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Effects of feed ratio on the product quality of SAME reactive distillation process

Abdulwahab Giwa[1] and Saidat Olanipekun Giwa[2]

[1]*Chemical and Petroleum Engineering Department, College of Engineering, Afe Babalola University, KM. 8.5, Afe Babalola Way, Ado-Ekiti, Ekiti State, Nigeria*
[2]*Chemical Engineering Department, Faculty of Engineering and Engineering Technology, Abubakar Tafawa Balewa University, Tafawa Balewa Way, Bauchi, Nigeria*

ABSTRACT

This research work has been carried out to investigate the effects of volumetric feed ratio of stearic acid and methanol on the purity of the stearic acid methyl ester (SAME) obtained from a reactive distillation processaccomplished through an esterification reaction. The investigation was carried out by developing a model of the process with the aid of Aspen Plus using RadFrac column having 32 stages including the condenser and the reboiler. Wilson model was used as the property package of the simulation. The feeds (top – stearic acid and bottom – methanol) were passed into the column at a temperature and a pressure of 25 ^{o}C and 1 atm, respectively. The esterification reaction of the process was modelled as an equilibrium type, the equilibrium constant of which was estimated using Gibbs free energy. In the simulation of the developed Aspen Plus model of the reactive distillation process, the volumetric feed ratio of the column was varied from 3 to 11, and the results obtained showed that the trends of the mole fraction profiles of the components of the process were very similar to one another except those of the feed ratios of 9, 10 and 11 that were a little bit different from the others. Also obtained from the results was that increasing the volumetric feed ratio of the column made the mole fraction of the desired product, which was stearic acid methyl ester and also known as methyl stearate, to decrease. The results obtained have thus revealed that there was an inverseproportional, but not linear, relationship between the volumetric feed ratio of the process and the mole fraction of the desired product. Furthermore, it was discovered from the results that the feed ratio that gave the highest mole fraction of the desired product was 3.

Keywords: Reactive distillation, SAME (stearic acid methyl ester), feed ratio, Aspen Plus, esterification.

INTRODUCTION

Fatty acid methyl ester, otherwise known as biodiesel, is currently receiving attentions both in academics and in industries because it has been discovered that it can serve as an alternative fuel. The need for the source foran alternative fuel occurred owing to the limited availability of conventional petroleum diesel as well as environmental concerns. Biodiesel can be directly used to replace petroleum diesel without any modification because their properties such as specific gravity, cetane number, viscosity, cloud point, and flash point, are similar ([1], [2],[3], [4]). This fuel is a very good promising alternative to conventional petroleum based diesel fuel because it can be derived from a renewable domestic resource (e.g., waste cooking oil), it reduces carbon dioxide emissions by about 78%, and it is nontoxic and biodegradable. All these benefits have made the fuel a very good environmental friendly one ([5], [6],[2],[3],[4]). Another good thing about this fuel is that it can be produced using an integrated process known as reactive distillation.

Reactive distillation is known to be a process that has the capability of combining both separation and chemical reaction in a single unit. It is very attractive whenever conversion is limited by reaction equilibrium ([7],[8],[9],[10],[11],[4]). Also, it is an excellent alternative to conventional flowsheets with different reaction and

separation sections ([12], [13],[4]) as it combines the benefits of equilibrium reaction with distillation to enhance conversion ([14],[15],[4]). Combining reaction and distillation, as found in this reactive distillation process, has several advantages such as (a) shift of chemical equilibrium,(b) increase of reaction conversion, (c) suppression of side reactions and (d) utilization of heat of reaction for mass transfer operations ([16], [4]). Consequently, this process has low external energy consumption and, as such, reduced investment and operating costs ([17], [4]).

