giwa and Giwa, 2016).

There are various types of fuel additives. These include oxygenates, ethers, antioxidants (stabilizers), antiknock agents, fuel dyes, metal deactivators, corrosion inhibitors. Oxygenates, as the name implies, contain oxygen as a part of their chemical structure. They are used to reduce the carbon monoxide emissions created when burning fuel and can be based on either alcohol or ethers such as diisopropyl ether (DIPE), ethyl *tert*-butyl ether (ETBE), ethanol, methanol, n-butanol, *tert*-butyl alcohol (TBA) and tertiary-amyl methyl ether (TAME). Antioxidants are the molecules that inhibit the oxidation of other ones; they are used as fuel additives when creating fuel blends. Normally, oxidation reactions produce free radicals leading to chain reactions. Antioxidants are used to terminate the chain reaction by disrupting radical intermediates. Some antioxidants are also used as a stabilizer in fuel to prevent oxidation. Examples of these are butylated hydroxytoluene (BHT), 2, 4-dimethyl-6-*tert*-butylphenol, p-phenylenediamine and ethylenediamine.

An antiknock agent is a gasoline additive that is used to reduce engine knocking and increase the octane rating of a fuel by raising the temperature and pressure at which auto-ignition occurs (Shekhawat and Padwa, 2015). All these fuel additives can be produced very economically and with high conversion through the use of a novel process known as "reactive distillation" (Giwa and Giwa, 2013b; Giwa and Giwa, 2016).

Reactive distillation is a process that combines both separation and chemical reaction in a single unit (Giwa, 2012; Giwa, 2013; Giwa *et al.*, 2013a). It has a lot of advantages, especially, for those reactions occurring at temperatures and pressures suitable for the distillation of the resulting components (Sneesby *et al.*, 1997; Giwa and Karacan, 2012b; Giwa and Karacan, 2012d; Giwa and Karacan, 2012e; Giwa and Giwa, 2013a; Giwa *et al.*, 2013b; Giwa and Giwa, 2013b; Giwa, 2014; Giwa *et al.*, 2014; Giwa *et al.*, 2015a; Giwa *et al.*, 2015b; Giwa and Giwa, 2016). This process actually combines the benefits of equilibrium reaction with a traditional unit operation (known as distillation) to achieve a substantial progress in not only promoting the reaction conversion through constant recycling of unconverted materials and removal of products but also reducing the capital and operating costs as a result of the reduction of the number of equipment units (Giwa and Karacan, 2012a; Giwa and Giwa, 2013c, Giwa *et al.*, 2014; Giwa and Giwa, 2016) required for a process.

Basically, combining reaction and distillation has several advantages such as shift of chemical equilibrium and an increase of reaction conversion by simultaneous reaction and separation of products, suppression of side reaction(s) and utilization of heat of reaction for mass transfer operation. These synergistic effects result in significant economic benefits of reactive distillation compared to a conventional design. The economic benefits include lower capital investment, lower energy cost and higher product yields (Moritz and Hasse, 1999; Giwa and Karacan, 2012c; Giwa and Giwa, 2016).

Despite the economic benefits of reactive distillation, the combination of both reaction and separation in a single unit has made the control of the process very challenging (Giwa and Karacan, 2012c; Giwa and Giwa, 2016). Besides, due to the occurrence of both reaction and separation in a single equipment unit, the process exhibits some complex behaviours (Khaledi and Young, 2005; Giwa and Karacan, 2012b; Giwa and Giwa, 2016) such as steady state multiplicity, process gain sign changes (bidirectionality) and strong interactions between process variables (Jana and Adari, 2009; Giwa and Karacan, 2012b; Giwa and Giwa, 2016). These complexities have not only made the study of the process extremely difficult both theoretically and practically, especially in a situation whereby more than one reactions are involved in a particular process (Giwa and Giwa, 2016), but also its control. Thus, it is very necessary to obtain a concrete method of designing a controller for this process so that, at any point in time, the desired product can be obtained in high purity.

Researches concerning the control of reactive distillation processes, especially for fuel additive production, have been reported in literature. For instance, Sneesby *et al.* (1999) used an ETBE reactive distillation column as a case study to show how a two-point control configuration recognizing the importance of composition and conversion could be developed and implemented for a reactive distillation process with simple PI controllers. The combined composition and conversion control configuration developed in their work was tested using SpeedUp dynamic simulations, and it was proved to be effective in maintaining a high isobutylene conversion. Sneesby *et al.* (2000) developed an integrated control scheme for an ETBE reactive distillation column using only linear control loops. The results obtained from the dynamic simulations of their work indicated that the designed control system was stable for a range of process disturbances despite the cogent process non-linearity and the bidirectionality. Monroy-Loperena *et al.* (2000) studied the control of an ethylene glycol reactive distillation column in the presence of uncertainties in the dynamics of regulated output. The objective of their work was to regulate ethylene glycol composition in the product taking the reboiler boil-up ratio as the manipulated variable. Based on that, they designed a first-order output-feedback compensator which was equivalent to a PI controller. Using numerical simulations on a full dynamical model, they were able to show the ability of the controller in regulating the product composition. Al-Arfaj and Luyben (2002a) studied control structures for ethyl *tert*-butyl ether (ETBE) reactive distillation columns by exploring two process configuration designs: one with two fresh reactant feed streams and the other with a single mixed reactant feed. They carried out the optimum design for the double-feed case by minimizing the total annual cost and used a design given in the literature for the single-feed case. Using the double-feed system, they studied three basic control structures (the first one used direct composition control of two product purities; the second structure fixed the reflux ratio and controlled one end product; the third structure used temperature to infer product composition with a fixed reflux ratio). Furthermore, they used a single-feed control design from the literature with some modifications. They were able to discover in the work that the double-feed system required internal composition control to balance the stoichiometry along with temperature control to maintain product purity. They, however, discovered that the single-feed case, which was operated with an excess of ethanol, could be effectively controlled with only a temperature controller in the absence of large disturbances. Al-Arfaj and Luyben (2002b) carried out the control of an ethylene glycol reactive distillation column using a simple single-temperature proportional-integral (PI) structure. Their control objective was to maintain the ethylene glycol purity within the desired range. However, they used simple temperature measurement to infer composition because controlling product quality directly would require the use of an expensive and unreliable online composition analyzer. They controlled the temperature on tray 3

