Comparative Analysis of Process Flow Configurations for Ethanol Dehydration

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ABSTRACT

Air pollution as a result of smoke from vehicles is one of the leading sources of these greenhouse gases hence ways of reducing smoke (CO, SO_2, etc.) Produced by automobile became main objective to researchers. One of the ways of reducing this smoke from automobile is by mixing the fossil fuel used by these automobiles with ethanol to produce gasohol which is more environmental friendly. Production of this gasohol makes ethanol to become highly demandable and it's of high energy intensive. This work focuses on determining ethanol dehydration process of less energy intensive. Three different configurations of azeotropic distillation of ethanol dehydrating process were modeled using Aspen Hysys (version 7.1) with benzene as the entrainer. Anhydrous ethanol of 99.5% concentration was obtained. When the three configurations were compared to each other using their rate of energy consumption as the criteria,the configuration with the least total energy of 2.176*107Kj/hr was taken as the best case configuration. The effects of the four process parameters were investigated on the best case configuration and also were optimized using response surface methodology (RSM). The optimal points conditions generated by the design expert (RSM) were used to simulate the best case configuration, and the optimized total energy of the process is 1.8826*107Kj/hr which when compared with the total energy of the best case configuration (2.176*107Kj/hr), 13.5% of the total energy of consumption was saved. The RS-Model process configuration (optimized model) shows third (Cubic) order polynomial and are significant models with high R squares.

Keywords: azeotropic distillation, dehydration, ethanol, optimization, process parameter.

1.0 INTRODUCTION

In order to control air pollution from fossil fuels, biofuels are mostly use in automobiles in today's world (Paola et al, (9)).This increases the demand for anhydrous ethanol in industries hence has increased researchers interest in developing cheaper and more reliable methods of its production (Boggan (3)).Ethanol is also added to gasoline as an octane enhancer. For all these reasons many ethanol producers or engineering firms are today focusing on designing and building-up new plants as rapidly as possible in order to satisfy a growing demand (Inderwildi et al,(7)). Alcohol is second only to water in solvent value and is employed in nearly all industries. One of the chief difficulties in using alcohol in gasoline is that the usual 95% ethanol is not miscible with gasoline. Only absolute or 99.5% alcohol will mix the gasoline for gasohol, this requires costly extra processing, because simple distillation will not produce ethanol above 95% concentration. Many new methods for lower cost distillation or other ways of removing the water in the alcohol have been proposed, but so far absolute alcohol continues to cost more to produce than gasoline (Austin, (2)). The usual ratio of ethanol to gasoline is ninety (90) parts gasoline to ten(10) parts ethanol while that for methanol is ninety-seven (97) parts gasoline to three (3) parts methanol. Some cars have been designed to run on pure methanol.Gasohol has higher anti-knocking properties (higher octane) than gasoline, burns more slowly, coolly and completely. However, it is more expensive and energy intensive to produce and more friendly to the environment and people (Boggan, (3)).

Distillation is a process that uses different in boiling point to separate compounds. In the case of alcohol and particularly ethanol, knowledge that the boiling point of pure water is 100^{o}c while that of ethanol is 78.4^{o}C, entrainer allows the separation of the ethanol from the water by adjusting the distillation temperature to a point

slightly lower than that of ethanol and lower than that of water. Pure (anhydrous) ethanol cannot be obtained through conventional distillation of a water-ethanol mixture because a constant boiling mixture forms consisting of 95% ethanol, 5% water. Such a mixture is referred to as an azeotrope. Further concentration of the ethanol can be achieved by shifting the azeotropic point through vacuum distillation or addition of another substance (entrainer) to the mixture. Often times, the compound added is highly toxic such as benzene, toluene, heptane, etc., therefore absolute alcohol must never be consumed (Boggan, (3)). Optimization of the operating conditions of azeotropic distillation columns with pervaporation membranes was studied and it shows the hybrid process of a distillation column combined with pervaporation membranes which when compared to the classical two-column process for methyltert-Butyl ether production gives a result that shows a significant reduction in operating cost obtained by using a pervaporation membrane instead of the second column in the original process. Hoch, et al, (6).

