



# ECONOMIC ANALYSIS OF ANETHANOL-TO-HYDROCARBON PROCESSSET-UP THROUGH MODELLING AND SIMULATION USING ASPEN PLUS

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## ABSTRACT

This research work has been carried out to develop and simulate the reactive distillation and conventional models for production of hydrocarbon ether (diethyl ether) from ethanol for the purpose of economic analyses. The development of the models for the two process methods were achieved with the aid of Aspen Plus using RadFrac as the column for the reactive distillation process and an equilibrium reactor in addition to RadFrac for the conventional process method. The column used in both cases had 21 stages including a total condenser and a kettle reboiler, and the feed entered the column at the 11th stage of the column. For the two processes, Non-Random Two-Liquid activity coefficient model was used as the Property Method. From the results obtained, it was discovered that the performance of reactive distillation process was better than that of the conventional method of diethyl ether production from ethanol. This was because the mole fraction of liquid product given by the reactive distillation process was higher than the one obtained from the conventional method of production when the two of them were operated at approximately the same conditions. Furthermore, the observations made from the economic analyses of the two approaches of the production indicated that reactive distillation was a cheaper process to set up and operate because its total capital cost, operating cost, utilities cost, equipment cost and equipment installation cost were estimated to be less than those of the conventional method of the ethanol-to-diethyl ether process.

**Keywords:** ethanol, diethyl ether, modelling, simulation, economic analysis, aspen plus.

## 1. INTRODUCTION

The main chemical compounds in industry, which are hydrocarbons, are currently synthesized from petroleum resources. However, there are limited petroleum resources. Besides, the fact is that the combustion of these resources gives a greenhouse gas, which is carbon dioxide. As such, much attention has been paid to biomass as an alternative resource to petroleum because biomass is renewable, and its combustion does not lead to increased carbon dioxide in the atmosphere. One of these biomass-derived resources is ethanol [1]. This ethanol can be processed to give hydrocarbons.

The conversion of ethanol to hydrocarbons has received wide attention these days due to the global energy crisis and the heavy demand for hydrocarbons. The ethanol that is used as the raw material holds good promise as it can be obtained from fermentation of biomass, a renewable agricultural resource. Some countries that have large sugarcane cultivation can produce ethanol easily from fermentation of molasses, which is a by-product of the sugar industry [2].

Many researches have been carried out on this subject matter, but most of them were experimental. Studies on this topic involving modelling and simulation are very scarce, especially those involving reactive distillation that is being applied in this work.

Basically, reactive distillation is a process that combines chemical reaction and multi component separation inside a single piece of equipment [3-7]. It has been a focus of research in chemical process industries and academia in the last few years [8], and it is a very good alternative to conventional flow sheets with separate

equipment for reaction and separation [9]. This process has been used in a small number of industrial applications for many years, but an increase has been shown in both its research and applications in the last decade [10]. In order to apply reactive distillation, the volatilities of the reactant and the product must be in such a way that the products can be easily removed and reactants retained inside the column to undergo further reaction. Apart from that, the temperature levels for both reaction and vapour-liquid-equilibrium of the process must overlap [11-20]. By carrying out chemical reaction and separation in one process step, just as it is obtainable in reactive distillation process, operating and investment costs can be greatly minimized [20-22]. Other benefits of this novel process include [23-27]: (i) increased yield, due to overcoming chemical and thermodynamic equilibrium limitations, (ii) improved selectivity via suppression of side reactions, (iii) reduced energy consumption, owing to effective utilization of reaction heat, especially in the case of exothermic reactions, (iv) avoidance of hot spots by simultaneous liquid evaporation, and (v) ability to separate close boiling components. As a result of these advantages, in addition to growing understanding of the process, the chemical process industries have developed an increasing number of processes based on this reactive distillation.

This work has been carried out to investigate the economic advantage of reactive distillation over the conventional method of producing a hydrocarbon from ethanol through developing the model of the process and simulating it with the aid of Aspen Plus. The hydrocarbon produced in this work as a case study was a hydrocarbon ether named as diethyl ether.



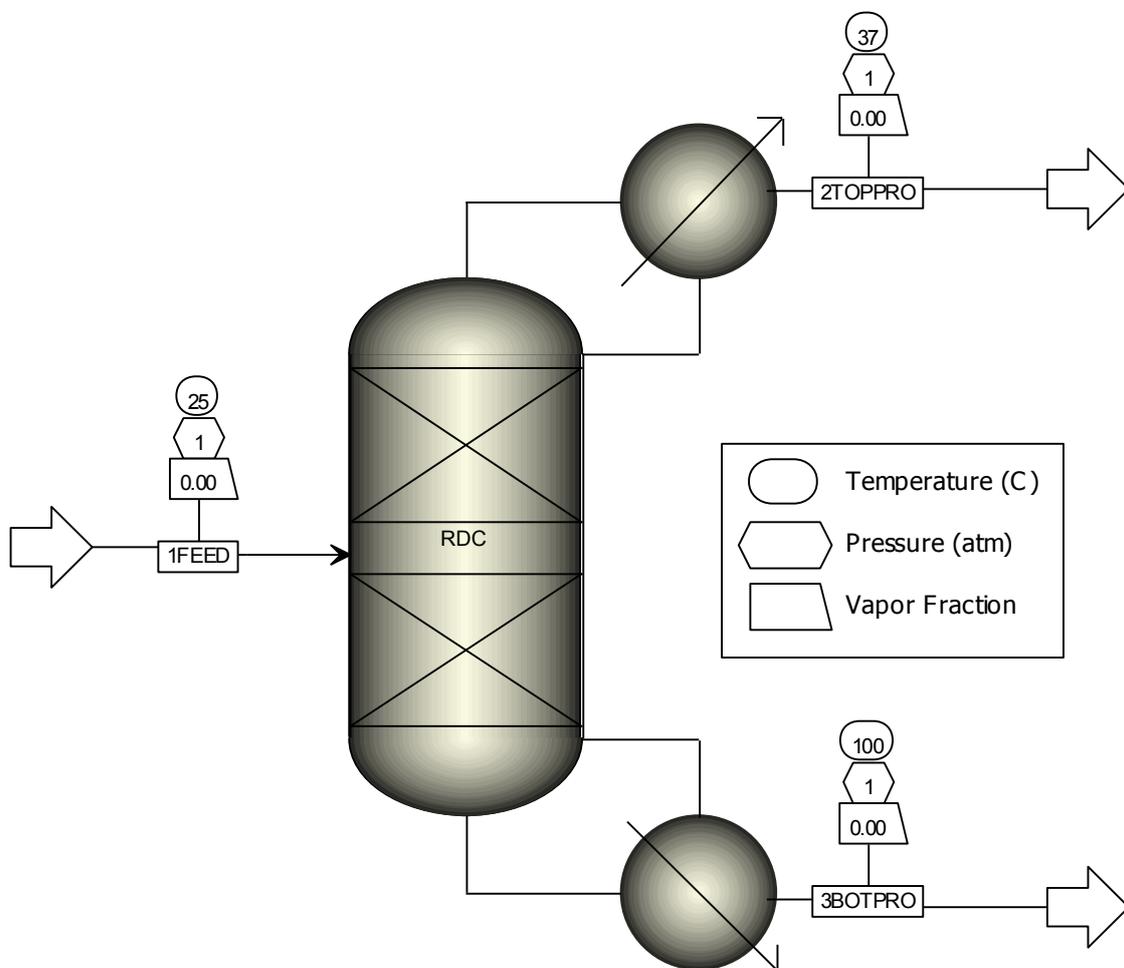
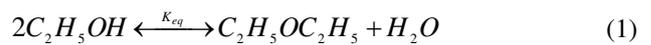
## 2. METHODOLOGY