(numbered from the bottom) of the column by manipulating the reboiler heat input, and they were able to demonstrate that ethylene glycol reactive distillation columns could be controlled effectively using a simple PI controller because the structure used in the work was able to achieve the stoichiometric balancing of the reactants and maintained the product purity within reasonable bounds. Bisowarno *et al.* (2003) developed and implemented a model gain scheduling on one-point control (product purity) for an ethyl *tert*-butyl ether reactive distillation column. The scheduling used in the work employed a set of derived simplified input-output first-order models that was able to cope with the nonlinear characteristics of the process. The simple models were integrated with the aid of a proper switching scheme. The results they obtained showed that this control strategy outperformed the standard proportional-integral control in both set-point tracking and disturbance rejection. Tian *et al.* (2003) developed a pattern-based predictive control (PPC) to maintain the purity of ethyl *tert*-butyl ether (ETBE) synthesized in a pilot-scale reactive distillation column. The control algorithm of the work was developed in order to alleviate the requirement of good process models, which were essential for modern model-based control. To obtain the pseudo input-output linear process gain, a non-linear transformation, which needed only a rough and easily obtained knowledge of the steady state characteristics of the process, was designed. Four types of process feature patterns were extracted from the time series of the controlled variable and the transformed manipulated variable. Fuzzy logic rules driven by the extracted feature patterns were then developed for process prediction. The case studies unto which the control algorithm was implemented revealed that the PPC could provide improved control performance for both set-point tracking and disturbance rejection. As such, it was concluded that PPC was a promising tool for complex processes, especially where good process models are difficult to obtain or to implement for real-time control. Khaledi and Young (2005) investigated the nonlinear ETBE reactive distillation process, and developed a 2 x 2 unconstrained model predictive control scheme. In the control configuration, reflux flow rate was used to control the reaction zone temperature difference, which inferred isobutylene conversion, and reboiler duty was used to control the temperature of stage 7, which inferred bottom product ETBE purity. The models used in the MPC of the work were approximated by first-order-plus-dead-time approach. It was discovered that the model predictive controller designed was able to handle the process interactions very well. The controller was also found to be very efficient in disturbance rejection and set-point tracking. The MPC controller performance was further compared with a simple single-point control scheme and a 2 x 2 PI control structure. The simple control structure was found to show a faster response as compared to MPC and the 2 x 2 PI control structures, but it was discovered not to be as stable as the 2 x 2 PI and MPC in maintaining isobutylene conversion. Also, the MPC controller was slightly slower than the conventional 2 x 2 PI controller, however, it was found not to be affected by loop interactions. Wang and Wong (2006) used steady state and dynamic simulations to investigate the process characteristics and control strategy of a reactive distillation column for isopropanol (IPA) synthesis by direct hydration of propylene with the aid of PI controllers. They found a robust nominal operation of the process by maintaining an excess of propylene feed to the column and recycling the unreacted propylene to the feed instead of the top stage. Stage temperature and propylene composition with one-to-one relationship with reboiler duty and propylene feed were respectively selected as the controlled variables for maintaining bottom purity and feed ratio in the presence of possible measurement bias. High nonlinearity between the selected input–output pair was reduced by using variable transformation. Dynamic simulations demonstrated that such a control scheme with nonlinear transformed variable was capable of providing much superior control performance than the one using natural variable.

So far from the literature review, no work has been found that compared the different controller tuning techniques to a reactive distillation system producing a fuel additive. Therefore, in order to bridge this gap, this research work has been carried out to perform closed-loop dynamic (control) simulations of a reactive distillation process used for the production of isopropyl alcohol (a fuel additive) using PI and PID controllers tuned with Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols techniques.

PROCEDURE

Data generation

In order to develop the transfer function model required for the control of the reactive distillation process for fuel additive production, data were generated using the prototype plant shown in Figure 1 that was developed with the aid of Aspen HYSYS (Aspen, 2012) by employing a Distillation Column Sub-Flowsheet having two (upper and lower) feed streams and 21 stages. The lower feed stream of the column, entering through the 14th stage, consisted of propylene flowing at a rate of 30 mL/min and at a temperature and a pressure of 25 ^{o}C and 12.30 atm respectively. The second reactant of the process, which was water, entered the column from the upper feed stream, which was the 7th stage of the column, at the same flowrate and temperature as that of the lower feed stream but at a pressure of 1.1 atm. The pressure of the column condenser was 1.0 atm while that of the reboiler was 1.5 atm. The fluid package used for the development of the Aspen HYSYS prototype plant of the process was non-random two-liquid (NRTL). After developing the prototype plant of the column, it was run using Sparse Continuation Solver.

The two reactions involved in the process were equilibrium types given in Equations (1) and (2). Equation (1) was for the main reaction of the process giving the desired product that was isopropyl alcohol while Equation (2) was a side reaction yielding diisopropyl ether that was

expected to be suppressed in the reactive distillation column. The two reactions were modelled to occur in liquid phases and their equilibrium constants were estimated using Gibbs free energy.

$$C_3H_6 + H_2O \xleftrightarrow{K_{eq}} C_3H_8O \quad (1)$$

$$C_3H_8O + C_3H_8O \xleftrightarrow{K_{eq}} C_6H_{14}O + H_2O \quad (2)$$

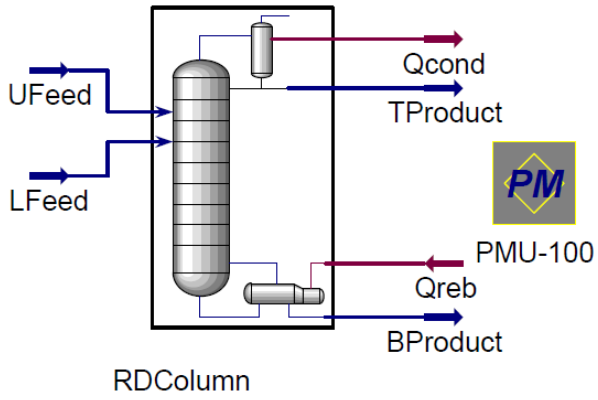

Figure-1. Fuel additive reactive distillation process prototype plant.

After running the prototype plant to convergence using the initial values given in Table-1, the Parametric Utility of Aspen HYSYS was inserted (see Figure-1). The input variables of the utility were chosen to be the reflux ratio and the reboiler duty of the column while the output variable was the mole fraction of isopropyl alcohol (a fuel additive) obtained from the top product of the column. Thereafter, the input variables were varied within the ranges given also in Table-1, and the corresponding output variable value was recorded in each case, and that was what made up the process variable data.

Table-1. Values and ranges of the input variables used.

Parameter	Initial value	Low limit	High limit
Reflux ratio	4	2	6
Reboiler duty (kW)	0.21	0.11	0.31

Process transfer function model development

After obtaining the data from the prototype plant of the process, it was loaded into MATLAB and, with the aid of System Identification Toolbox, a transfer function model of the plant having two input variables and an output variable was developed using *pem* command of the Toolbox. The format of the transfer function model developed was as given in Equation (3).

$$x_{fa}(s) = \frac{K_p e^{(-T_{dp}s)}}{\tau_p s + 1} R(s) + \frac{K_d e^{(-T_{dd}s)}}{\tau_d s + 1} Q(s) \quad (3)$$

Open-loop dynamics study

The transfer function model of the system obtained with the aid of System Identification Toolbox of MATLAB (Mathworks, 2015) was used to develop a Simulink model of the system in the form shown in Figure-2. As can be seen from the figure, the Simulink model of the system had two input variables each denoted by a step block named R and Q. The block named R was the reflux ratio, which was selected as the manipulated variable while the block Q was specified as the disturbance variable of the process. After the Simulink model of the process was developed and the variables specified, steps were applied to the input variables and the responses of the output variable were recorded accordingly.