Actually, there are some factors that affect the operation of this process such as reflux ratio, feed ratio and reboiler duty. The relationship of between this process and the operating conditions (reflux ratio, feed ratio and reboiler duty) have been investigated to some extent by some researchers. For instance, Karacan and Karacan (2014)[18] applied Aspen HYSYS to simulate and obtain the optimum parameters for some operating conditions of a reactive distillation process used for the production of a fatty acid methyl ester. In the work, canola oil and methanol were used as feedstocks while potassium hydroxide and potassium methoxide were used as catalysts, and the operating conditions optimized were reflux ratio, reboiler duty and condenser pressure. Also, Simasatitkul *et al.* (2011)[1] carried out the simulation of a reactive distillation process for a fatty acid methyl ester production from transesterification reaction of soybean oil and methanol, catalysed by sodium hydroxide. They applied HYSYS to find the optimum values of molar feed ratio of methanol and oil, reflux ratio and reboiler duty. Furthermore, Samakpong *et al.* (2012)[19] simulated and optimized a fatty acid methyl ester production using reactive distillation of rubber seed oil with the aid of Aspen Plus. They studiedthe effects of operating parameters (molar distillate rate and molar reflux ratio) in order to find the optimum conditions required by the process. Giwa *et al.* (2014)[2] investigated the performances of some fatty acids used for the production of fatty acid methyl esters in a reactive distillation column with the aid of Aspen HYSYS. The fatty acids considered were oleic acid, which was discovered, according to Kusmiyati and Sugiharto (2010)[20], to give fatty acid methyl ester that had the quality required to be a diesel substitute, and some other ones (stearic acid, linoleic acid and palmitic acid) found to be present in jatropha oil. Methanol was used as the alcohol for the reaction. Nwambuonwo and Giwa (2015)[21] modelled, simulated and optimized a reactive distillation process used for the production of fatty acid methyl ester (FAME) by considering an esterification reaction between palmitic acid and methanol to give methyl palmitate and water (by-product) with the aid of Aspen HYSYS. They used the optimizer tool of Aspen HYSYS to obtain theoptimum operating conditions of the process using three different algorithms (Box, Mixed and Sequential Quadratic Programming).Santander *et al.* (2010)[22] used response surface methodology and Aspen Plus process simulator to investigate biodiesel production in a reactive distillation using castor oil.They employed the programs to simulate the process for castor oil biodiesel production with the aim of obtaining a deep understanding of the process as well as finding the best conditions forproducing very large amount of fatty acid esters and assess its viability. Giwa and Giwa (2015)[4]studied the effects of reflux ratio and reboiler duty on a reaction integrated distillation process used for the production of stearic acid methyl ester (SAME) that was obtained from the esterification reaction between stearic acid and methanol using Aspen Plus.

Considering the information obtained in the literature, Giwa and Giwa (2015)[4] only studied the effects of reflux ratio and reboiler duty on the operation of a reactive distillation process, but did not consider the effects of feed ratio, particularly how it was affecting the profile(s) of the column. As such, this work has been carried out to investigate the effect of volumetric feed ratio on the performance of a reactive distillation process producing stearic acid methyl ester (methyl stearate) from the esterification reaction between stearic acid and methanol. The performance of the process was taken to be a function of the purity of the products, especially the desired one, obtained from the column.

MATERIALS AND METHODS

The developed Aspen Plus [23] model that was used to represent the reactive distillation process producing stearicacid methyl ester (SAME) studied in this work was as shown in Figure 1. The process was carried out using the esterification reaction between stearic acid and methanol as shown in Equation (1). In the model, the heavy feed, that is, stearic acid, was fed from the top feed stage while the other one, methanol, was introduced into the column through the bottom feed stage of the column. The condenser and the reboiler types were total and kettle respectively while the valid phases in the column was vapour-liquid. Given in Table 1 are the data used to carry out the simulation of the developed Aspen Plus model of the process.

$$C_{18}H_{36}O_2 + CH_3OH \xleftrightarrow{K_{eq}} C_{19}H_{38}O_2 + H_2O \quad (1)$$

Table 1. Simulation parameters of the reactive distillation process for stearic acid methyl ester production

Parameter	Value
Stearic acid feed	
Purity (%)	100
Temperature (^oC)	25
Pressure (atm)	1
Methanol feed	
Purity (%)	100
Temperature (^oC)	25
Pressure (atm)	1
Fluid Package	Wilson
Column	
Total number of stages	32
Stearic acid feed stage	11
Methanol feed stage	20
Top product stage	1
Bottom product stage	32
Reflux ratio	3
Reboiler duty (kW)	0.9
Reaction	
Type	Equilibrium
Segment	11 – 20 and reboiler
Phase	Liquid
K_{eq} source	Gibbs free energy
Basis	Molarity