In order to achieve the goal of this work, Aspen Plus process simulator V8.8 [28] was employed. In applying the process simulator, the components involved in the process, which were ethanol, diethyl ether and water, were first selected by finding them in the Specifications Section of the Components under Properties. All the components selected were Conventional Types.

Thereafter, Non-Random Two-Liquid (NRTL) activity model was chosen as the Property Method from the Specifications Section of the Methods under Properties also. The parameters required by the NRTL were generated automatically by the process simulator after the property method had been selected.

Upon the selections of the components and the property method of the process simulation, the Simulation Environment of the process simulator was entered and the Aspen Plus model of the process was developed by picking RadFrac column from the Columns Section of the

Model Palette. After that, the input and output Material Streams were added appropriately before specifying the operations conditions. The column was specified to have 21 stages including the condenser, which is Total in type, and the reboiler, which is a Kettle type. The valid phase of the process was set to be Vapour-Liquid, and its Convergence was chosen to be Standard. Furthermore, the pressure of the condenser was fixed to be 1 atm with negligible pressure drop throughout the column. After developing the reactive distillation process model (Figure 1), the column was divided into five sections, viz. the condenser, the rectifying, the reaction, the stripping and the reboiler sections. The reaction section was made to be between the 7th and the 14th stage of the column. The reaction occurring in the reaction section was an equilibrium type, which is given in Equation (1).



**Figure-1.** Aspen plus reactive distillation model of the ethanol-to-hydrocarbon process.

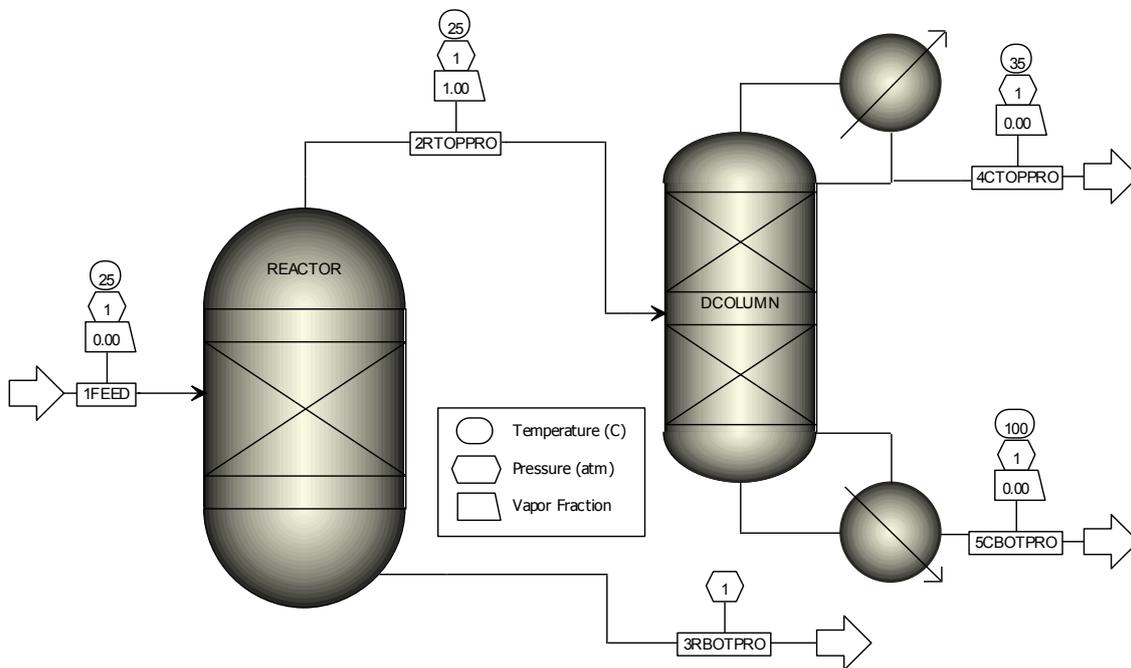
The feed, which was ethanol, was passed into the reactive distillation column at room temperature and

atmospheric pressure on the 11<sup>th</sup> stage at the rate of 50 mL/min.



On the completion of the model development of the process shown in Figure 1, it was run by clicking the Run Button of the process simulator and the results were thereafter given after convergence.

After simulating the reactive distillation process of the diethyl ether production, the conventional method of the production was also modelled and simulated. Given in Figure-2 is the developed Aspen Plus model of the conventional method of the production.