Garcia, et al, (4), researched on "Numerical Optimization Applied to the Design of An Extractive Distillation System for the Production of Fuel Grade Alcohol", the optimal design of an extractive distillation system is developed for the separation of the ethanol - water azeotropic mixture using ethylene-glycol as entrainer. The system is made up by an extractive distillation column and a recovery column, each one with total condenser and reboiler. The extractive distillation column is fed with an ethanol /water mixture which composition is close to the azeotrope and a high purity stream of ethylene-glycol; this column produces as distillate ethanol with purity higher than 99.5% molar and as bottom product a mixture composed mainly by water and ethylene glycol. Predicting Minimum Energy Conditions for a Distillation Column by Design of Experiments and Process Simulation was carried out using Aspen Plus and according to their report, the energy consumption of the distillation column is dependent on several operation variables, optimization of these variables minimized the energy demand while maintaining good product quality Adela, et al (1). Vasconcelos, et al (10), studied Optimization, Dynamics and Control of a complete Azeotropic Distillation: New Strategies and stability considerations. It was found out that Heterogeneous azeotropic distillation process is widely used in industries to separate non- ideal mixtures in order to obtain high purity components. The processes were optimized in terms of energy consumption using factorial design and Respond Surface Methodology.

This research work centers on the azeotropic distillation of the ethanol dehydration process plant.In thisprocess plant, a lot of energy is consumed by the plant to produce absolute ethanol. This research work focuses on determining a dehydration process of less energy intensive. The best process incures less investment cost during initial deployment of the technology. The energy consumption and capital investment cost are competitive and represent important saving in final cost of ethanol plant.This study gives the current trend in the process design and operations of ethanol dehydration plant in terms of energy efficiency

2.0 MATERIALS AND METHODS

2.1 PROCESS MODELING OF THE ETHANOL DEHYDRATION PLANT USING ASPEN HYSYS

Hysys is a powerful Engineering simulation tool. The software is used in research, development, modeling and design. HYSYS serves as the engineering plat form for modeling processes, Hamid (5). In Aspen Hysys simulation environment, there are steps involved in modeling a chosen process. Some of these steps include; selecting the components for the process, choosing the fluid package for the process, laying out the unit operation, specifying the specification for the unit operation.

2.2 PROCESS DESCRIPTION OF ETHANOL DEHYDRATION PLANT

An ethanol Process plant consists of three (3) main sections;

First Section

This is where fermentation process of the plant is carried out. Depending on the type of process approach used, which could be sugarcane, sorghum, molasses, grain, or cassava to produce ethanol using yeast as an activator. In this division, the main equipments are fermentor or a reactor where the fermentation is carried out and a storage tank where the broth (product from the fermentation) produced is stored. The fermentation process is always carried out in batches.

Second Section

The broth in the storage tank is taken as feed to the carbon dioxide (CO2) separator where the CO2 formed during the fermentation process that are embedded in the broth are evolved from the CO2 separator through the upper outlet and the remaining (mixture of ethanol / water) is taken to the distillation unit through the bottom outlet. In the distillation unit heat is applied and ethanol having a lower boiling point temperature than water leaves the distillation column through the upper outlet and water leaves through the bottom outlet. The water is taken to the water treatment plant. The ethanol distilled in this unit is not an absolute (anhydrous) ethanol because it still contains some percentages of water of about 5% - 6% which makes it unfit for wide industrial use except for few beverage company or consumption. To make the ethanol fit for industrial uses; it is taken to azeotropic distillation unit where it is further distilled. The main equipments in this section of the plant are separator and distillation columns.

Third Section

In this section, dehydration process of the ethanol is carried out using azeotropic distillation method. The ethanol produced in the first distillation unit of the plant still contains some percentages of water (94% - 95% ethanol, 6% - 5% water). They are sent from the first unit to the azeotropic distillation unit where heat is applied and some quantity of entrainer is added. The presence of the entrainer (benzene) forms ternary in the azeotropic column. The ternary boils at 78.2oC and leaves the column from the upper outlet into a decanter (note that; water boils at 100oC, Ethanol boils at 78.4oC, and Benzene boils at 80.1oC). The absolute (anhydrous) ethanol of about 99.5% or 99.6% concentration leaves the column from the bottom outlet and is stored in the anhydrous ethanol tank.