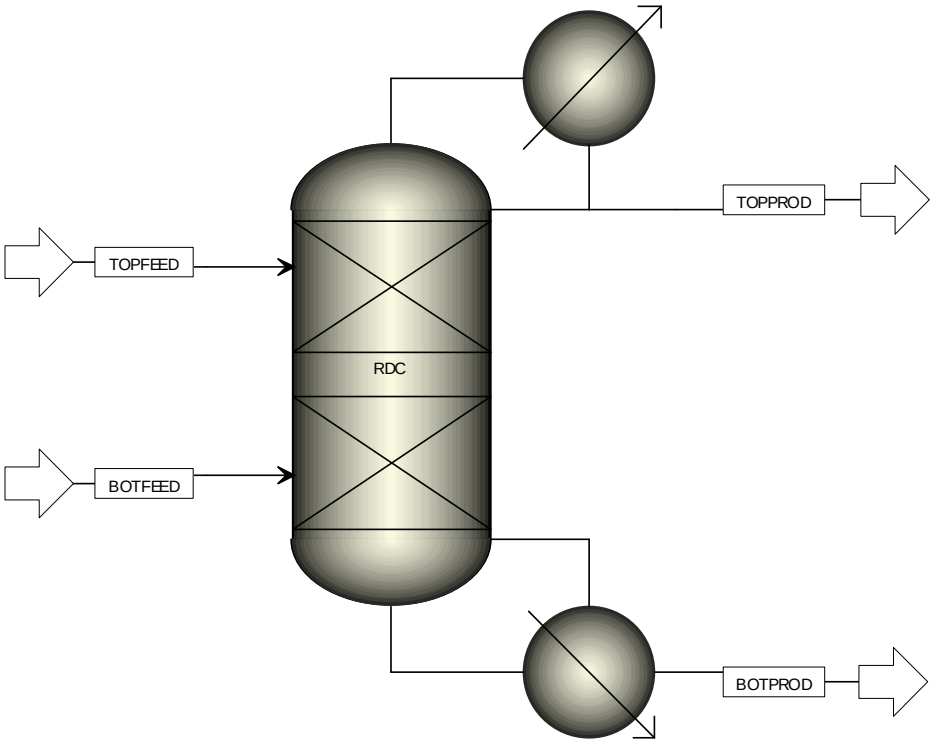

Figure 1. Aspen Plus model of the reactive distillation process producing stearic acid methyl ester

In order to investigate the effects of the proportions of the feed on the performance of the column, which was obtained by considering the mole fraction profiles of the components involved in the process after steady-state simulation, the ratio of the volumetric flow rates of stearic acid and methanol was varied from 3 to 11, and the mole fraction profile of the column for each volumetric feed ratio used was recorded and plotted.

RESULTS AND DISCUSSION

The mole fraction profiles obtained from the simulations of the developed Aspen Plus model of the reactive distillation process used for the production of methyl stearate, with water as a by-product, from the esterification reaction between stearic acid and methanol are given in Figures 2 – 10.