**Figure-2.** Aspen Plus conventional model of the ethanol-to-hydrocarbon process.

The flowrate of the feed entering the reactor was the same as the one fed into the reactive distillation column. The reactor temperature was 25 °C, and the reaction (Equation 1) was set to occur in vapour phase. Also, the parameters used in the simulation of the distillation of the conventional method were the same as those of the reactive distillation column except that no reaction was occurring in the distillation column of the conventional method.

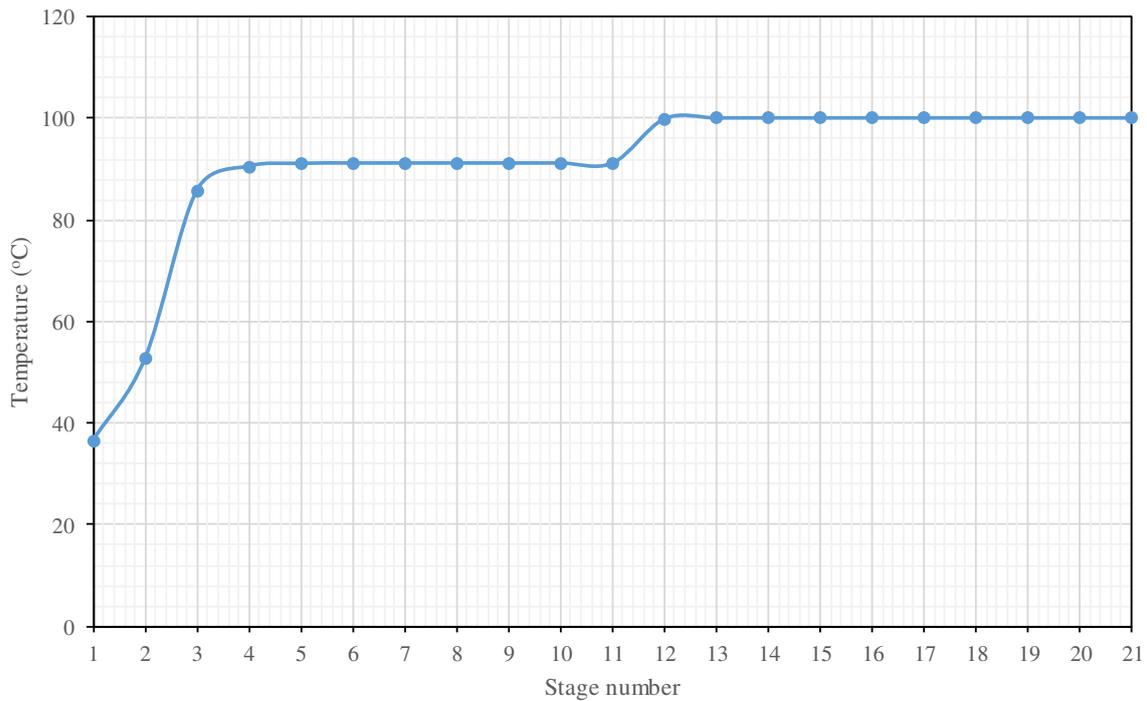
Finally, in order to achieve the aim of this work, the economic analyses of the two processes were carried out with the aid of Aspen Process Economic Analyser (APEA), which is also present within the Aspen Plus.

### 3. RESULTS AND DISCUSSIONS

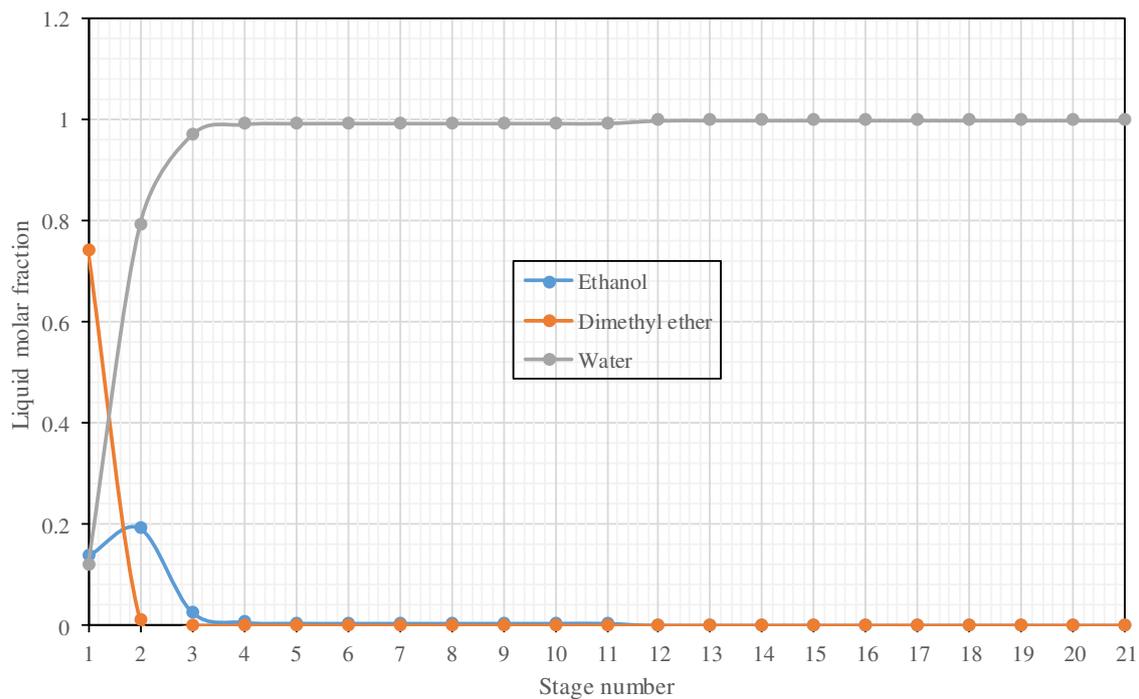
The temperature profile of the reactive distillation process used for the production of diethyl ether, which is a hydrocarbon ether, from ethanol is given in Figure-3. The figure showed that the lowest temperature of the process occurred at the condenser section while the highest temperature was found to be in the reboiler section of the

column. This observation was found to be in agreement with the principle of distillation in which low- and high-boiling components are expected to be collected at the condenser and the reboiler sections respectively. It was also observed from the profile shown in Figure 3 that the temperature of the column was found to decrease down the column with the temperature of the stripping section towards the reboiler found to be approximately constant.