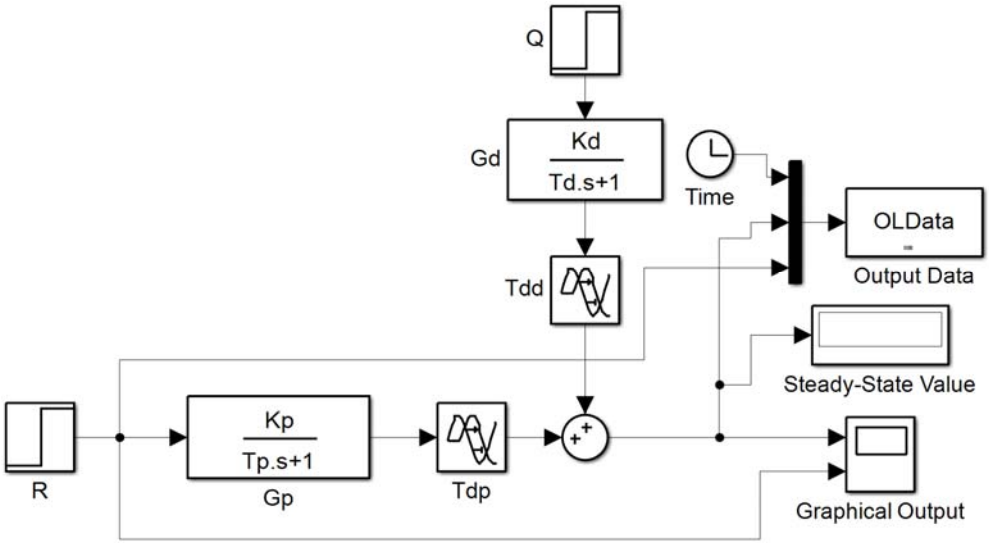

Figure-2. Fuel additive reactive distillation Simulink model for open-loop simulation.

Closed-loop dynamics study

After developing and simulating the open-loop Simulink model of the process, its closed-loop model was also developed with the aid of Simulink in MATLAB by incorporating a controller block, a transfer function block for the final control element and another one for the measuring element as well as a sum (error computing) block. Shown in Figure-3 is the developed closed-loop Simulink model of the reactive distillation process used for the production of isopropyl alcohol in this work.

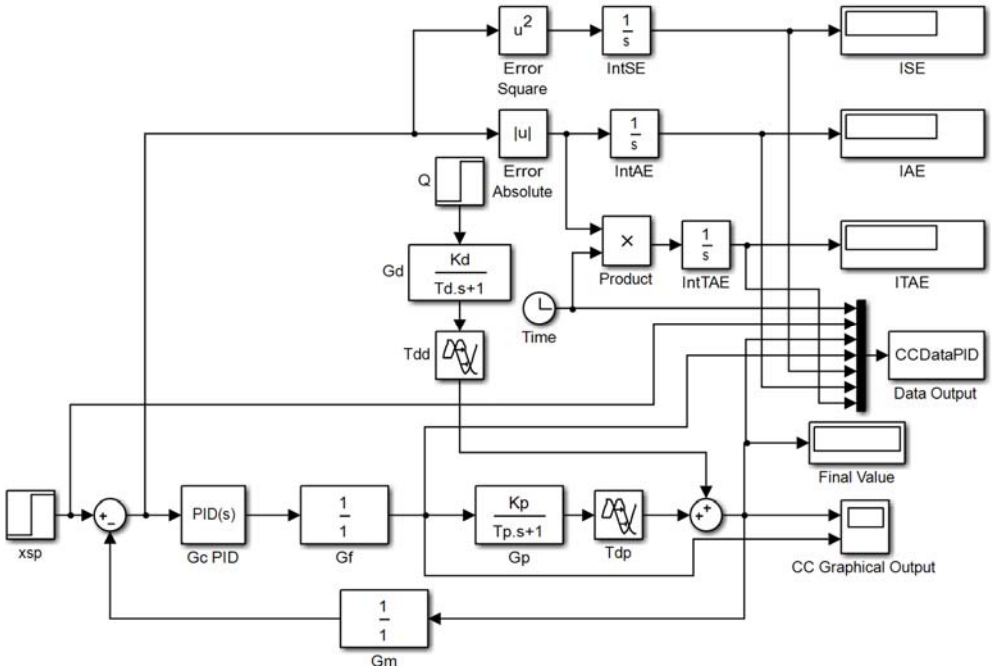

Figure-3. Fuel additive reactive distillation Simulink model for closed-loop simulation.

In order to study the dynamics of the closed-loop Simulink model of the system, three different (Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols) tuning techniques were considered and used with proportional-integral (PI) and proportional-integral-derivative (PID) controllers.

$$G_c(s) = K_c\left(1 + \frac{1}{\tau_I s} + \tau_D s\right) \quad (4)$$

Table-2. Tuning parameter expressions.

Type of control	Cohen-Coon tuning technique[1]	Ziegler-Nichols tuning technique[1]	Tyreus-Luyben[2]
Proportional-Integral (PI)	$K_c = \frac{1}{K_p}\frac{\tau_p}{T_{dp}}\left(0.9 + \frac{T_{dp}}{12\tau}\right)$ $\tau_I = T_{dp}\frac{30 + 3T_{dp}/\tau_p}{9 + 20T_{dp}/\tau_p}$	$K_c = \frac{K_u}{2.2}$ $\tau_I = \frac{P_u}{1.2}$	$K_c = 0.31K_u$ $\tau_I = 2.2P_u$
Proportional-Integral-Derivative (PID)	$K_c = \frac{1}{K_p}\frac{\tau_p}{T_{dp}}\left(\frac{4}{3} + \frac{T_{dp}}{4\tau_p}\right)$ $\tau_I = T_{dp}\frac{32 + 6T_{dp}/\tau_p}{13 + 8T_{dp}/\tau_p}$ $\tau_D = T_{dp}\frac{4}{11 + 2T_{dp}/\tau_p}$	$K_c = \frac{K_u}{1.7}$ $\tau_I = \frac{P_u}{2}$ $\tau_D = \frac{P_u}{8}$	$K_c = 0.45K_u$ $\tau_I = 2.2P_u$ $\tau_D = \frac{P_u}{6.3}$

Source: [1]Stephanopoulos (1984), [2] Seborg *et al.* (2004)

In order to estimate the parameters required by each of the techniques for the PI and the PID controllers, the general transfer function of the controller was taken to be as given in Equation (4) and the relationships used were as given in Table-2.

RESULTS AND DISCUSSIONS

The random data generated, from the Aspen HYSYS prototype plant of the process, for the reflux ratio, which was one of the input variables of the process, were as given in Figure-4. As can be seen from the figure, the generated reflux ratio data were found to be within the range of 2 to 6 used as the low and the high limit of the variable. This was discovered to be an indication that the Aspen HYSYS prototype plant developed was able to recognize the limits entered into it, and that it was also able to represent the process very well.

