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Studying the Dynamics of a Fame Reactive Distillation System towards some input types

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Abstract : This work has been carried out to study the dynamics of a fatty acid methyl ester reactive distillation process upon the application of some input types. The fatty acid methyl ester used as a case study was methyl oleate, which was produced from the esterification reaction between methanol and oleic acid. The dynamics study was accomplished using the first order transfer function model of the process developed with the aid of System Identification Toolbox of MATLAB from the data generated using the prototype plant of the process set up with the aid of Aspen HYSYS. The results obtained from the data generation showed that Aspen HYSYS was successfully used to study this system, the experimental setup of which was not available. In addition, the results obtained from the simulation of the transfer function model revealed that the system was a stable one because it was able to get to a steady state when each of constant, step and pulse input variable changes were applied to it. Therefore, it has been demonstrated that, besides the step input that is most commonly used in studying the dynamics of a system, other input types such as constant, ramp, pulse and repeating sequence can as well be applied.
Keywords: Reactive distillation, fatty acid methyl ester (FAME), Aspen HYSYS, transfer function model, MATLAB, constant input, step input, pulse input.

1.0 Introduction

The variables that are capable of independently stimulating a process and inducing changes in its internal conditions are referred to as the input variables of that process. The changes that occur in the internal state of the process are usually apparent from the observation of the changes in the output variables.The magnitude and the nature in which the process responds to a change in anyinput variable clearly depends on the nature of the input changethat has been applied. In addition, this also depends on the intrinsic nature of the process itself [1]. For example, the response of 5 L of water being heated using a hot plate will not be the same as that being heated with the aid of sunlight. In the same vein, the cooling of liquid using a refrigerator will not give the response if the same liquid is cooled in an open atmosphere.

Generally, for any given input change, the observed process response provides information about the intrinsic nature of the process under investigation. Similarly, if there is proper knowledge about the intrinsic nature and the characterization of a process, then,its response to any input change can be predicted under the subject that is referred to as process dynamics[1].

Process dynamics is a phenomenon that is concerned with analysing the dynamic (that is, the time-dependent) behaviour of a process in response to various types of inputs. A wide variety and limitless number of actual processes are able to be characterized into a relatively small number of well-defined categories through studying process dynamics, and the advantages of such process characterization cannot be overemphasized[1]especially when the process in question is a complex one like reactive distillation.

Reactive distillation can be defined as a process that combines both separation and chemical reaction in a single piece of equipment([2], [3], [4], [5]). The process has a lot of benefits, especially, for those processes having reactions occurring at temperatures and pressures suitable for the distillation of the process components ([6-17]). Actually, the process combines the benefits of equilibrium reaction with a separation operation (in this case, 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 ([18], [19], [14], [17]) that are required for a process. The combination of reaction and separation gives this process several advantages that also result in significant economic benefitsin comparison to a conventional design, and these economic benefits include lower capital investment, lower energy cost and higher product yields ([20], [21], [17]). Based on the benefits of this process, it will be very good in the production of fatty acid methyl ester, otherwise known as biodiesel, which is a renewable energy source[22] that has superior properties than that of petro-diesel fuel([23], [24]) such as nontoxicity [25]. The research involving the production of fatty acid methyl esters are being embarked on nowadays becauseit is very important for today's world to identify an alternative tofossil fuel to meet the future demands for energy([26-28]), based on the fact that diesel fossil fuel reserves dwindling and at a time will run out[29], especially for use in internal combustion engines, which reducethe peak flame temperature and thereby reduction in various emissions[30],as it (biodiesel) is an alternative fuel that can be prepared from renewable biological sources such as vegetable oils both(edible and nonedible oil) and animal fats([31], [32]).