Shown in Figure-4 are the molar fraction profiles of the components present in the liquid flowing in the column. As can be seen from the figure, the mole fraction (0.7411) of the desired product, which was diethyl ether, was the highest in the condenser section of the column while the by-product was the one that dominated the reboiler section with a mole fraction of approximately 1. The mole fraction of ethanol through the column was found to be very low. In fact, it was approximately zero as from stage 4 of the column downwards towards the reboiler. This was an indication that very high conversion of the feed was achieved in the reaction section of the column.



**Figure-3.** Temperature profile of the ethanol-to-diethyl ether reactive distillation process.



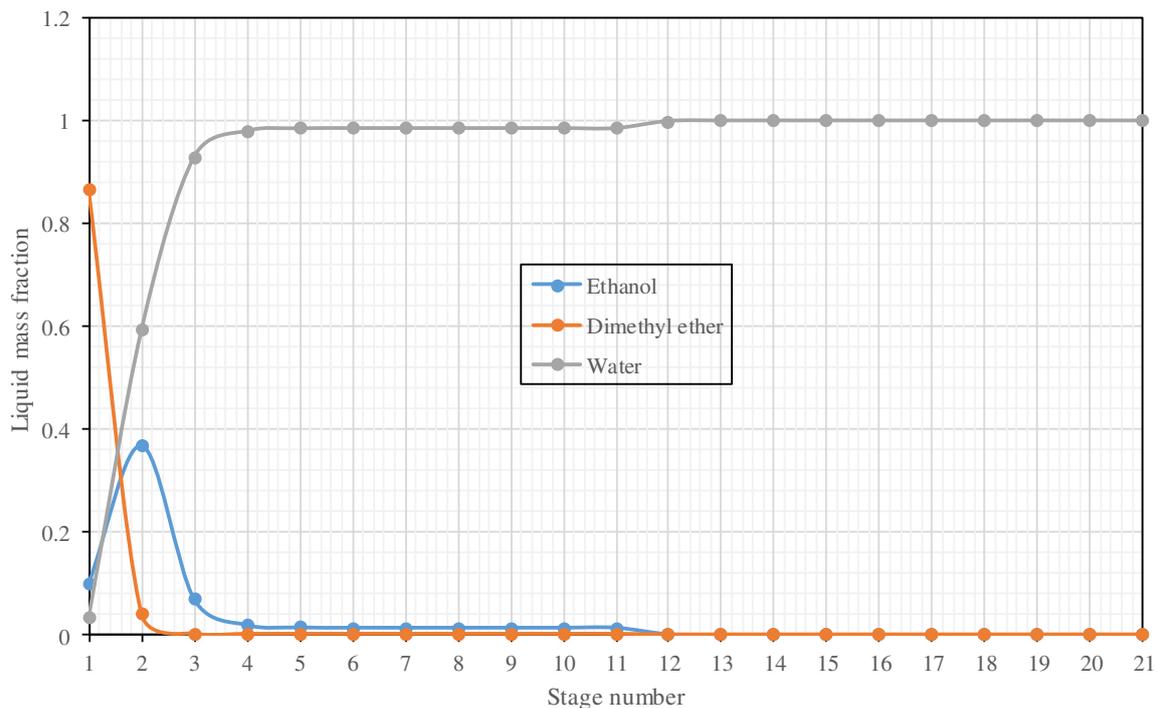
**Figure-4.** Liquid molar fraction profiles of the ethanol-to-diethyl ether reactive distillation process.

Also considered in this work was the mass fraction profile of the liquid present in the column at steady state for the production of diethyl ether from ethanol, and the results of this consideration are given in Figure-5. From the profile given in Figure-5, it was discovered that the diethyl ether had a mass fraction of approximately 0.8656 at the condenser section of the

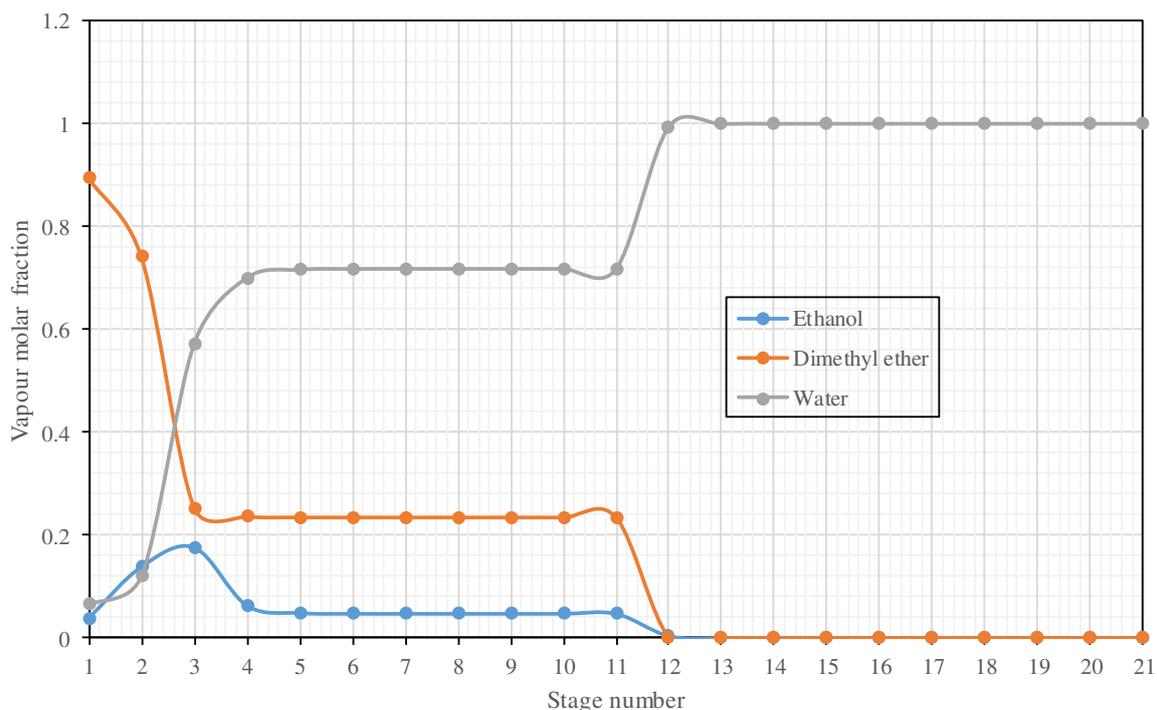
column, and that was the highest in that section of the column. Furthermore, the mass fraction of water was found to be very low in that (condenser) section, although it (water) had a mass fraction that was approximately unity (1) at the reboiler section. Also, the mass fraction of the reactant (ethanol) was found to be low both in the condenser and the reboiler section. The results given by