In decanter, the azeotropic mixture settles into two phases, organic and aqueous phases. The organic phase (mainly benzene) leaves the decanter from the upper outlet and is recycled to mix with the benzene make-up. The aqueous phase leaves from the lower outlet and is taken to column 3 for further heating.

In column 3, the aqueous phase is heated up and another azeotropic mixture is formed (mainly benzene, and ethanol) which is recycled back to mix up with azeotropic mixture 1 coming from column 2 into the decanter. The remaining feed in the column 3 leaves from the lower outlet as aqueous alcohol (mainly water and ethanol) into column 4 for further distillation.

In column 4, the light phase (mainly ethanol) leaves the column from the upper outlet and is recycled back to mix up with the feed (hydrated ethanol) entering column 2. The remaining leaves as water through the lower outlet into the waste water tank

The main equipment in this section includes: Reboiled Absorber (Azeotropic column), Decanter, Distillation column (Stripper or solvent recovery column), Storage tanks

2.2.1The Three Different Configurations:

Configuration 1: has 4 columns at which the light phase (comprising mainly of ethanol) leaves the column as distillate product from the upper outlet and is recycled back to mix with the feed (hydrated ethanol) entering column 2.

Configuration 2: has 3 columns, in the column 3, the light phase (comprising mainly of ethanol) leaves the column from the upper outlet and is recycled back to mix with the feed (hydrated ethanol) entering column 2.

Configuration 3: has 3 columns, at the third column, the aqueous phase is further heated and the light phase (comprising mainly of ethanol) leaves the column from the upper outlet into the organic storage tank from where they are recycled back to mix with the benzene make-up unit.

Ethanol plant of different configurations has different rate of energy consumption. In this study, three process configurations were simulated and studied. The process configuration with the least rate of energy consumption was taken as the best case and is used in the parameter optimization.