So far from the literature, Roat *et al.*[33] discussed dynamic simulation of reactive distillation with an equilibrium model using the Eastman methyl acetate process as a case study. Ruiz *et al.*[34] developed a generalized equilibrium model for the dynamic simulation of multicomponent reactive distillation. A simulation package called REActive Distillation dYnamic Simulator (READYS) was used to carry out the simulations of their work. Several test problems were studied and used to compare the work with those of others. Alejski and Duprat [35] developed a dynamic equilibrium model for a tray reactive distillation column. Similarly,Sneesby *et al.* [36] developed a dynamic equilibrium model for a tray reactive distillation column used for the production of ethyl *tert*-butyl ether (ETBE). In their own work, chemical equilibrium on all reactive stages and constant enthalpy were assumed in order to simplify the model that was implemented in Speed Up and simulated. Kreul *et al.* [37] developed a dynamic rate-based model for a reactive packed distillation column for the production of methyl acetate. All the important dynamic changes except the vapour holdup were considered in the model developed in the study. The dynamic rate-based model was evaluated in ABACUSS large-scale equation-based modelling environment. Dynamic experiments were carried out and the results obtained were compared to those of simulations. Peng *et al.* [38] developed dynamic rate-based and equilibrium models for a reactive packed distillation column for the production of *tert*-amyl methyl ether (TAME). The two types of models, consisting of differential and algebraic equations, were implemented in gPROMS and dynamic simulations were carried out to study the dynamic behaviour of the reactive distillation of the TAME system. Giwa and Karacan [18] used AutoRegressive with eXogenous Inputs (ARX) and AutoRegressive Moving Average with eXogenous Inputs (ARMAX) models they developed from generated experimental data to study the dynamics of a reactive distillation column used for ethyl acetate production. Also, Giwa and Karacan [21]developed dynamic models from first principles for a reactive packed distillation column, and solved the models with the aid of MATLAB. The results they obtained from the simulation were compared with the experimental ones.

Based on the information obtained from the literature review carried out, it has been discovered that some researchers have worked on the studies of dynamics of reactive distillation system, but very few of them used a developed transfer function model to do that. Besides, the dynamics studies carried out by some other researchers were based just on using step inputs. It should be noted that step input is not the only input variable that are available in studying the dynamics of a process in Chemical Engineering.

Therefore, this work has been carried out to investigate the dynamic response of a reactive distillation system used for the production methyl oleate towards some input variables including the commonest one, which

is the step input, using a transfer function model developed with the generated data obtained from the prototype plant of the process set up with the aid of Aspen HYSYS.

2.0 Methodology

2.1 Data Generation for Modelling

The data used for the development of the model equation of the oleic acid methyl ester reactive distillation system considered in this work were obtained from the prototype plant of the process developed with the aid of Aspen HYSYS[39]. The Aspen HYSYS prototype plant, which was developed using UNIQUAC as the Fluid Package, had seventeen (17) stages, excluding the condenser and the reboiler, which was divided into three sections - rectifying, reaction and stripping sections. The condenser used, which was a total type, as well as the reboiler were taken to operate at atmospheric pressure without any drop. The plant had two feed streams that were acid (oleic) feed and alcohol (methanol) feed entering the column at stages 6 and 11 respectively. In addition, the oleic acid feed entered the column at a temperature and a pressure of 350 ^{o}C and 1 atm, respectively while the methanol stream was fed into the column at a temperature of 35 ^{o}C and a pressure 1 atm.

The reaction occurring in the column was an equilibrium type, given in Equation (1), occurring in liquid phase whose basis was taken to be molarity and the equilibrium constant of which was estimated using Gibbs Free Energy.

$$C_{18}H_{34}O_2 + CH_3OH \leftrightarrow C_{19}H_{36}O_2 + H_2O \quad (1)$$

In order to use the prototype plant of the process to generate the data required for model development, Parametric Utility (designated in Figure 1 as PMU) of Aspen HYSYS was added to the developed prototype. The input variable of the Parametric Utility and, of course, that of the process, was the reboiler duty while the output variable was the mole fraction of the methyl oleate obtained from the bottom section of the column. Before generating the data for the output variable, a random data set between 1.1 and 1.7 kJ/s was first built for the input variable.