this mass fraction profiles were observed to be similar, though with different steady-state values, to that of the mole fraction profiles (see Figure-4) of the components.



**Figure-5.** Liquid mass fraction profiles of the ethanol-to-diethyl ether reactive distillation process.



**Figure-6.** Vapour molar fraction profiles of the ethanol-to-diethyl ether reactive distillation process.

Given in Figure-6 are the component molar fraction profiles for the vapour present in the column. The natures of the profiles obtained, in this case of the vapour, were found to be different from those of the liquid components. For instance, liquid molar fraction of both

diethyl ether and ethanol in the middle of the rectifying section was observed to be zero (Figure-4) whereas for the vapour mole fraction profiles, their values were not zero. However, the component with the highest vapour mole fraction in the condenser was still diethyl ether while, in



the reboiler section of the column, water, which is referred to as steam in this case, still had the highest vapour mole fraction.

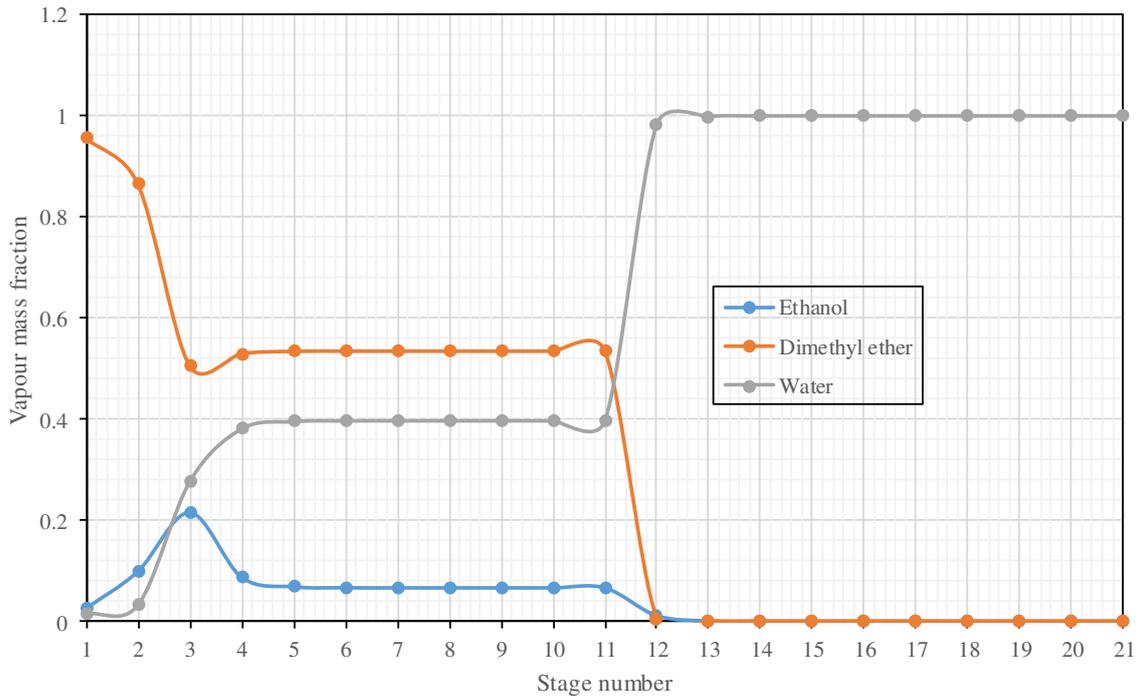


Figure-7. Vapour mass fraction profiles of the ethanol-to-diethyl ether reactive distillation process.