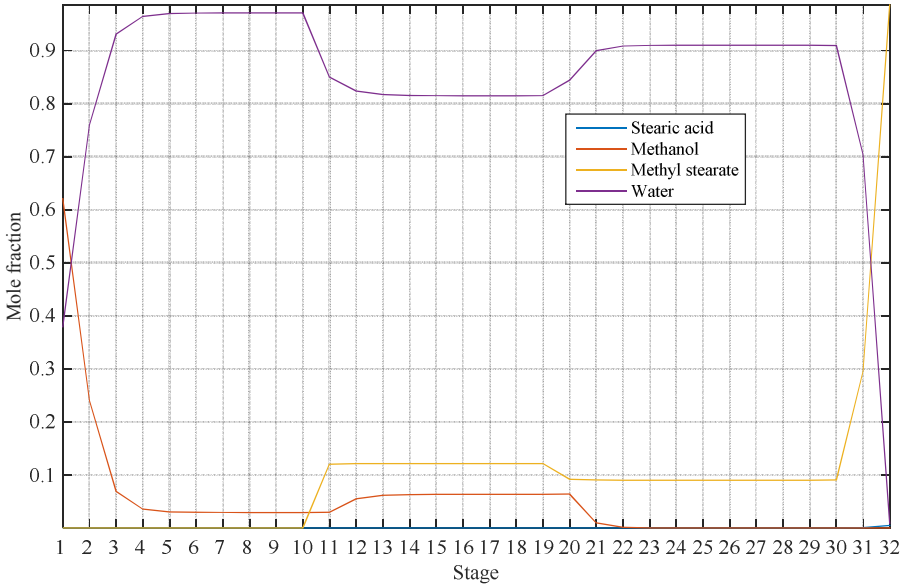

Figure 2. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 3

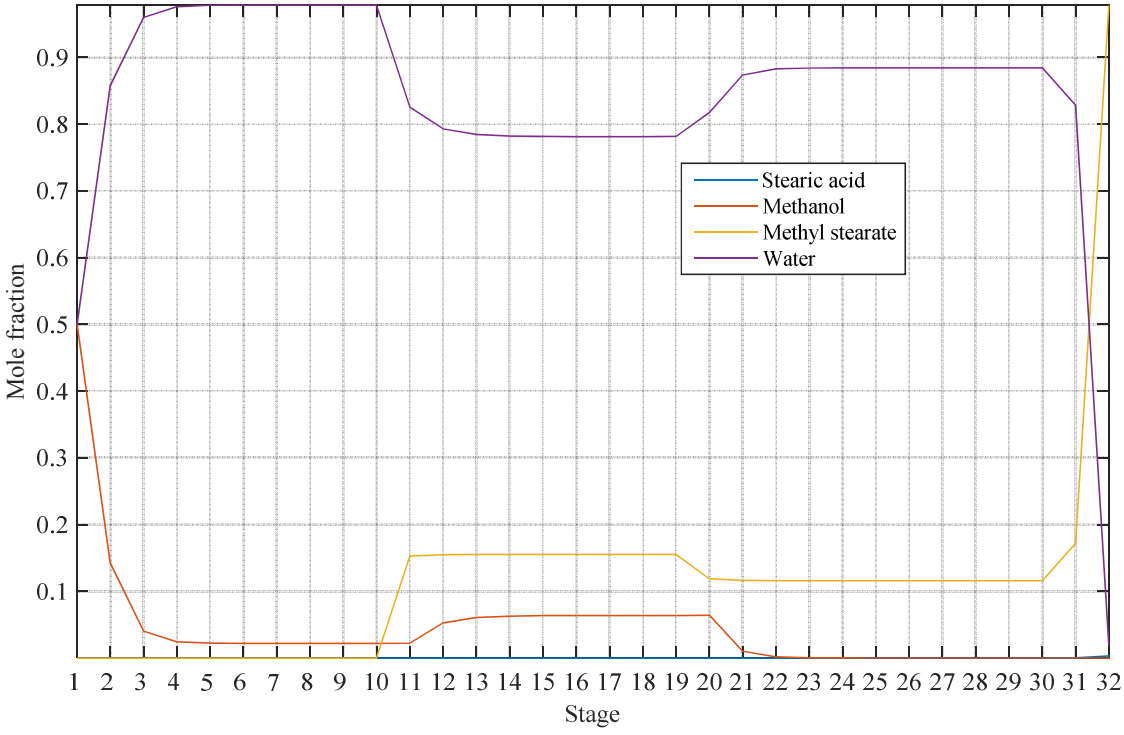

Figure 3. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 4

Given in Figure 2 are the mole fraction profiles of the components in the process when a volumeetric feed ratio of 3 was used to carry out its simulation. According to the figure, very high purity of the desired product of the process, which was methyl stearate, was found to be obtained from the bottom section of the column. Actually, methyl stearate was obtained in high purity at the bottom section of the column because it was one of the heavy components of the process. From the information given by the figure, it was discovered that the mole fraction of the by-product

of the process, water, was higher than that of the desired product in almost all the stages of the column except in the reboiler.