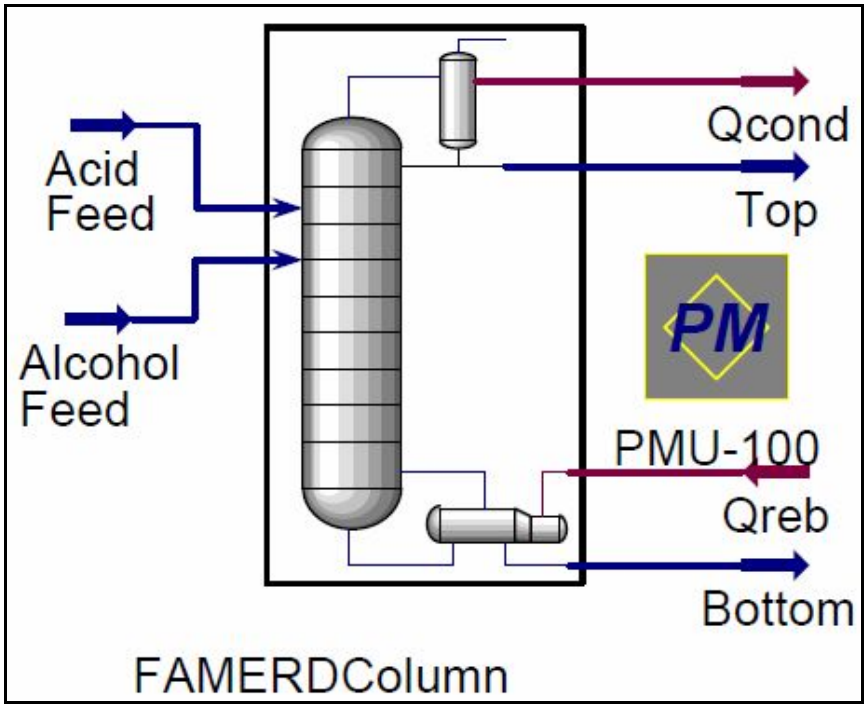

Figure 1. Fatty acid methyl ester reactive distillation process column

2.2 Model Development

After generating the data required for the development of the reactive distillation process model, MATLAB [40] codes were written, specifically, using the *pem* command to obtain a single input – single output with delay transfer function model of the process having the form given in Equation (2).

$$G_p(s) = \frac{x_{fame}(s)}{Q(s)} = \frac{K_p e^{(-T_{dp}s)}}{\tau_p s + 1} \tag{2}$$

2.3 Dynamics Study

The dynamics study of the reactive distillation system considered in this work was carried out by representing the process transfer function model in Simulink environment using appropriate blocks. Different input types (Constant, step, ramp, pulse andrepeating sequence inputs) were used to carry out the study and the Simulink models of all of them are given in Figures 2 – 6.

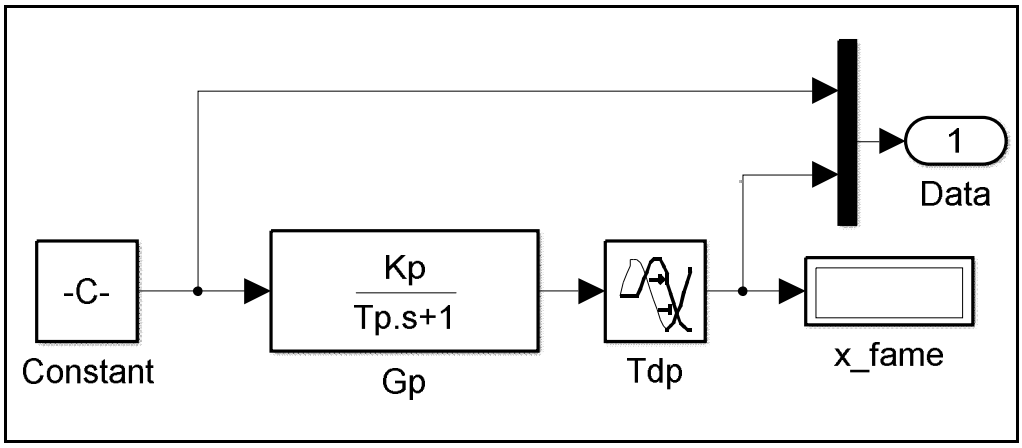

Figure 2. Simulink model of the reactive distillation process with constant input