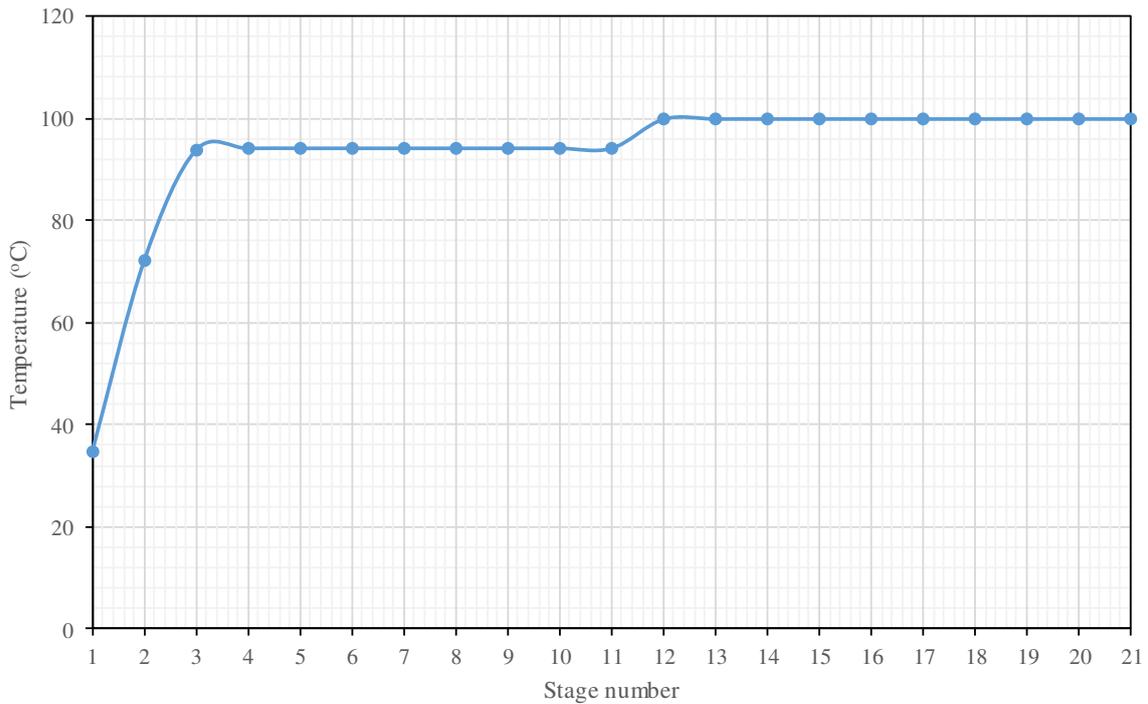


Figure-8. Temperature profile of the ethanol-to-diethyl ether conventional process.

The vapour mass fraction profiles were also obtained and were as given in Figure-7 for components involved in the process for the production of diethyl ether from ethanol, with water as the by-product. The trends of

the vapour mass fraction profiles were, actually, found to be similar to those of the vapour molar fractions, but their steady-state values were different. For instance, the steady-state of vapour mass fraction for diethyl ether



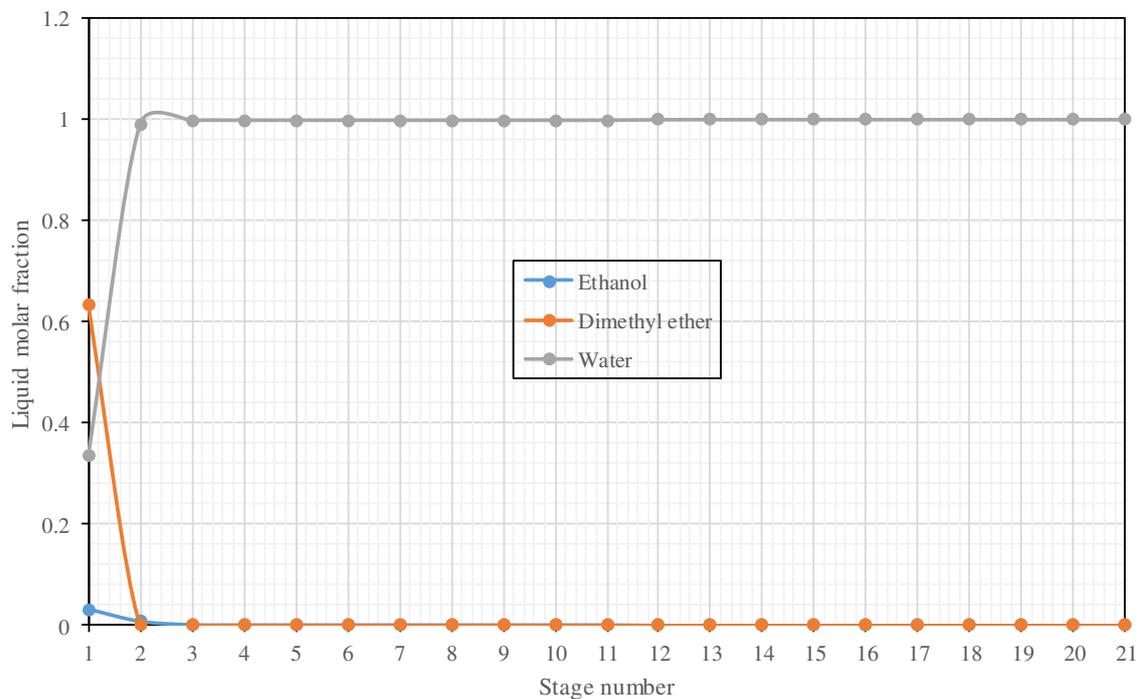
present at the condenser section of the column was approximately 0.9570 while that of its molar fraction was about 0.8952. Similar variations were observed to occur in the compositions of the other two components involved in the process.

After simulating the reactive distillation process of diethyl ether production using ethanol as the feedstock, the conventional method of production of the material was also simulated, and the results obtained showed that a diethyl ether output having a mole fraction of 0.4881 could be obtained as the top product of the reactor when the equilibrium constant was 419.78 at the reaction temperature of 25 °C.

In order to increase the purity of the product obtained, it was passed into a distillation column, and the temperature profile of the conventional distillation process of diethyl ether production is given in Figure 8. From the figure, it was discovered that the trend of the temperature

profile in this case was like that of the reactive distillation given (cf. Figure-3). Also, it was discovered in this conventional system that the lowest and the highest temperatures of the distillation operation occurred at the top and the bottom sections of the column respectively. Of course, this observation was in line with the principles of distillation operation.