Process Configuration 1

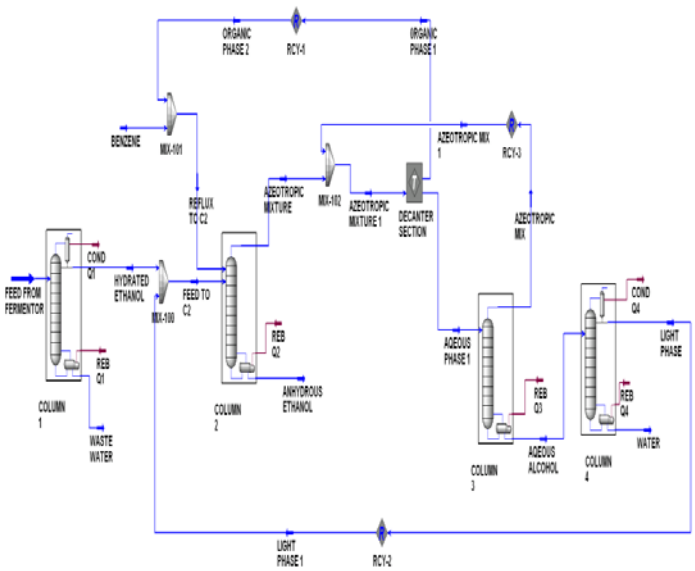


Figure 1: Process Flow Diagram of Configuration 1

Process Configuration 2

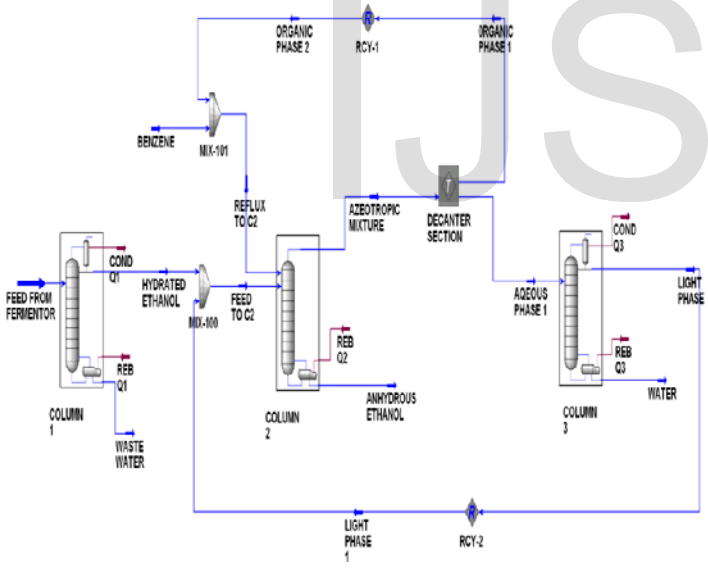


Figure 2: Process Flow Diagram of Configuration 2

Process Configuration 3

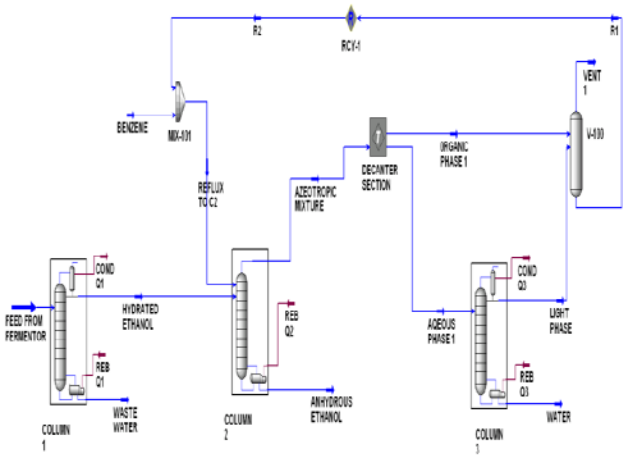


Figure3: Process Flow Diagram of Configuration 3

3.0 RESULTS AND DISCUSSION

3.1 PROCESS MODELLING OF THE ETHANOL DEHYDRATION PLANT (BASE CASE SCENARIO)

The ethanol dehydration process involves the separation of three compounds namely; ethanol, water and benzene. These three compounds were selected and specified as the components of the simulated process in Aspen HYSYS basis environment.In the azeotropic distillation process, the Vapour – Liquid Equilibrium (VLE), Vapour – Liquid – Liquid Equilibrium (VLLE), and Liquid – Liquid Equilibrium (LLE) must be considered. NRTL of different basis were used as fluid package to simulate the process and the result obtained from each of them was compared with actual industrial data to ascertain their suitability to predict the vapour-liquid interactions of the process. The three NTRL basis include; VLE basis (case 1), VLLE and LLE basis (case 2) and General (case 3). Table1shows the temperature values for specified stages of the azeotropic column for each of the cases and was also validated by comparing the results obtained from simulation with actual industrial temperature data from a distillery reported by Vasconcelos *et al*. (10).

The results were approximately the same and indicated that the data obtained from simulation were within $\pm 5^0$C of the industrial data. When other things such as the equilibrium phases were considered, case 2 (NRTL – VLE & LLE) was chosen because its calculations addressed both the Vapor – liquid equilibrium (VLE)

and the liquid – liquid equilibrium (LLE) which gives a better condition for the process calculation throughout the simulations.

Table 1: Comparison of Simulation data with industrial data

Stage No	Case 1: NRTL (VLE basis) Temp (°C)	Case 2: NRTL (VLE & LLE basis) Tempe (°C)	Case 3: NRTL (General) Temp (°C)	Industrial data from a distillery* Temp (°C)
25	86.90	86.90	86.90	83.30
17	75.54	75.88	75.87	73.20
5	66.54	67.33	67.33	66.00

*Source: Vasconcelos *et al.* (10)

The simulation is satisfactory and the simulation results acceptable when all the design specifications for all the various process equipments in the plant are met. These design specifications are discussed in table 2 and 3 for azeotropic distillation column (column 2) (reboiled absorber) andsolvent recovery column (column 3) respectively. The decanter's temperature was set at a constant value of 58°C, a temperature lower than the azeotropic mixture temperature. This is to enable the mixture coming from the azeotropic distillation column 2 to cool down and separate into two phases; the organic and the aqueous phases. The organic phase; has three components in which benzene is more. The ratio of the organic stream is; benzene (82.35%), Ethanol (17.23%) and water (0.42%). The aqueous phase has three components in which water has a percentage of 35–40 %, ethanol is 53.61% and benzene is 11.26%.