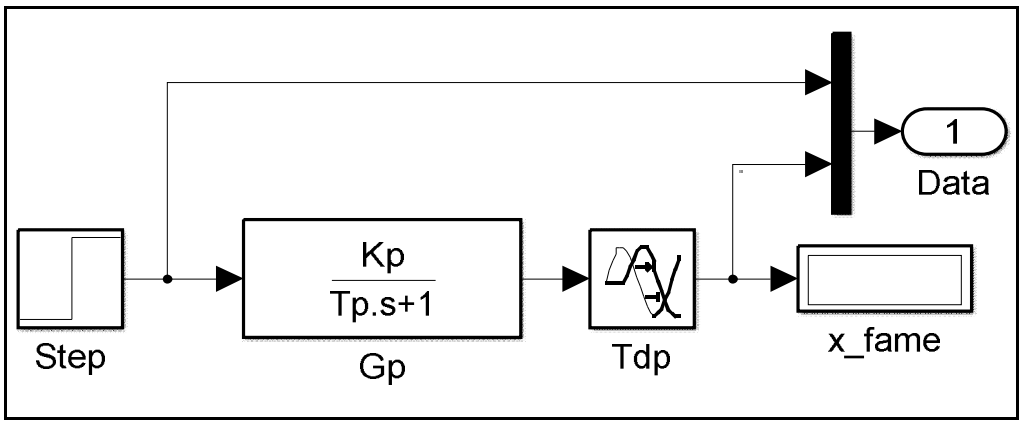

Figure 3. Simulink model of the reactive distillation process with step input

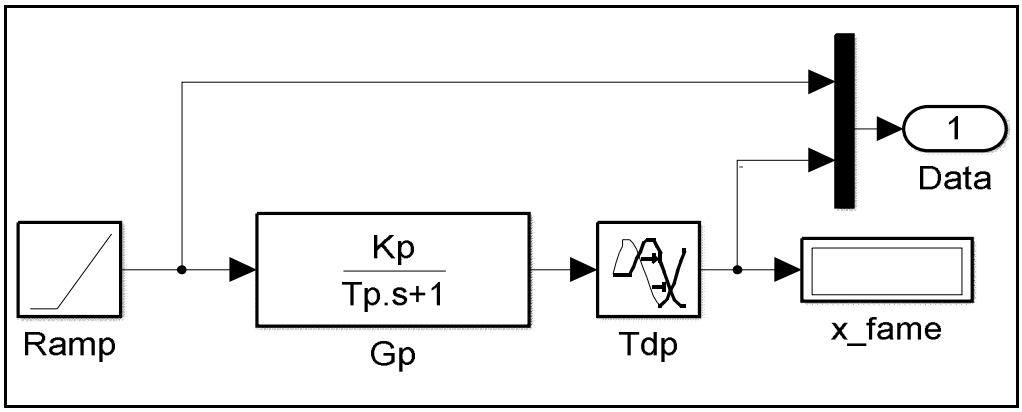

Figure 4. Simulink model of the reactive distillation process with ramp input

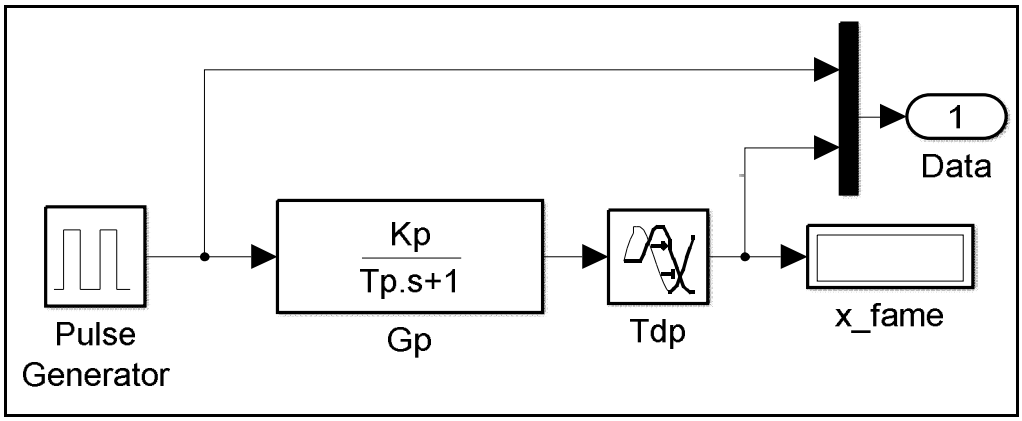

Figure 5. Simulink model of the reactive distillation process with pulse input

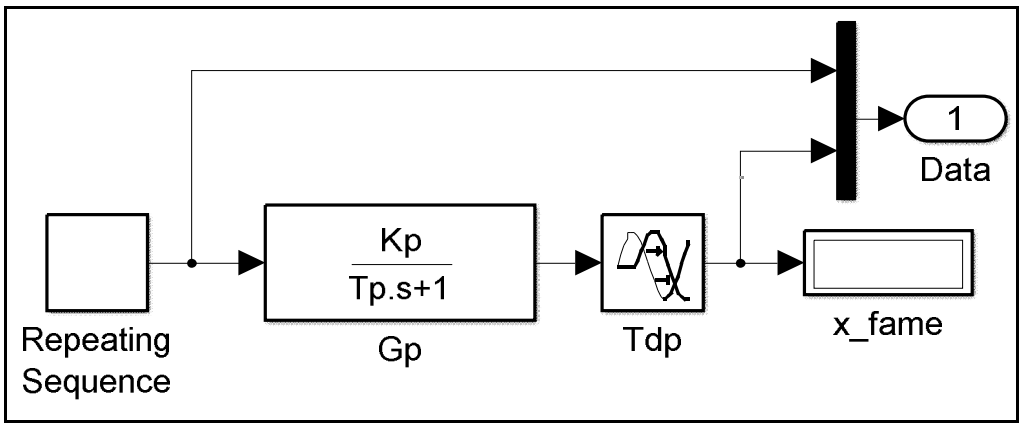

Figure 6. Simulink model of the reactive distillation process with repeating sequence input