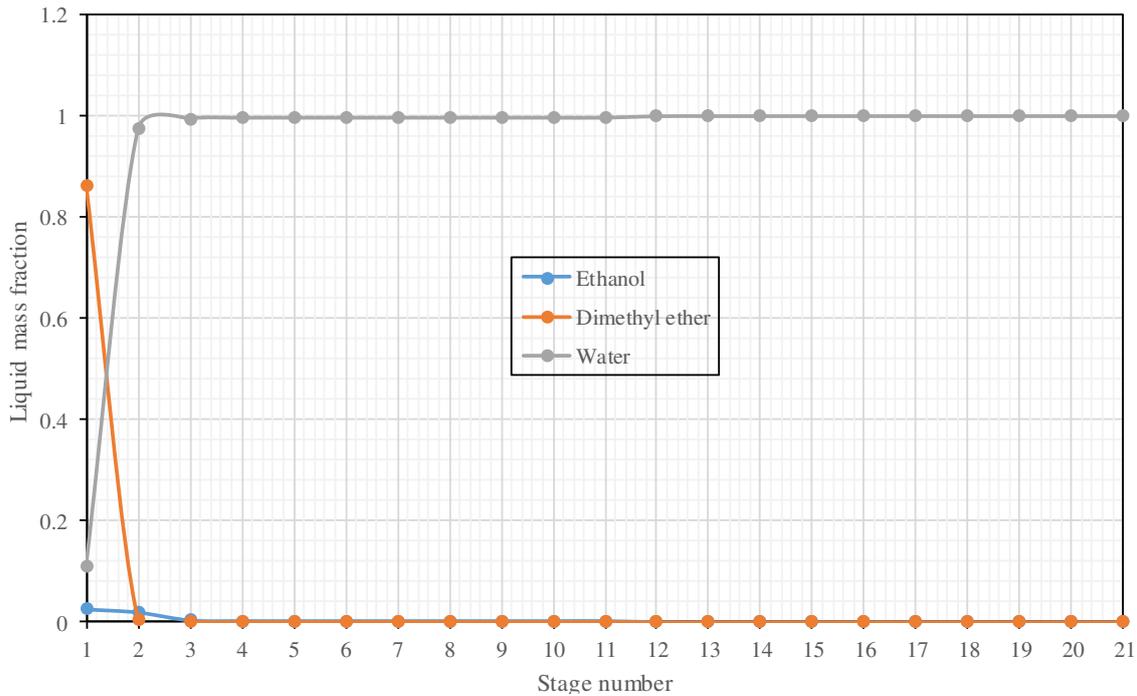
Figure-9 gives the molar fraction profiles of the liquid involved in the conventional distillation operation of this hydrocarbon production process. As can be seen from the figure, diethyl ether had the highest mole fraction in the condenser section of the column followed by water while ethanol had the least mole fraction in that section. At the bottom section of the column, the dominant component was found to be water, with a mole fraction of approximately 1, while the remaining two components were very negligible there.



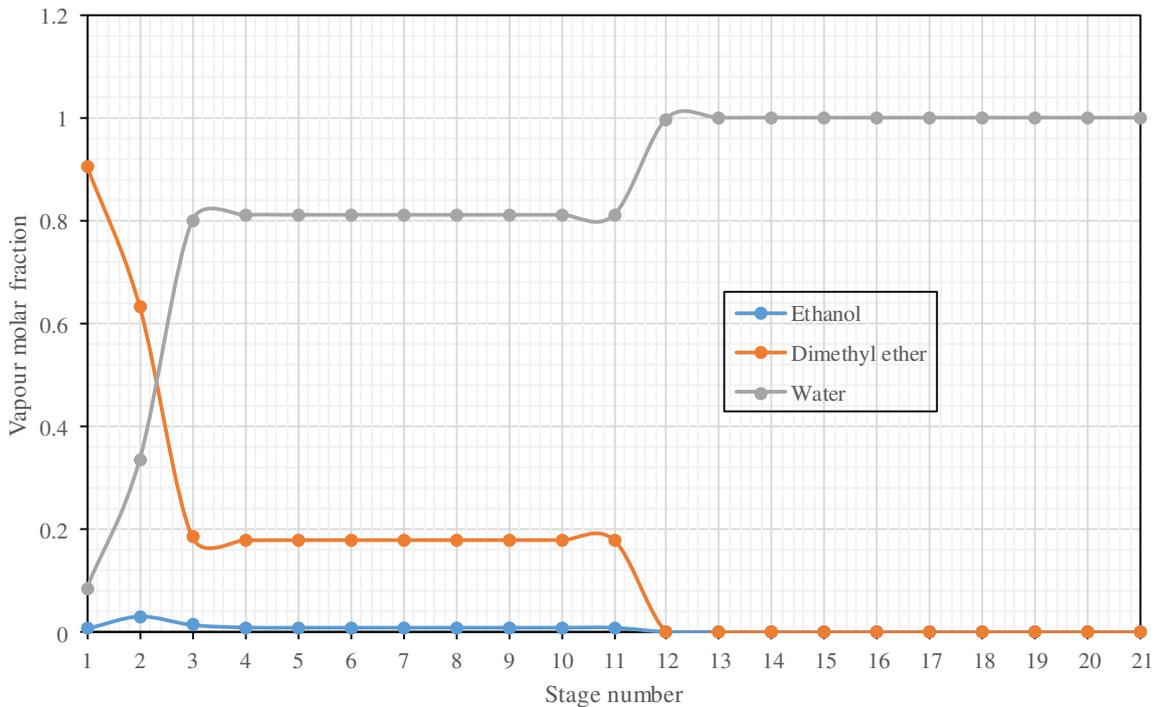
**Figure-9.** Liquid molar fraction profiles of the ethanol-to-diethyl ether conventional process.

The liquid mass fraction profiles of the components involved in this process being considered were as given in Figure-10. Based on the information given by this figure, in terms of mass, the component with the highest fraction at the condenser section of the column

was still found to be diethyl ether, which was the desired product of the process. The nature of the mass fraction (Figure-10) of the components at the reboiler section of the column were the same as those of their mole fraction values (Figure-9).