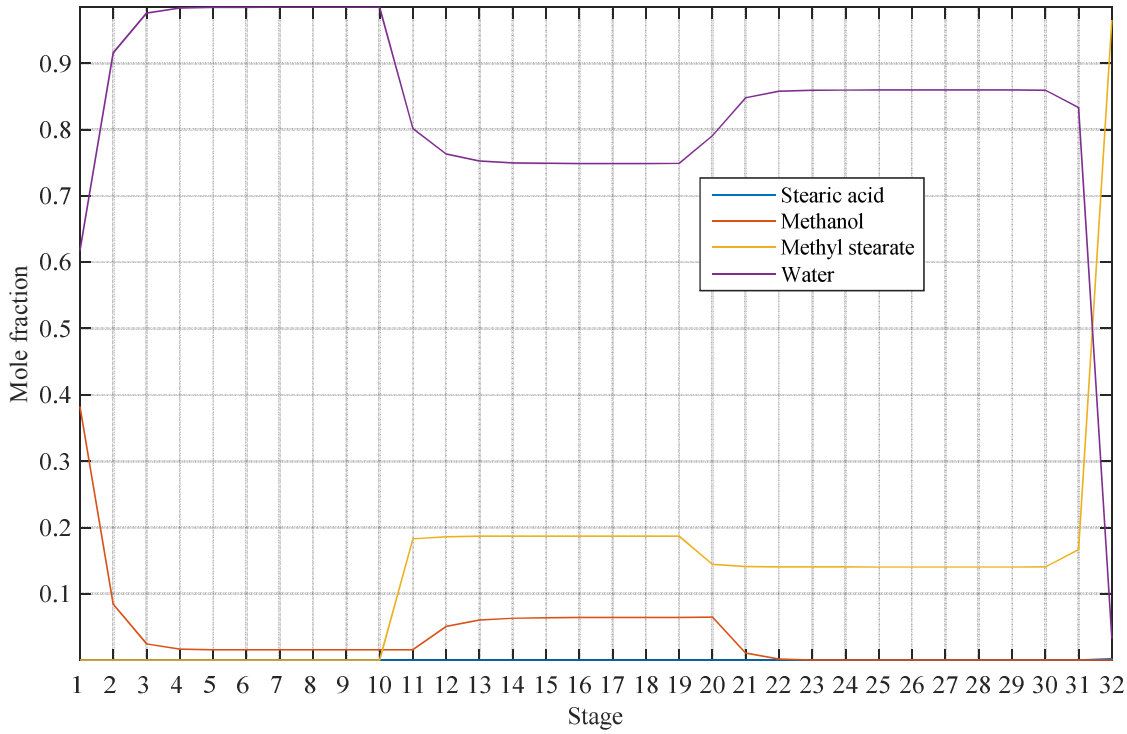

Figure 4. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 5

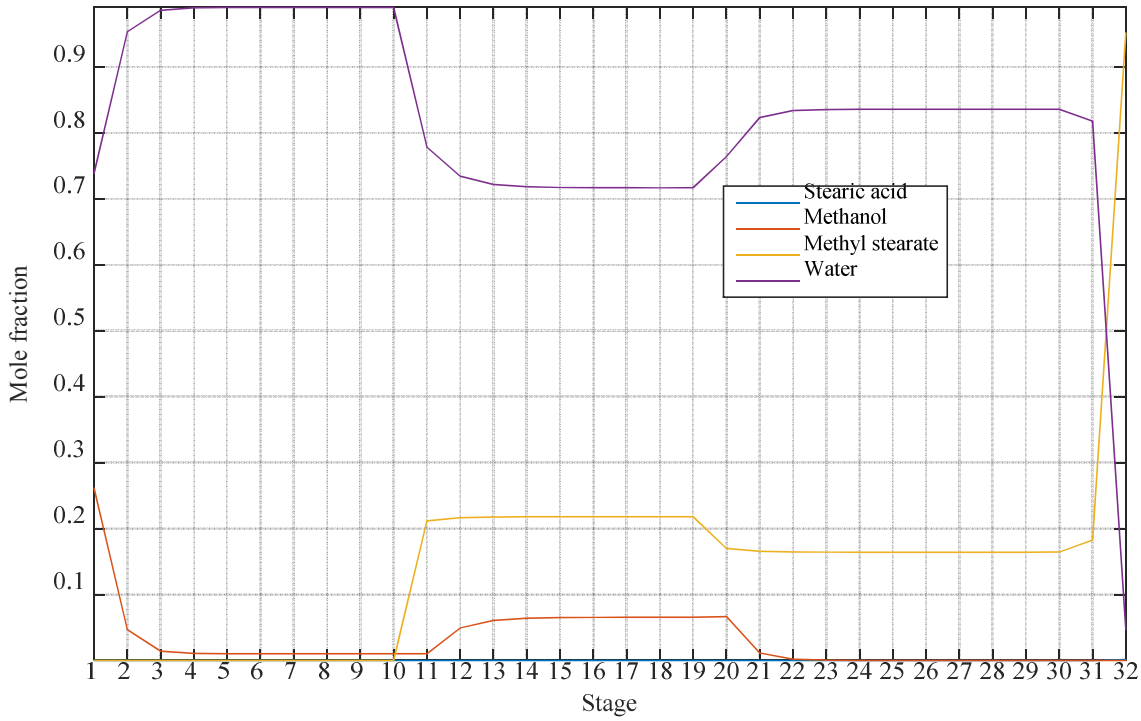

Figure 5. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 6

Regarding the conversion of the reactants of the process, from the results obtained and shown in Figure 2, it was clear that stearic acid was more used up in the process than methanol because its mole fraction found in the column stages after the steady-state simulation was found to be almost zero. In addition, the mole fraction of the two reactants were found to be negligible at the stripping and the bottom (reboiler) section of the column.

In Figure 3, the mole fraction profiles of the components of the process simulated using a feed ratio of 4 are given. The observations made in this case were found to be very similar to those of the simulation carried out using a feed

ratio of 3, as shown in Figure 2. Another thing noticed in this figure (Figure 3) was that the mole fraction of the desired product obtained in this case was less than that of the feed ratio of 3.