3.0 Results and Discussion

The values of the reboiler duty generated randomly using Aspen HYSYS, which were used to run the developed prototype plant, is given in Figure 7. It can be noticed from the results given in Figure 7 that the values of the reboiler duty were actually random in nature. Normally, the values of the input values are made random in order to know how the process would respond under different operating conditions.

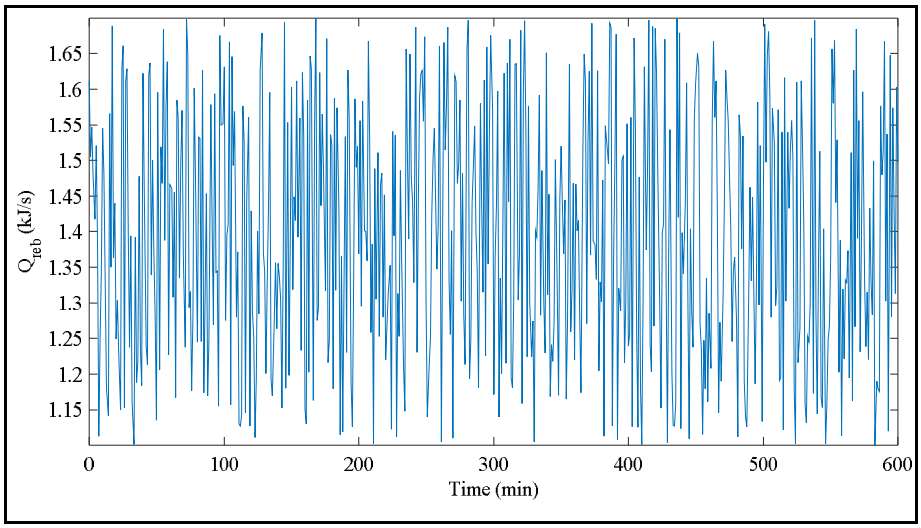

Figure 7. Randomly generated reboiler duty values

Also, given in Figure 8 are the values of the mole fraction of methyl oleate obtained from the bottom section of the column when the generated random reboiler duty values were used to run the developed prototype plant. As it is known that the nature of the response of an output variable to a particular input variable is a function of the nature of that input variable. Since the input variable of the process was random in nature (see Figure 7), the nature of the output variable given was also observed to be random (Figure 8). This observation was an indication that the developed prototype plant of the process was working in line with the principles of process dynamics.