Table 2: Specifications for Azeotropic Distillation Column (Column 2) (specified & simulated values)

Specification	Desired Value	Simulated Value
Benzene in bottom(kgmole/hr)	$1.000*10^{-04}$	$1.000*10^{-04}$
Ethanol in bottom (kgmole/hr)	0.9950 (99.50%)	0.9951(99.51%)
Water in bottom (kgmole/hr)	$5.000*10^{-04}$	$4.79*10^{-04}$

Table 3: Specification for Solvent Recovery Column

Specification	**Desired Value**	**Simulated Value**
Ethanol Recovery (kgmole/hr)	0.9999 (99.99%)	0.9999 (99.99%)
Benzene recover (kgmole/hr)	0.9999 (99.99%)	1.00
Water in bottom (kgmole/hr)	0.9999 (99.99%)	0.9998 (99.98%)

3.2 COMPARISON OF THE THREE PROCESS FLOW CONFIGURATIONS OF ETHANOL DEHYDRATI0N PLANT

The three process flow configurations (1, 2, & 3), were simulated. The simulated data were taken, studied and compared. From the simulation results presented in Table 4, it was deduced that process configuration 1 has the highest flow rate of anhydrous ethanol (158.6kgmole/hr), 99.5% concentration of ethanol, the highest energy consumption rate of $2.619*10^{07}$kJ/hr with 93.2% ethanol recovery in the solvent recovery column and four distillation units. Process configuration 2 consumed the least energy of $2.176*10^{07}$kJ/hr, 99.5% of ethanol concentration, a flow rate of anhydrous ethanol of 126.5kgmole/hr with 99.97% ethanol recovery in the solvent recovery column and has three distillation units. The criteria of selecting the best process configuration is based on the rate of energy consumption of the process model obtained from simulation since this will imply a favorable economics. Process configuration 2 was selected as the best (base) process configuration because it has the least energy consumption rate. Also table5 shows the operating conditions with which the best case scenario was simulated.

Table 4: Simulation Results of the Different Process Configurations

Factors	**Process Configurations**

	1	2	3
Reboiler duty Column 2, (kJ/hr)	1.179*10^{07}	9.122 *10^{06}	1.103 *10^{07}
Reboiler duty Column 3, (kJ/hr)	1.458 *10^{06}	1.264 *10^{07}	1.396 *10^{07}
Reboiler duty Column 4, (kJ/hr)	1.294 *10^{07}	-	-
Total Energy (KJ/hr) consumed by the Process Model	2.619 *10^{07}	2.176 *10^{07}	2.499 *10^{07}
Ethanol Concentration (%)	99.5	99.5	99.5
Anhydrous Ethanol Flow rate (Kgmole/hr)	158.6	126.5	147.3
Ethanol Recovery (%)	93.2	99.97	91.6

Table 5: operating conditions of the Best Case Configuration

Factors	Conditions
Entrainer	Benzene
No of Stages in column 2	25
Feed stage in Column 2	3
No of stages in column 3	13
Feed stage in Column 3	9
Reboiler energy Column 2 (Kj/hr)	9.120*10^{06}
Reboiler energy Column 3 (Kj/hr)	1.264*10^{07}
Total energy (Kj/hr)	2.176*10^{07}

4.0 OPTIMIZATION OF THE PROCESS PARAMETERS

In optimizing the process parameters using RSM, the values of four process parameters were varied simultaneously between the low and high levels. Table 6 shows the factors levels used in the RSM optimization. A standard RSM design called Box Henken design was used to design the simulation experiment generating twenty five (25) simulation runs from a combination of the values of the variables between the low and high levels and the value of the three responses (reboiler energy in column 2, reboiler energy in column 3 and total energy consumed by the process) for each of the run was obtained.