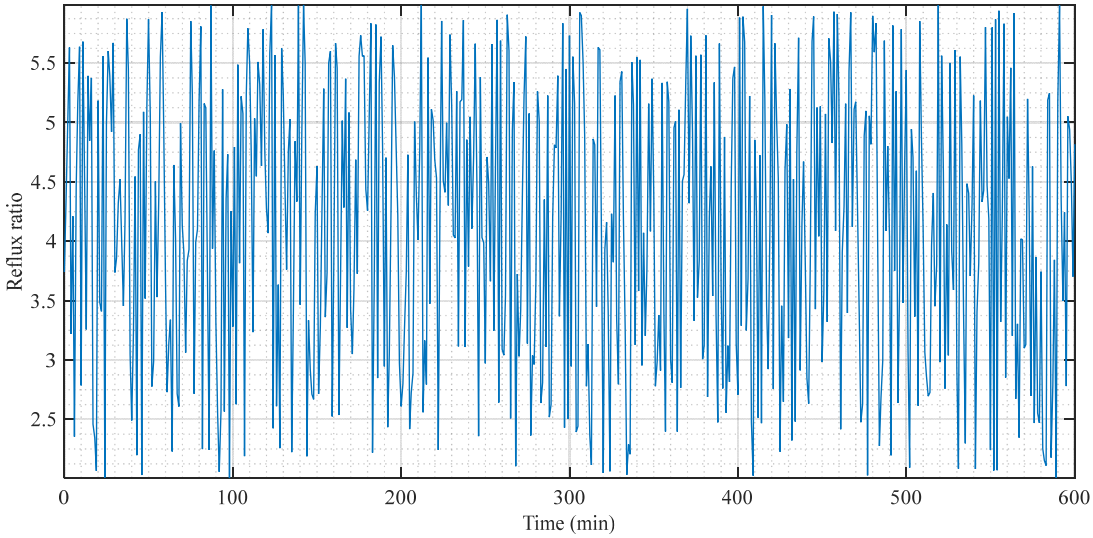

Figure-4. Reflux ratio data generated for the running of the Aspen HYSYS fuel additive reactive distillation process prototype plant.

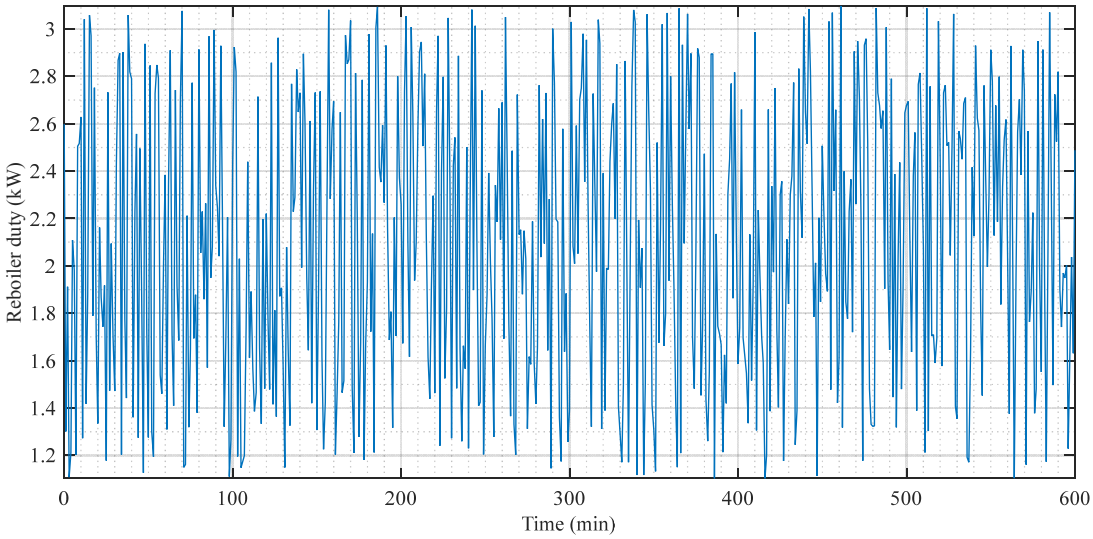

Figure-5. Reboiler duty data generated for the running of the Aspen HYSYS fuel additive reactive distillation process prototype plant.

Given in Figure-5 are the random data generated for the second input variable of the process, which was the reboiler duty. Just as it was observed in the case of the reflux ratio data given in Figure-4, the data for the reboiler duty were also found to be within the range chosen and entered into the Aspen HYSYS prototype plant of the process. This was found to be another evidence that the developed Aspen HYSYS prototype plant of the process was working appropriately.

In addition, the input data generated were made to be random in nature so that the behaviour of the developed Aspen HYSYS model of the process could be tested under various conditions and, as such, the robustness of the prototype plant could be ascertained.

When the generated input data were then used to run the developed Aspen HYSYS prototype plant of the process, the obtained output data, that is, the mole fraction of isopropyl alcohol (IPA) given from the top segment of the column were as shown in Figure-6. From the Figure, it was clear that the generated output data were also random in nature in resemblance to the data of the input variables used. This observation has shown that the output obtained from the fuel additive reactive distillation prototype plant was a function of the input variables used to run the plant.

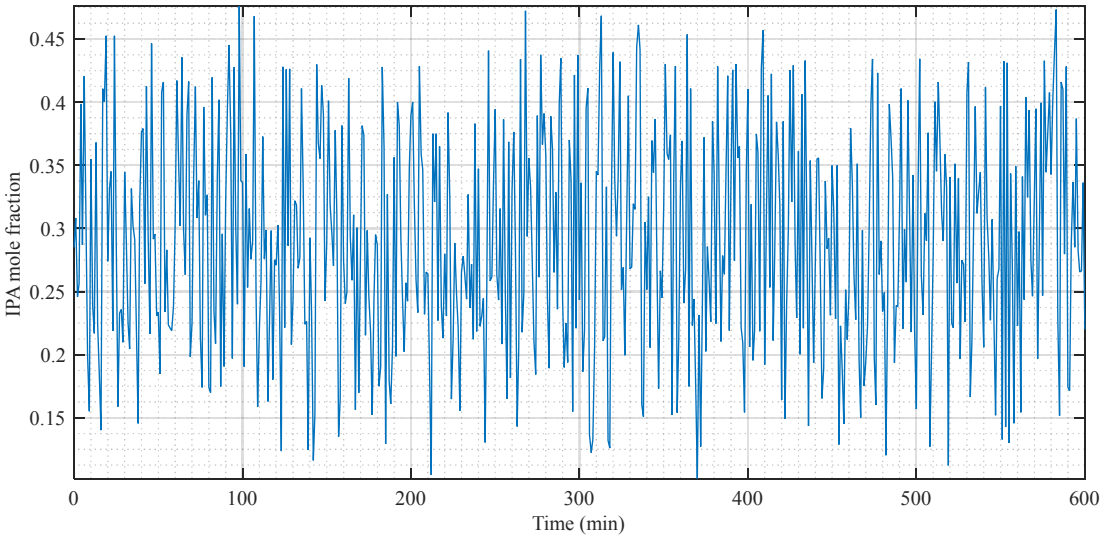

Figure-6. IPA mole fraction estimated from the simulation of the Aspen HYSYS fuel additive reactive distillation process prototype plant.