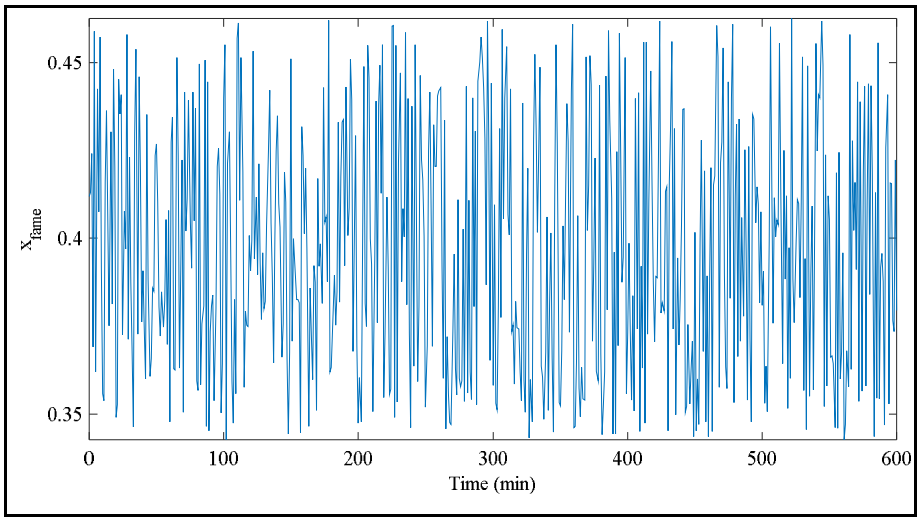

Figure 8. Generated bottom methyl oleate mole fraction values

Now, using the generated input and output data, with the aid of the System Identification Toolbox of MATLAB, the developed transfer function model was obtained as given in Equation (2). Based on the configuration used for the model development, the transfer function model was found to be a single-input single-output (SISO) with delay model having the input and the output variables to be the reboiler duty of the column and the mole fraction of methyl oleate (a fatty acid methyl ester) obtained through the bottom section of the column, respectively.

$$x_{fame}(s) = \frac{0.2845e^{-9.2}}{373.8s+1}Q(s) \qquad (2)$$

From the developed transfer function model of the process, it was observed that the system might take some time to get to steady state because its time constant is somehow high. However, the value of the process at steady state would depend on the nature and the value of the input variable applied to the system.

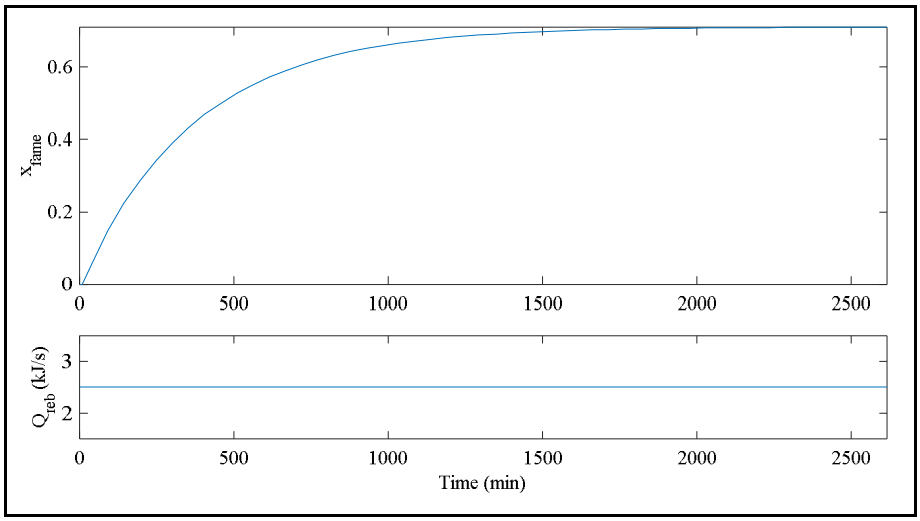

Figure 9. Process response to a constant input of magnitude 2.5 kJ/s

To start with, a constant input of magnitude 2.5 kJ/s was applied to the system and the results, both the input applied and the output given, obtained were as given in Figure 9. From the figure, it was observed that the system followed a smooth transient nature to get to its steady state value of approximately 0.71. Also, considering the kind of the input changed that was applied to the system and based on the figure, the response given by the system was found to be very comparable to that of a first order system, and this was found to be in good agreement with the type of the transfer function model of the system that was developed and given in Equation (2).

Given in Figure 10 is the response of the system as well as the applied step input change of 2.5 kJ/s, which was passed to the input variable of the system. Observing the figure, it was discovered that the response of the system to a step input was similar to that given when a constant input was applied to the system (see Figure 9). In addition, the steady-state values of the two (constant input simulated and step input simulated) systems were found to be exactly the same within the simulation time used. The only difference between these two systems was found to be just the nature of the input applied.