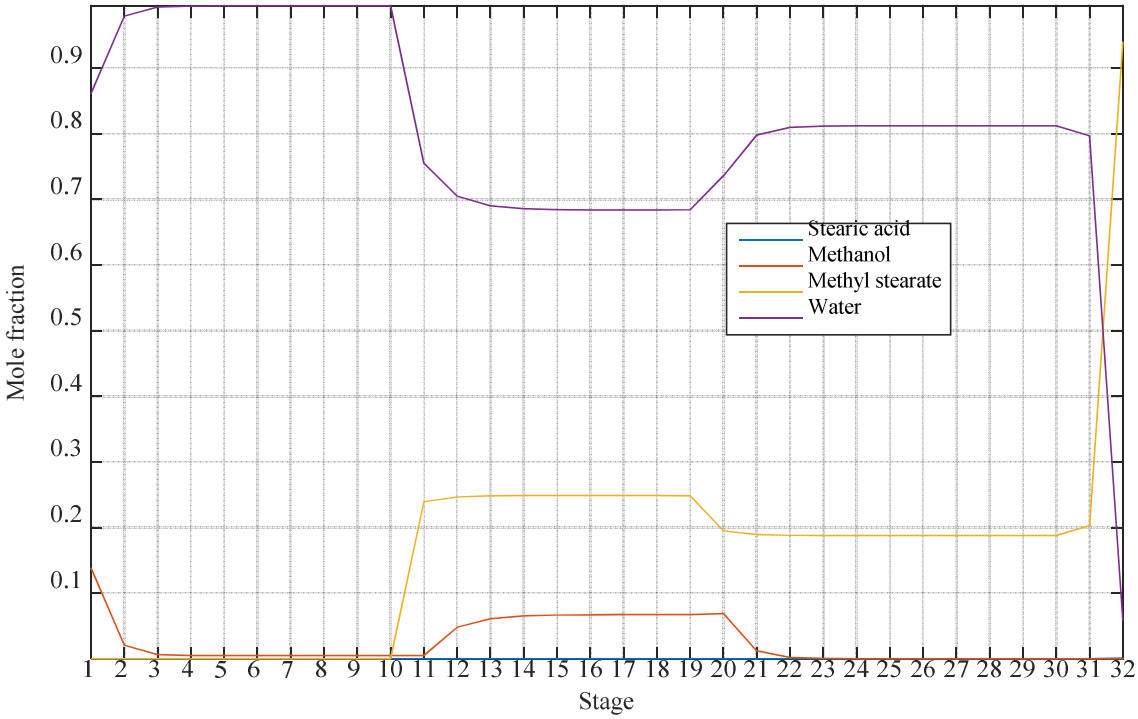

Figure 6. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 7

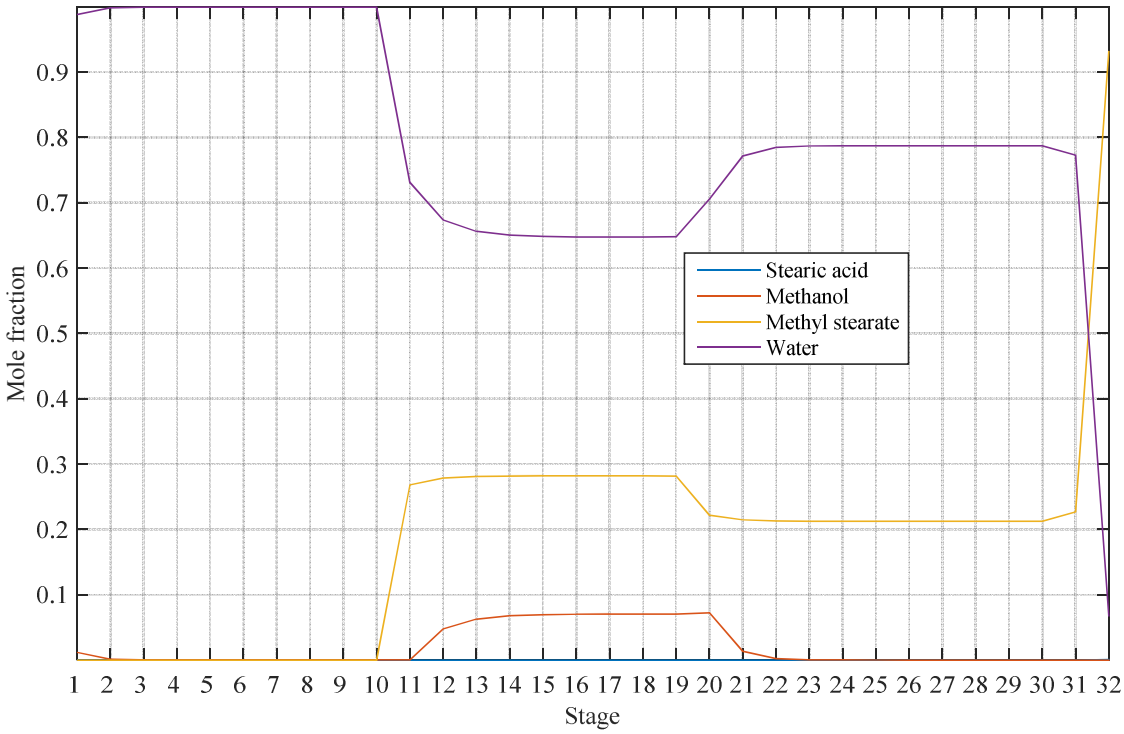

Figure 7. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 8

The mole fraction profiles obtained for the components when the simulation of the Aspen Plus model of the reactive distillation process was carried out using a feed ratio of 5 were as shown in Figure 4. The information obtained from the trend of the profiles given in the figure was found not to be too different from those of Figures 2 and 3.