Table 6: Factor Levels used in the RSM Optimization

Factor	Name	Low	High
A	No of stages in Azeotropic column 2	25	45
B	Feed Tray Stage in Column 2	3	9
C	No of stages in the Solvent Recovery column 3	10	20
D	Feed tray Stage in the Solvent Recovery Column 3	2	8

The combination of the four variables for the twenty five simulation runs are generated using the Box Henken design in RSM design expert. Each simulation run represents a unique combination of values for the four variables and the value of the three responses were obtained for each of these specified points by simulation. The values of the three responses obtained by simulation for each of the twenty five runs are also studied.

4.1 Statistical modeling and analysis

Based on the simulation results obtained, the regression models have been constructed by mean of OLS (ordinary least square) method in order to determine the functional relationship for approximation and prediction of responses. The response variables (Y_1, Y_2, and Y_3) were fitted by a cubic order polynomial model in order to correlate the response variable to the design variables (x_1, x_2, $x_3$and x_4).

Statistical modeling and analysis of total energy of the process (response 3, (Y3))

The RS-model for response 3 (Total energy of the process model) was found significant as the computed F-value (F-model = 60.73) with very low probability value (p = 0.0198) indicated the high significance of the fitted model at 95% confidence level. These results show that the cubic RS-model is satisfactory for predicting the total energy consumed by the columns.The goodness-of-fit of the cubic RS-model for response 3 is illustrated in Fig 4. On the other hand, a relatively low value of the coefficient of variation (C.V = 1.72%) reveals a better

precision and reliability of the simulation results of the presently fitted model.

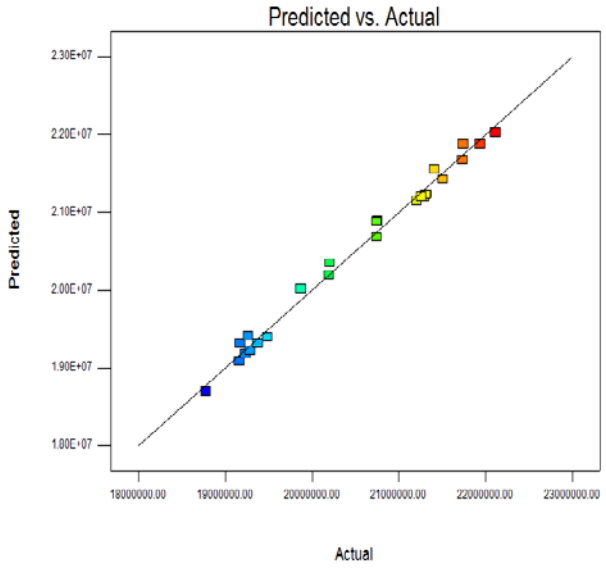


Figure 4: Goodness-of-fit of RS-model for response 3

Statistical Significance of the Model for the total energy of the process (response 3, (Y3))

Figure 5 to Figure 10 show the Response surface 3D graphs of the interaction of effects of the process variables on the total energy for the columns (Response 3). From the graphs the reboiler energy for column 2 generally increases in one part and decreases in the other part as its variables varies though its energy level of increase differs as the variables interactions differs in the graphs.

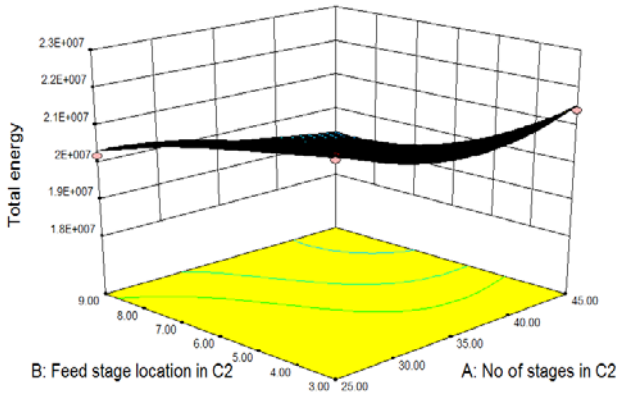


Figure 5: Response surface 3D graph of the interaction of effects of the number of stages in column 2 and the feed stage location in column 2 on the total energy for the process columns (Response 3)