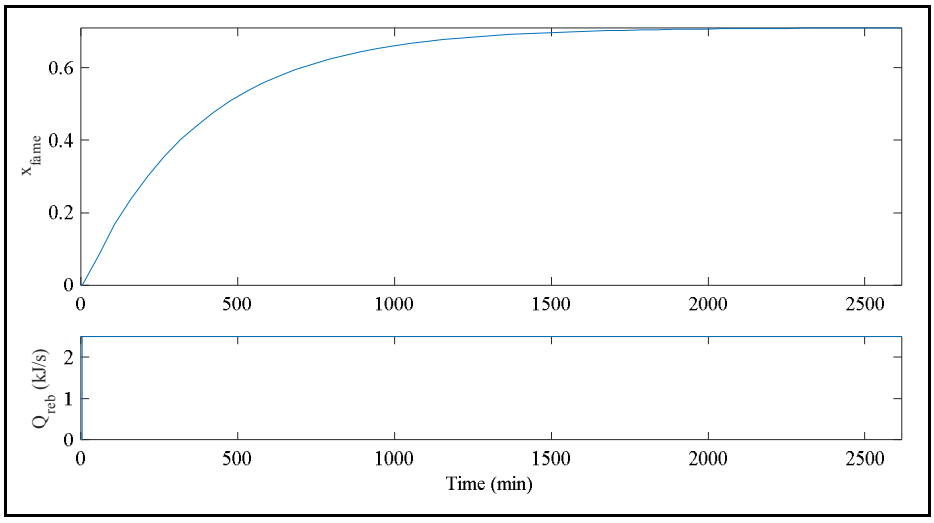

Figure 10. Process response to a step input change of magnitude 2.5 kJ/s

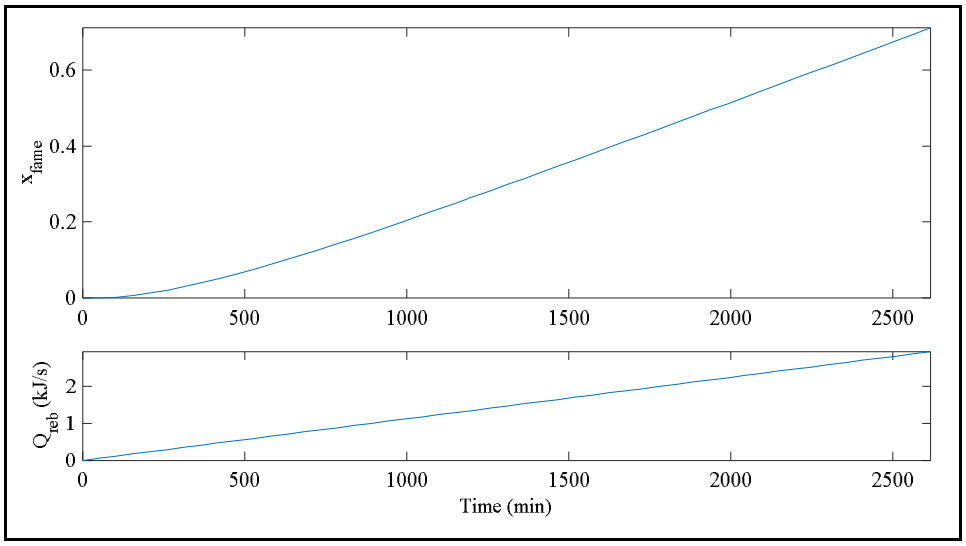

Figure 11. Process response to a ramp input

In Figure 11, the dynamic response of the reactive distillation system towards a ramp input, which is another input type that can be used in process dynamics, is shown. Recalling the principle of a system giving a response that is a function of the nature of the input applied, it was discovered from Figure 11 that the response given by the system upon the application of a ramp input change was different from the other two considered before. In this case also, the nature of the output response of the system was discovered to be similar to that of the input used. This was found to be another evidence that the developed system under investigation was showing dynamics that was in line with the theoretical principles of the subject. Furthermore, in order to obtain a final methyl oleate mole fraction of approximately 0.71, which would be very close to the steady-state values given by the system when constant and step inputs were applied, the slope of the ramp input was set to be 0.0011191 kW/s applied at time zero with zero initial output.

The response given by the system upon the application of a pulse input variable that was achieved through the use of a pulse generator block of Simulink is given in Figure 12. With the pulse input having an amplitude of 2.5 kJ/s, a period of 50 min, a width of 99.5 min and without any phase delay, a steady-state mole fraction of approximately 0.71 was as well achieved.