Using the generated input and output data, the parameters of the transfer function model of the process were estimated with the aid of *pem* command MATLAB to be as given in Equation (5).

$$x_{fa}(s) = \frac{0.10e^{(-0.64s)}}{30.99s+1}R(s) + \frac{0.14e^{(-0.53s)}}{5.61s+1}Q(s) \quad (5)$$

Considering the model given in Equation (5), it could be observed that the time constant of the model relating the output variable to the selected manipulated variable (reflux ratio) was higher than that of the one relating the output variable to the disturbance variable (reboiler duty) of the process. This was found to be an indication of the fact that the main equation of the process would be slower.

In order to investigate how the process would behave dynamically, its open-loop Simulink model was developed and simulated, and the results obtained were as given in Figures 7-9.

Shown in Figure-7 is the response of the system when a unit step was applied to the reflux ratio alone. According to the figure, the system was able to respond to the change in the reflux ratio and become steady at an IPA mole fraction of approximately 0.10 within about 180 min of the simulation time.

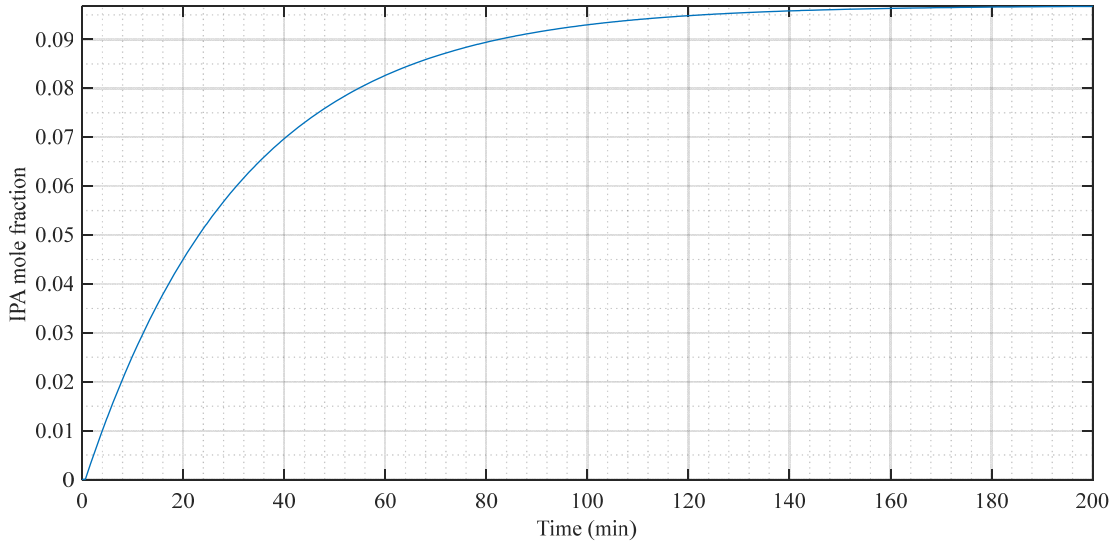

Figure-7. Open-loop dynamic response of the system to a unit step change in the reflux ratio.

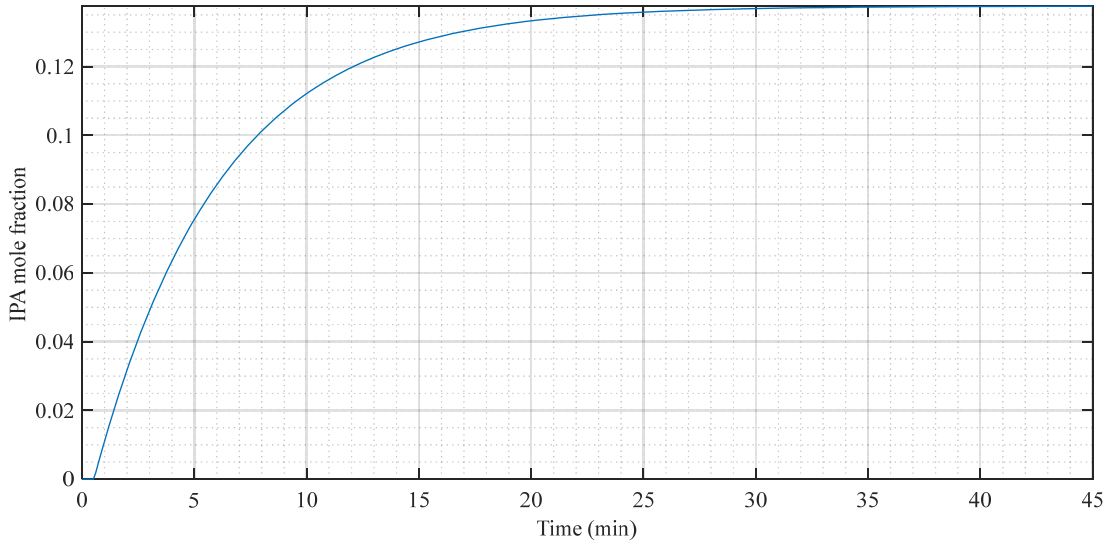

Figure-8. Open-loop dynamic response of the system to a unit step change in reboiler ratio.

Similarly, the response given by the system when a unit step was applied to the second input variable of the process, which was the chosen disturbance variable (reboiler duty), is shown in Figure-8. Based on the information obtained from the figure, the steady-state value of approximately 0.14 was attained within about 35 min of the simulation time.

It should be noted that the difference between the response times of the two model parts was as a result of the difference in their time constants. Generally, the higher the time constant of a process, the higher its response time. Furthermore, applying a unit step to each of the input variables (reflux ratio and reboiler duty), the response given by the fuel additive reactive distillation process is shown in Figure-9. It could be deduced from the figure that the system was able to attain its steady-state value of approximately 0.23 within about 175 min of the simulation time used.

Based on the open-loop dynamic responses of the system obtained and given in Figures 7-9, it was thus established that the process being considered in this work was a stable one because its responses obtained upon the application of steps to the input variables were able to get settled after some time. However, it was still deemed necessary to control the system so as to increase its steady-state value in an attempt to get higher mole fraction of the isopropyl alcohol being produced as the fuel additive.