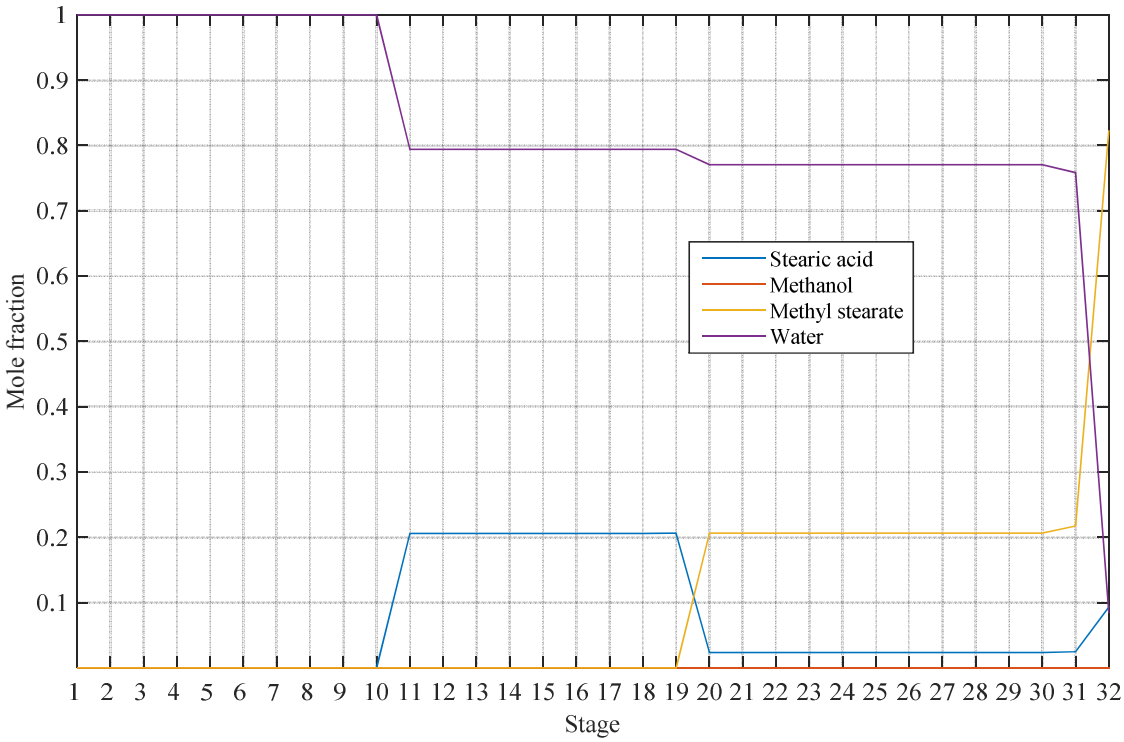

Figure 8. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 9

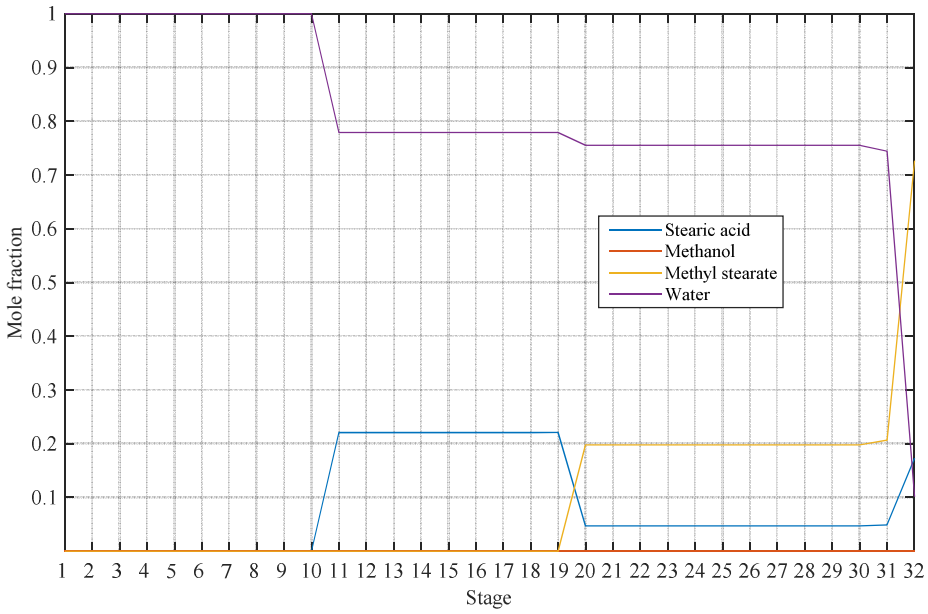

Figure 9. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 10

When the simulation of the developed reactive distillation process was carried with feed ratios of 6, 7 and 8, the mole fraction profiles obtained were as given in Figures 5, 6 and 7, respectively. The trend of the profiles given in the figures were found to be similar to those obtained earlier in Figures 2, 3 and 4. However, it was discovered from the figures that as the feed ratio was increased, the mole fraction of water given by the process through the top section of the column was increasing and the mole fraction of the methyl stearate obtained from the bottom section of the column was decreasing.