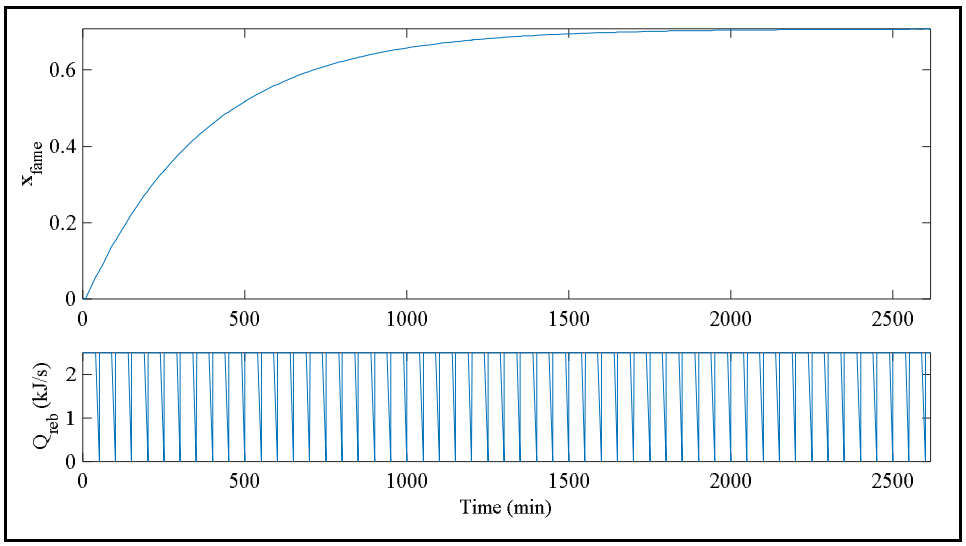

Figure 12. Process response to a pulse input

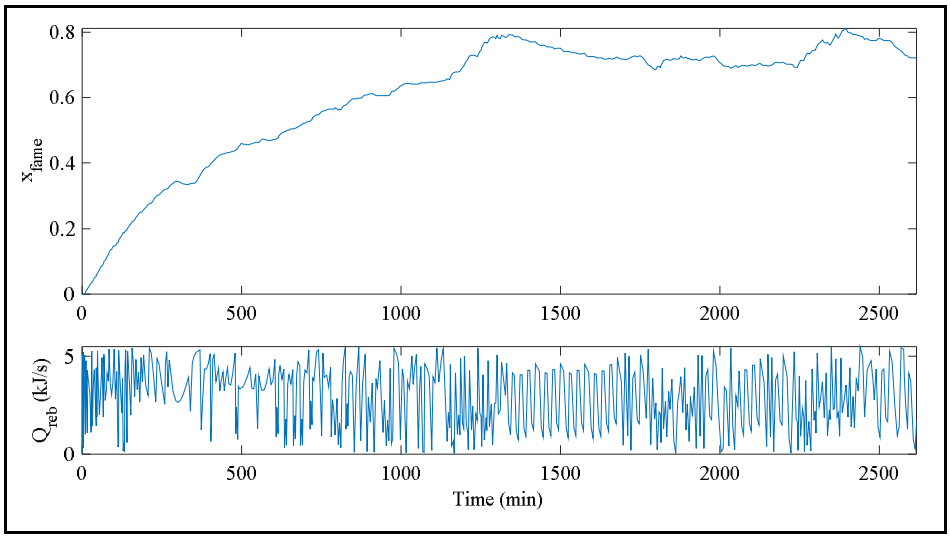

Figure 13. Process response to a repeating sequence input

Another input type whose effect on the system was also investigated in this work was a repeating sequence type, and the response of the system upon its application was as given in Figure 13. According to the figure, the response of the system towards the repeating sequence input seemed to be a kind of a step type, but it was not in a smooth manner. Within the same simulation time used for the all the systems with the different input types, the response of the system with repeating sequence input was observed not to get to any steady state. However, for this repeating sequence input having time values of [0 2] and output values of [0 5.5], the final mole fraction of the methyl oleate given by the system was found to be approximately 0.72, which was observed to compare very well the with the values obtained using the other input types with their corresponding appropriate parameters.

4.0 Conclusion

The good data generated from the prototype plant of the reactive distillation processused for the production of methyl oleate from the esterification reaction between methanol and oleic acid developed with the aid of a process simulator known as Aspen HYSYS showed that it (Aspen HYSYS) can be used to study a system whose experimental setup is not available. Also the results obtained from the simulation of the transfer function model developed with the System Identification Toolbox of MATLAB revealed that the system was a stable one because the application of constant, step and pulse input variable changes could make the response to become steady within the simulation period considered. It has, thus, been demonstrated in this work that, apart from the step input variable that is most commonly used in studying the dynamics of a system, other input types such as constant, ramp, pulse and repeating sequence can also be applied.

Nomenclature

FAME Fatty acid methyl ester
G_p Transfer function model of the process
K_p Static gain of the transfer function model of the process
Q_{reb} Reboiler heat duty (kJ/s)
x_{fame} Bottom fatty acid methyl ester (methyl oleate) mole fraction
T_{dp} Delay time of the transfer function model of the process
T_p Time constant of the transfer function model of the process

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