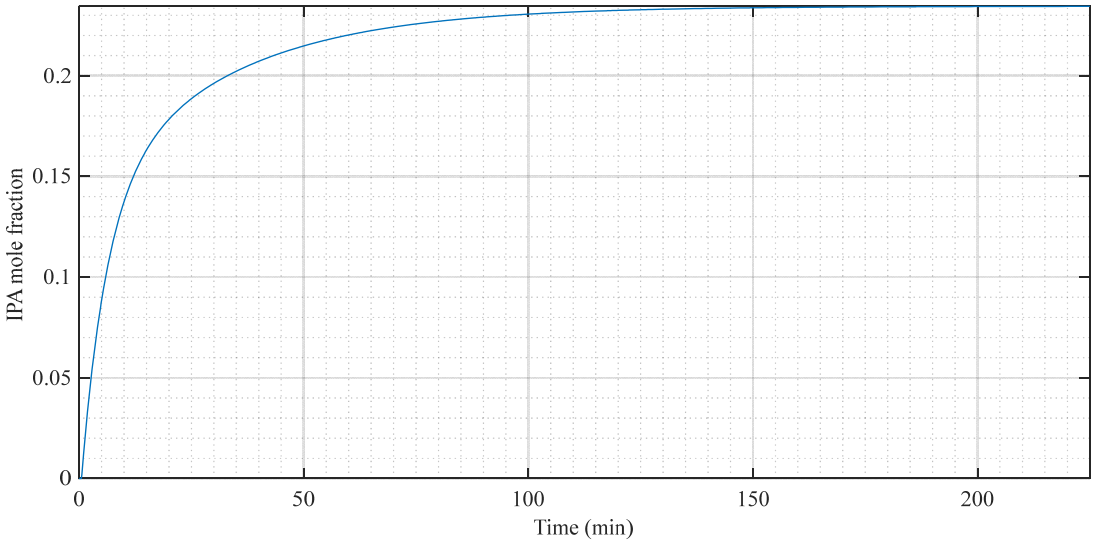

Figure-9. Open-loop dynamic response of the system to unit step changes in reflux ratio and reboiler duty.

Consequently, three different control techniques (Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols methods) were applied using PI and PID controllers in a set-point tracking manner to the process and the closed-loop dynamic responses were recorded and plotted. In the closed-loop simulation aspect of this work, the controlled variable was the mole fraction of isopropyl alcohol (IPA) obtained from the top section of the column while the manipulated variable was the reflux ratio. Also, the reboiler duty of the column was chosen as the disturbance variable of the process, even though the regulatory control aspect of the work has not been simulated in this work.

Shown in Figure-10 is the closed-loop dynamic response of the fuel additive reactive distillation system to a PI controller when a 0.25-unit step change was applied to the set-point of the controlled variable and when the open-loop steady-state value of the IPA mole fraction was 0.10. As can be seen from the figure, within the simulation time of 25 min considered, the system was able to get to its steady state. For this case of PI controller being used to regulate the system, the method that gave the minimum overshoot and less oscillations was found to be Tyreus-Luyben technique. On the other hand, the overshoot and the number of oscillations recorded in the case of Cohen-Coon technique were discovered to be the highest. This, therefore, implied that, for this case, Cohen-Coon was good because it made the system to get settled within the simulation time used, but the best tuning technique for this process was obtained to be Tyreus-Luyben.

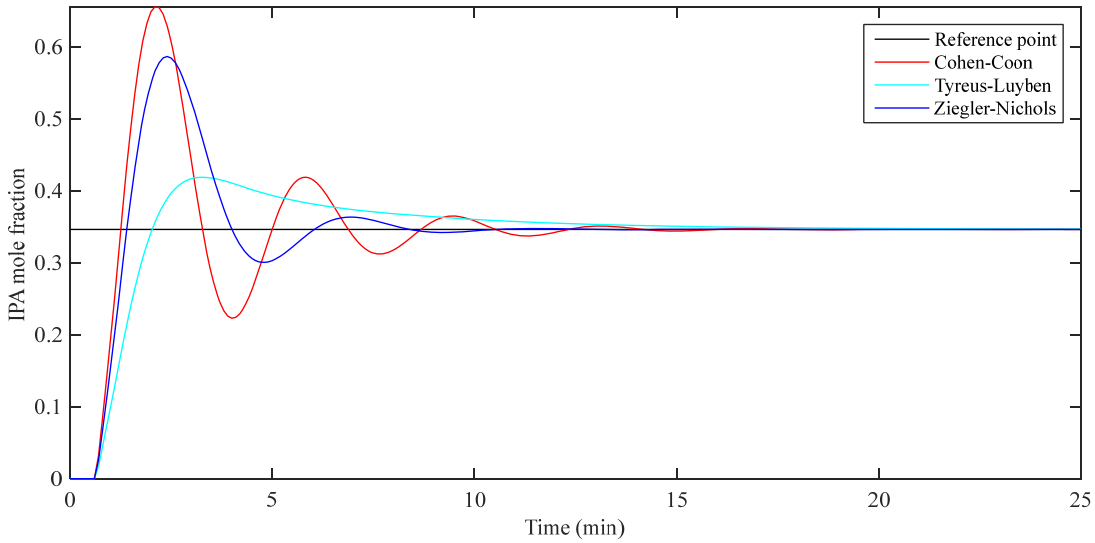

Figure-10. PI closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.10.

Shown in Figure-11 is the response of the fuel additive reactive distillation system to a PID controller under a set-point tracking simulation upon the application of a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value of the system was 0.10. As can be from the figure, the performances of the three tuning techniques considered were in the same order as that obtained from the PI control simulation of the same system. In addition, the level of the overshoot given, especially by the Ziegler-Nichols and Tyreus-Luyben tuning techniques, were lesser than those given by the PI control system.

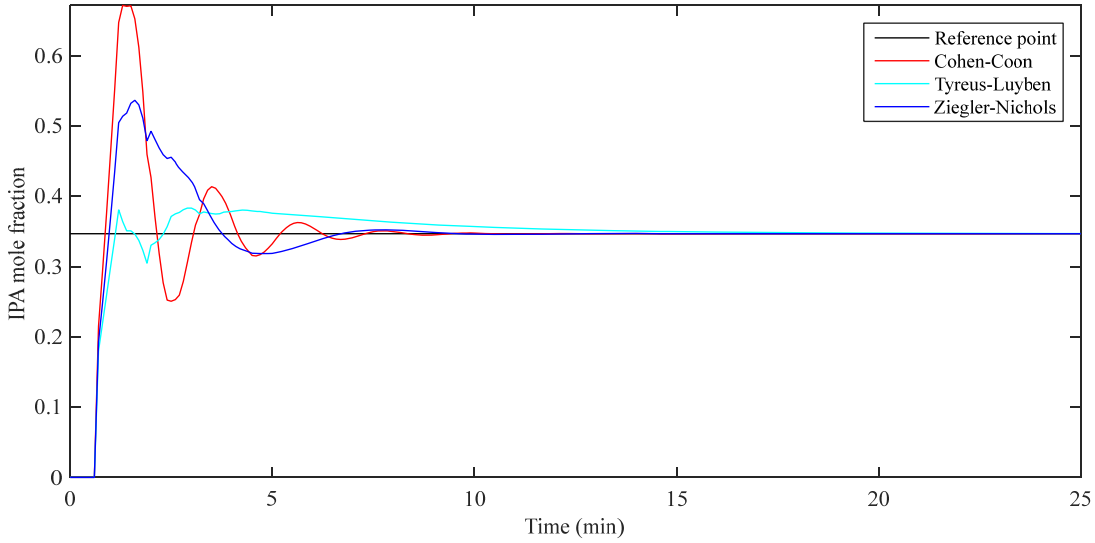

Figure-11. PID closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.10.