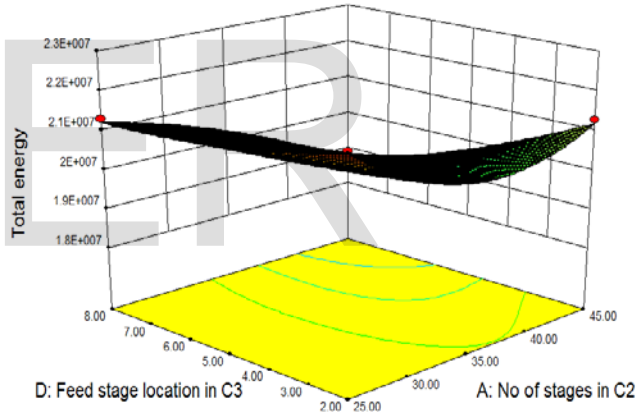


Figure 6: Response surface 3D graph of the interaction of effects of the number of stages in column 2 and the feed stage location in column 3 on the total energy for the process columns (Response 3)

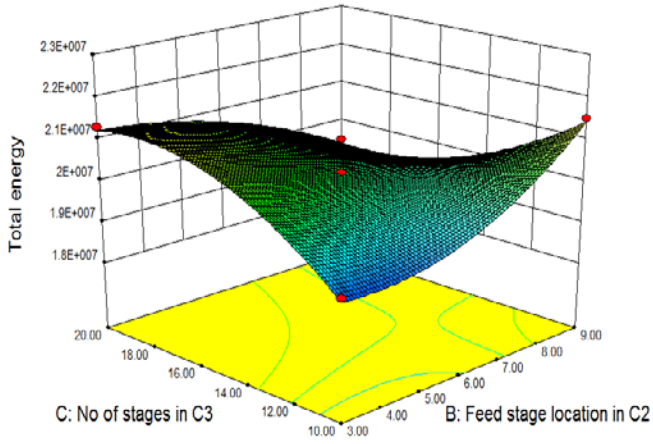
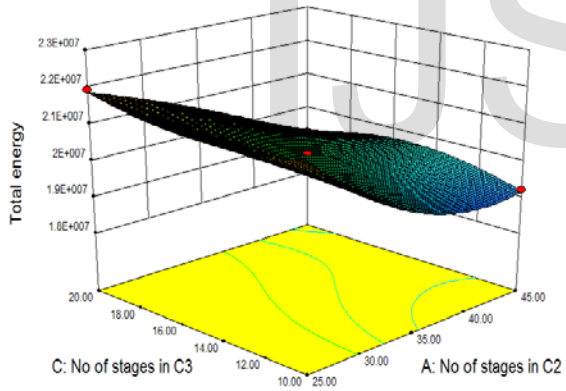


Figure 7: Response surface 3D graph of the interaction of effects of the feed stage location in column 2 and the number of stages in column 3 on the total energy for the columns (Response 3)

Figure 8: Response surface 3D graph of the interaction of effects of the number of stages in column 2 and the number of stages in column 3 on the total energy for the process columns (Response 3)



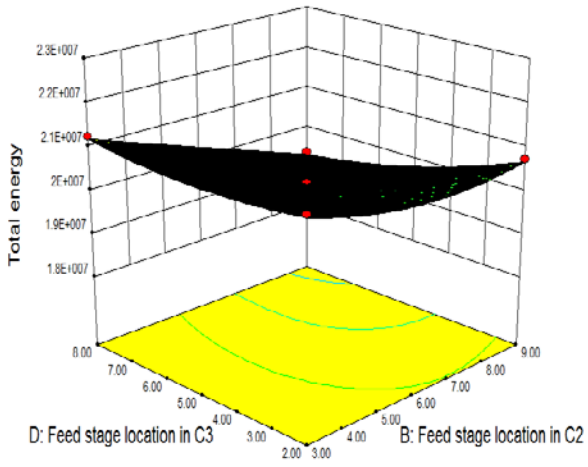
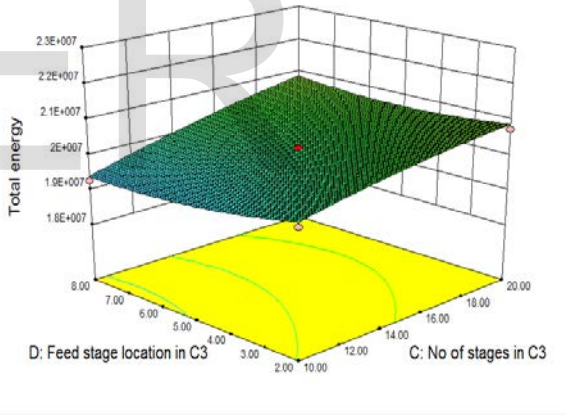