**Figure-10.** Liquid mass fraction profiles of the ethanol-to-diethyl ether conventional process.



**Figure-11.** Vapour molar fraction profiles of the ethanol-to-diethyl ether conventional process.

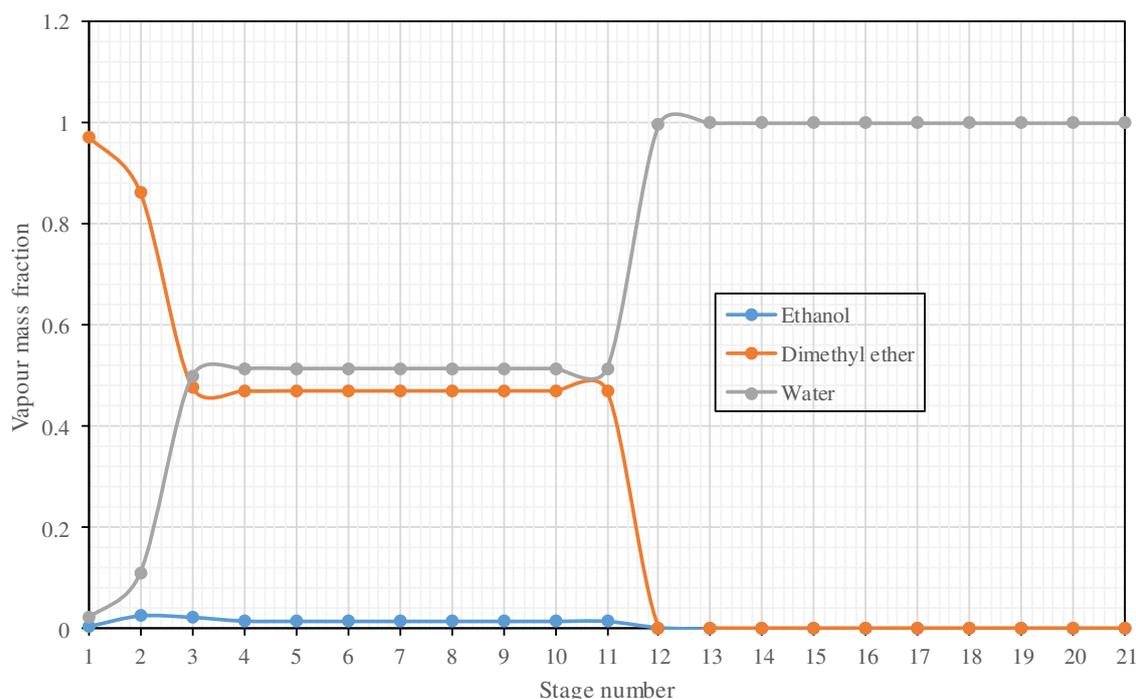
Considering the vapour molar fraction profiles of the components involved in the conventional distillation operation of this process, which are given in Figure-11, it was discovered that diethyl ether still had the highest value. However, the trends of the vapour mole fraction profiles were found to be different from those of the liquid mole fraction profiles of this particular process. For

instance, in the liquid molar fraction profiles, the mole fraction of diethyl ether in some parts of the rectifying section was zero, whereas in this case, diethyl ether has been seen not to have a vapour mole fraction of zero in the rectifying section. The mole fraction of ethanol for both the liquid and the vapour phases were observed to be approximately zero in most part of the rectifying section



and in the stripping section. This was found to be an indication that the ethanol passed into the reactor was well

consumed in the reactor and, as such, negligible amount of ethanol was entering the column.



**Figure-12.** Vapour mass fraction profiles of the ethanol-to-diethyl ether conventional process.

The profiles of the vapour mass fraction of these process components were also plotted and given as in Figure-12. It was observed from the figure that, as usual, diethyl ether and ethanol has the highest and the lowest values respectively. In fact, the mass fraction of diethyl ether in the condenser section of the column was very close to unity (1). Moreover, water still dominated the reboiler section with diethyl ether and ethanol very negligible there. Also noticed was that the mass fraction of diethyl ether in the rectifying section was somehow high (above 0.4).

Comparing the final products obtained from the two methods of diethyl ether production, it was discovered that reactive distillation was better because it could give higher molar fraction of the desired product (diethyl ether) in liquid form. For instance, the liquid mole fractions obtained from the reactive distillation process and the conventional process were obtained to be 0.7411 and 0.6348, respectively.

Furthermore, the economic analyses of the two processes for handling 50 mL/min of ethanol were considered using Aspen Process Economic Analyser (APEA), and the results obtained were as given in Table-1.

**Table-1.** Results of the economic analyses of the processes.

Name	Amount			
	Reactive distillation process		Conventional process	
	USD	Naira	USD	Naira
Capital Cost	353,885.00	126,160,002.50	406,886.25	145,054,948.13
Operating Cost / Year	121,061.88	43,158,558.44	163,061.25	58,131,335.63
Utilities Cost / Year	4,491.64	1,601,268.77	4,556.18	1,624,276.39
Equipment Cost	13,362.50	4,763,731.25	16,012.50	5,708,456.25
Installation Cost	46,012.50	16,403,456.25	64,762.50	23,087,831.25
Total	538,833.51	192,087,037.21	655,298.68	233,606,867.64

According to the results given in Table-1, it can be seen that the reactive distillation process is better than the conventional method for the conversion of ethanol to

diethyl ether, even, economic wise because the capital cost, the operating cost, the utilities cost, the cost of equipment and the cost for installing the equipment



required by the reactive distillation process were found to be lower than those of the conventional production method. Hence, the total amount of money required for the running of the reactive distillation process per year was found to be less than that required by the conventional method of diethyl ether production from ethanol.

#### 4. CONCLUSIONS

The results obtained from the simulation of the ethanol-to-diethyl ether processes carried out in this work has revealed that reactive distillation process was better than the conventional method for the production of diethyl ether because higher mole fraction of liquid product was achieved from the reactive distillation at approximately the same operating conditions. Furthermore, it was observed from the economic analyses of the two approaches of the production that reactive distillation would be cheaper to set up and operate than the conventional method because the total capital cost, the operating cost, the utilities cost, the equipment cost and the installation cost of the reactive distillation process were found to be less than those of the conventional method of the process.

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#### NOMENCLATURE

APEA	Aspen Process Economic Analyser
BOTPRO	Bottom product of reactive distillation column
CBOTPRO	Bottom product of distillation column of conventional method
CTOPPRO	Top product of distillation column of conventional method
NRTL	Non-Random Two Liquid
RBOTPRO	Bottom product of reactor of conventional method
RTOPPRO	Top product of reactor of conventional method
TOPORO	Top product of reactive distillation column
USD	United States Dollar

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