In order to gain a better understanding on the performances of the different controllers considered in this work, their performance values were calculated. The performance values estimated for each of the controllers were integral of the square error (ISE), integral of the absolute value of the error (IAE) and integral of the time-weighted absolute error (ITAE).

Table-3. Performance values of the controllers when the open-loop steady-state IPA mole fraction was 0.10.

Tuning technique	PI			PID		
	ISE	IAE	ITAE	ISE	IAE	ITAE
Cohen-Coon	0.22	1.02	2.86	0.16	0.65	1.03
Tyreus-Luyben	0.14	0.80	2.64	0.09	0.50	1.67
Ziegler-Nichols	0.18	0.82	1.69	0.12	0.60	1.04

The results obtained from the calculations of the performance values are given in Table-3. From the table, it was discovered that the control tuning technique with the lowest ISE and IAE was Tyreus-Luyben. Furthermore, Ziegler-Nichols had the lowest ITAE for the PI controller while, in the case of PID controller, Cohen-Coon had the lowest ITAE. The results given in Table-3 were found to be indications of the fact that, for this fuel additive reactive distillation process, Tyreus-Luyben tuning technique was the best in suppressing large and small errors whereas it was not the best in suppressing errors persisting for a long period of time.

Also simulated and the results of which are given in Figures 12 and 13 were the closed-loop fuel additive reactive distillation system using PI and PID controllers tuned with Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols techniques when the open-loop steady-state mole fraction of the fuel additive was 0.14. The observations made in this situation were found to be similar to those of the PI and PID controllers tuned with the different techniques when the open-loop steady-state value was 0.10. For instance, for this case also, the tuning technique that gave the lowest overshoot and number of oscillations was still found to be Tyreus-Luyben.

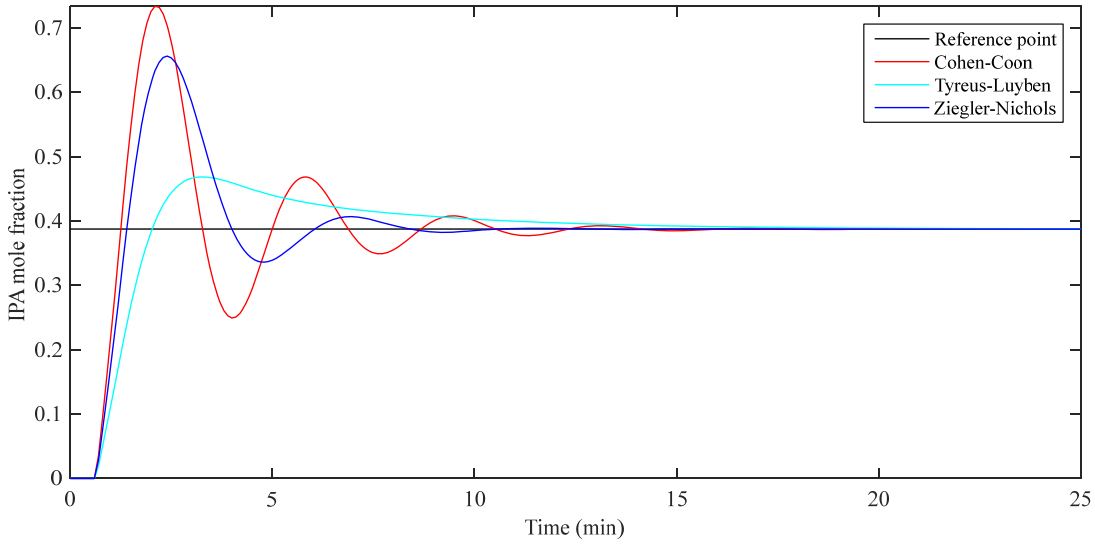

Figure-12. PI closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.14.

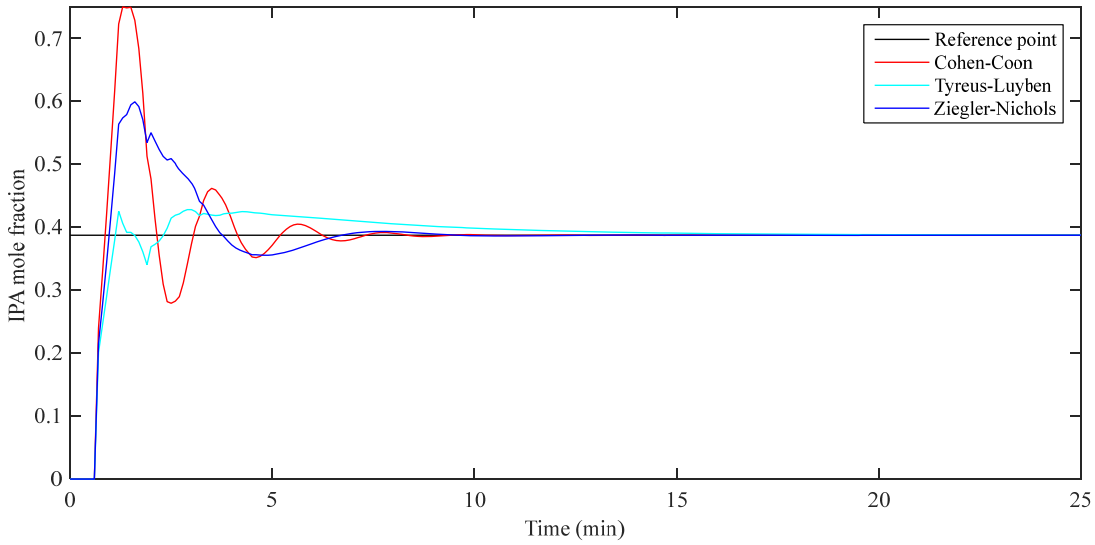

Figure-13. PID closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.14.

Considering the performance values given in Table-4 for the closed-loop simulations carried out when the open-loop steady-state value of the mole fraction of isopropyl alcohol was 0.14, Tyreus-Luyben technique was still the one that was found to be the best in suppressing large and small errors because it was the tuning technique that gave the lowest ISE and IAE values among the methods considered. Regarding ITAE, for the PI and the PID controllers, the techniques with the lowest values were found to be Ziegler-Nichols and Cohen-Coon, respectively.

Table-4. Performance values of the controllers when the open-loop steady-state IPA mole fraction was 0.14.