Based on the results given as the mole fraction profiles of the process components in Figure 8, when a feed ratio of 9 was used to simulate the developed Aspen Plus model, water of 100% purity was obtained from the top section of the column while the mole fraction of the desired product, stearic acid methyl ester (methyl stearate), was found to decrease a little bit further.

The trends of the mole fraction profiles obtained from the simulation of the process using a feed ratio of 10, shown in Figure 9, were found to be similar to those obtained when the simulation was carried out with a feed ratio of 9. Also noticed from the results given in Figure 9, obtained using a feed ratio of 10, was that the mole fraction of methyl stearate decreased further from that obtained with a feed ratio of 9.

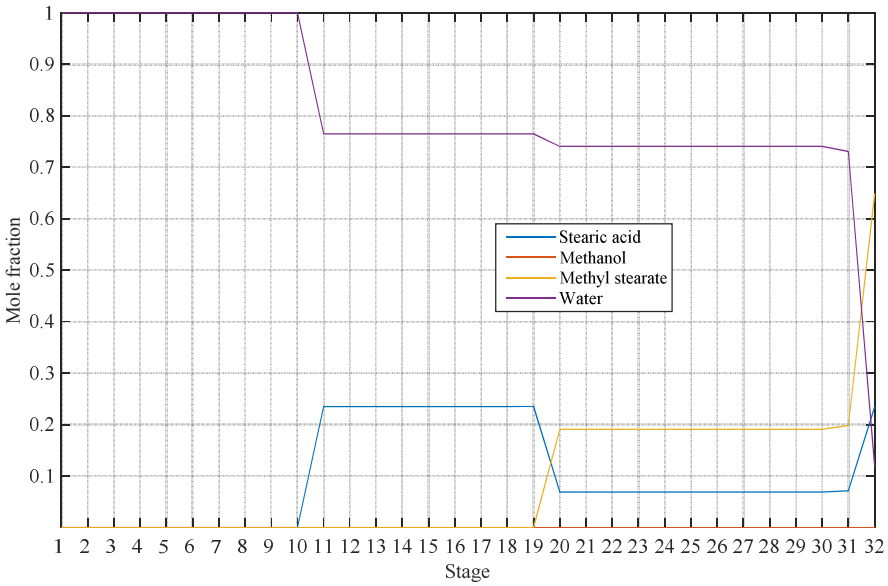

Figure 10. Mole fraction profiles of the reactive distillation process obtained using a feed ratio of 11

The simulation of the reactive distillation process was also carried out using a volumetric feed ratio of 11, and the profiles obtained from this simulation were as given in Figure 10. It was observed from the results shown in Figure 10 that the mole fraction profiles of the components in this case were similar to those obtained when the process was simulated using reflux ratios of 9 and 10, and the results of which are shown in Figures 8 and 9.

Table 2. Variation of the mole fraction of methyl stearate with volumetric feed ratio

Volumetric feed ratio	Methyl stearate mole fraction
3	0.9862
4	0.9763
5	0.9640
6	0.9511
7	0.9394
8	0.9313
9	0.8221
10	0.7256
11	0.6476

Given in Table 2 is the summary of the how the mole fraction of the desired product of the process was varying with the change in the volumetric feed ratio.From the table, it was found that that the relationship between the volumetric feed ratio of the process and the mole fraction of methyl stearate, which was the desired product obtained from the process,was inversely proportional, though not linear. For instance, as the volumetric feed ratio was varied from 3 to 11, the mole fraction of the desired product obtained from the bottom section of the column was found to decrease from 0.9862 to 0.6476.

CONCLUSION

From the results obtained when the Aspen Plus model of the reactive distillation process developed was simulated by varying the volumetric feed ratio from 3 to 11, it was found that the trends of the mole fractions of the components of the process were very similar except those of feed ratios of 9, 10 and 11 that were a little bit different from the others. Also, it was obtained from the results that as the feed ratio was increasing, the mole fraction of the desired product, methyl stearate, was decreasing. This revealed that the volumetric feed ratio of the process was inversely proportional, though not linear, to the mole fraction of the desired product.

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NOMENCLATURE

BOTFEED	Bottom feed of the column
BOTPROD	Bottom product of the column
K_{eq}	Equilibrium constant
RDC	Reactive distillation column
SAME	Stearic acid methyl ester
TOPFEED	Top feed of the column
TOPPROD	Top product of the column

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