Figure 9: Response surface 3D graph of the interaction of the effects of the feed stage location in column 2 and the feed stage location in column 3 on the total energy of the process columns (Response 3)

Figure 10: Response surface 3D graph of the interaction of effects of the number of stages in column 3 and the feed stage location in column 3 on the total energy for the process columns (Response 3)



4.2 Optimal Point for the Process

The optimal points obtained from the optimization simulation are presented in Table 7. The process was also simulated at these optimal points and the values obtained for the three responses from both the generated model and simulated data are also presented in Table 7.

Table 7: Optimal point obtained for the process

Factors	RSM Generated Data	Simulated Data
No of Stages in column 2	43.89	44
Feed stage in C2	7.21	7

No of stages in column 3	16.10	16
Feed stage in C3	6.57	7
Reboiler energy C2 (Kj/hr)	$8.8028*10^{06}$	$9.019*10^{06}$
Reboiler energy C3 (Kj/hr)	$1.0062*10^{07}$	$9.807*10^{06}$
Total energy (Kj/hr)	$1.8778*10^{07}$	$1.8826*10^{07}$

Desirability generated by the model is 0.888. Desirability values ranges from zero to one, values closer to one being more desirable.

The results in Table 7 shows that the values of the three responses predicted from the model are closely related to the simulation values. The slight changes are as a result of the approximation done on the number of stages (Columns 2 & 3) and their feed stages.The percentage error is 0.2556% which is very small and hence negligible.The percentage energy saving is 13.5% which means it maximizes the profit.

Table 8: Optimal operating Conditions of the best case

Factors	Conditions
Entrainers	Benzene
No of Stages in column 2	44
Feed stage in Column 2	7
No of stages in column 3	16
Feed stage in Column 3	7
Reboiler energy Column 2 (Kj/hr)	$9.019*10^{06}$
Reboiler energy Column 3 (Kj/hr)	$9.807*10^{06}$
Total energy (Kj/hr)	$1.8826*10^{07}$

5.0 CONCLUSION

Three different plant configurations of azeotropic distillation for ethanol dehydrating process were simulated using Aspen Hysys (version 7.1) with Non-Random Two-Liquid (NRTL) fluid package (Vapor Liquid Equilibrium (VLE) & Liquid-Liquid Equilibrium (LLE) basis) and benzene as the entrainer. The best configuration was selected out of the three configurations (1, 2, & 3) and its process parameters optimized. The optimal operating conditions of the model for the variable were obtained. These optimal points are the points where the model maximizes the yield of the anhydrous ethanol at a minimum rate of energy consumption. The models generated by the RSM were significant models with high R squares which indicate very strong models. Other factors such as f-value, P-value, desirability were obtained. An energy saving of 13.5% was achieved. The calculated % error of the predicted and simulated data is 0.2556% which is very small and it shows that the simulated data are within range and thus very significant. The model was validated by comparing the results obtained from simulation with actual industrial data from a distillery as reported by Vasconcelos et al. (2002) though factorial design was used as the optimization tool in that report. The results were approximately the same and indicated that the data obtained from simulation were within $+5^0$C of the industrial data. This study provides information on efficient design and optimal operation of ethanol dehydration plant. Since current trend in process design demands energy efficiency of all unit operation, this study highlights the necessary procedure for choosing the best technology using energy consumption as criteria.

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