Tuning technique	PI			PID		
	ISE	IAE	ITAE	ISE	IAE	ITAE
Cohen-Coon	0.27	1.15	3.20	0.20	0.73	1.15
Tyreus-Luyben	0.18	0.90	2.95	0.11	0.56	1.86
Ziegler-Nichols	0.23	0.92	1.89	0.15	0.68	1.17

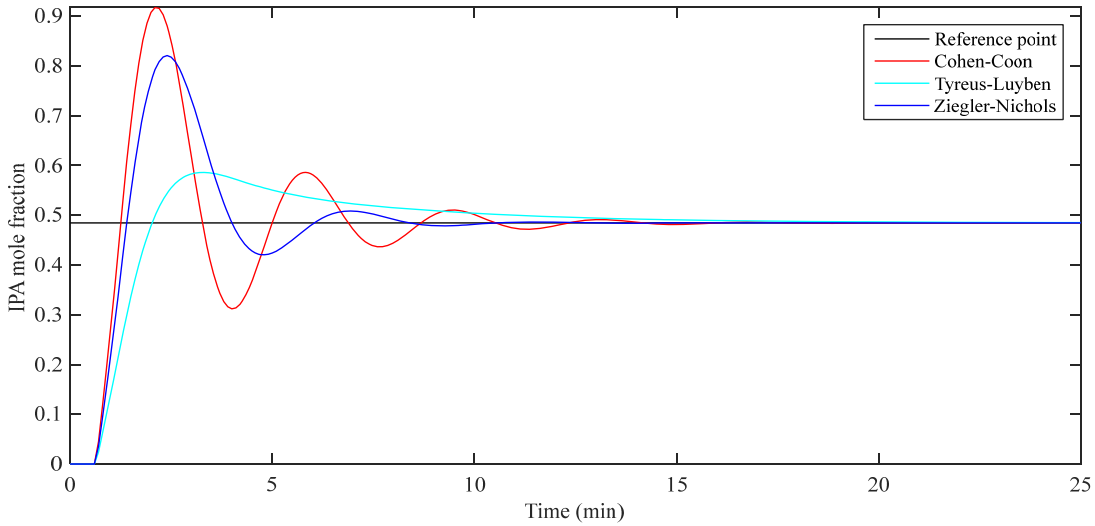

Figure-14. PI closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.23.

The results shown in Figures 14 and 15 that were obtained from the control simulations carried out with the PI and PID controllers using Cohen-Coon, Tyreus-Luyben and Ziegler-Nichols tuning techniques when the open-loop steady-state value of the mole fraction of isopropyl alcohol obtained from the top section of the column was 0.23 were found not to be too different from the ones obtained previously. In fact, their trends were the same as, in this cases of PI and PID also, the technique with the lowest overshoot and number of oscillations was still discovered to be Tyreus-Luyben.

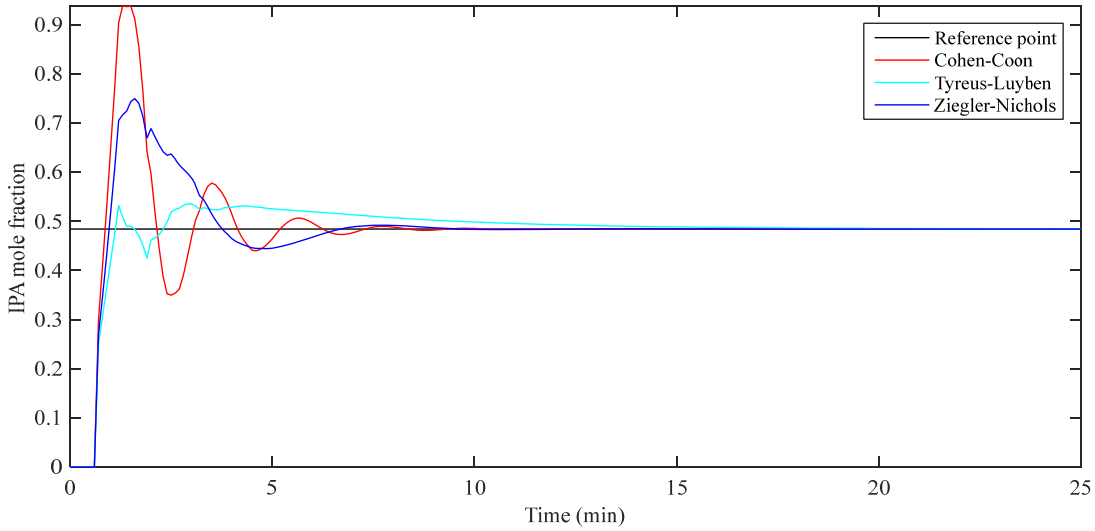

Figure-15. PID closed-loop dynamic response of the system to a 0.25-unit step change in IPA mole fraction when the open-loop steady-state value was 0.23.

Table-5. Performance values of the controllers when the open-loop steady-state value was 0.23.

Tuning technique	PI			PID		
	ISE	IAE	ITAE	ISE	IAE	ITAE
Cohen-Coon	0.42	1.43	4.00	0.31	0.91	1.43
Tyreus-Luyben	0.28	1.12	3.69	0.17	0.70	2.32
Ziegler-Nichols	0.35	1.15	2.36	0.24	0.84	1.45

The performance values of the controllers given in Table-5 were also found to be in agreement with the ones obtained earlier for the cases of initial steady-state IPA mole fraction values of 0.10 and 0.14. These results have, thus, pointed out that the performances of the controllers for the isopropyl alcohol reactive distillation system were not accidental at all because the same trends of results were observed for the three cases of different open-loop steady-state values that were considered.

CONCLUSIONS

The results obtained from the open-loop simulations of the reactive distillation process used for isopropyl alcohol (a fuel additive) production carried out revealed that the system was a stable one because it was able to get settled at steady states within the simulation times considered. Furthermore, the closed-loop system of the process simulated using PI and PID controllers showed that the best tuning method for the system in suppressing large and small errors was Tyreus-Luyben technique, but in suppressing any persistent error, Ziegler-Nichols and Cohen-Coon methods were found to be the best for PI and PID controllers respectively. Moreover, the comparison of the performance values of the controllers indicated that the PID controllers tuned with the different techniques used were better than the corresponding PI controllers because their (the PID controller's) ISE, IAE and ITAE values were found to be less than those of the PI controllers considered for the fuel additive reactive distillation process.

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Nomenclature

BProduct	Column bottom product
G_c	Transfer function of the controller
G_d	Transfer function of the disturbance
G_f	Transfer function of the final control element
G_m	Transfer function of the measuring element
IAE	Integral of the absolute value of the error
IPA	Isopropyl alcohol
ISE	Integral of square error
ITAE	Integral of time-weighted absolute error
K_d	Static gain of the disturbance
K_{eq}	Equilibrium constant
K_p	Static gain of the process
LFeed	Lower feed of the column
NRTL	Non-random two-liquid
PI	Proportional-integral
PID	Proportional-integral-derivative
Q	Reboiler duty (kW)
Q_{cond}	Condenser heat duty (kW)
Q_{reb}	Reboiler heat duty (kW)
R	Reflux ratio
RDColumn	Reactive distillation column
T_d	Time constant of the disturbance
T_{dd}	Delay time of the disturbance
T_{dp}	Delay time of the process
T_p	Time constant of the process
TProduct	Column top product
UFeed	Upper feed of the column
x_{fa}	Fuel additive (isopropyl alcohol) mole fraction
x_{sp}	Set-point of the mole fraction

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