The International Journal Of Engineering And Science (IJES)
|| Volume ||3 || Issue || 4 || Pages || 65-70 || 2014 ||
ISSN (e): 2319 – 1813 ISSN (p): 2319 – 1805

Investigation of behaviour of thermodynamic properties of cassava based ethanol-water system during azeotropic distillation process.

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ABSTRACT

This paper investigates the behaviour of properties of cassava based ethanol-water system during azeotropic distillation process. The product of fermentation is assumed to be binary mixture. The objective is to arrive at the optimum process conditions that will give the required percentage of purification using a new developed software. Simulations are performed with cassava as the biomass material and the parameters obtained from the beer produced from fermentation of cassava mash as the input for the software.The considered parameters were Reflux Ratio (R), Relative Volatility (RV), Minimum Reflux Ratio (R_{min}), Mole Fraction of the most volatile component in the distillate (x_D), Mole Fraction of the most volatile component in the bottom (x_B), Mole Fraction of the most volatile component in the feed (x_F), thermodynamics properties of the feed (q). The results obtained using the developed Software is compared with the predicted result from Central Composite Design model at various input levels and the new software is validated with published experimental results. The process simulation results show that the reflux ratio, relative volatility increases with increase in temperature at constant pressure and have significant effect on purification of ethanol compared to other parameters.

KEYWORDS: *Bioethanol, Cassava, Azeotropic Distillation, Design Expert, Simulation.*

Date of Submission: 10 February 2014 Date of Publication: 05 April 2014

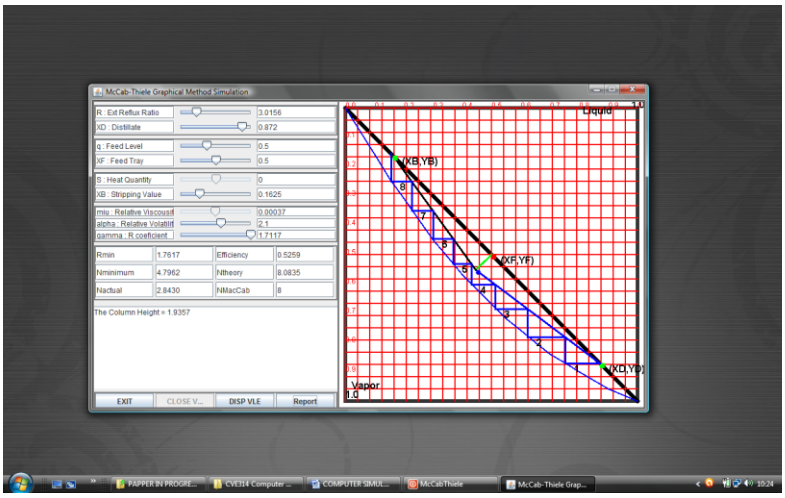
I. INTRODUCTION

The search of environment friendly solutions for the management, along with increasing costs of fuel and recent regulations on disposal, emissions leads toward the recovery of energy and demands research activities related to renewable energy such as biofuel which comprise of bioethanol and biodiesel [1]. Bio-ethanol is a distilled liquid produced by fermenting sugars from sugar plants and cereal crops such as sugarcane, corn, beet, cassava, wheat and sorghum. Several researchers have reported biofuel production from various agricultural materials including biogas from mixture of cassava peels and livestock waste [2], fuel from indigenous biomass wastes [3], as well as ethanol from non-edible plant parts [4].

Ethanol is a common ingredient in many solvents, perfume, disinfectants and alcoholic beverages. To produce bioethanol, it is necessary to separate ethanol from ethanol-water mixture after fermentation of alcohol. An azeotropic distillation is a widely practiced process to split one needed component from its heterogeneous system where the third component known as entrainer is incorporated. Azeotropic distillation columns are commonly used in industry to separate mixtures of close relative volatility and for breaking azeotropes such as bioethanol-water system. Process simulation is used for the design, development, analysis and optimization of the technical processes. It is a model-based representation of chemical, physical, biological, energy producing and transforming, in addition to other technical processes and unit operations using software. Process simulation always uses models which introduce approximations and assumptions, but allows the description of a property over a wide range of parameters which may not be covered by real data. Models also allow for interpolation or extrapolation, searching for conditions outside the range of known properties [5,6]. Many researchers have studied the production of bio ethanol from different feedstock but not much have taking coginizance of the behaviour of thermodynamic properties of the feed during distillation process.This paper investigates the behaviour of thermodynamic properties of cassava based ethanol-water system during distillation process.

II. MATERIALS AND METHODS

A new developed software [7] hinged on McCabe-Thiele method and the Fenske Equations [8] were used for the simulation of thermodynamics properties of azeotropic distillation of cassava based bioethanol method using Vapour- Liquid- Equilibrium (VLE) data of ethanol-water system obtained from literature [9]. The screen shot of the software used is as shown in Figure 3. Table 2 shows the output values obtained from.The Design Expert software was used to obtain the output values at different levels in the developed software. The central composite design is used to compare the values obtained from the developed software and the predicted values.



R : Ext Reflux Ratio 3.0156
XD : Distillate 0.872
q : Feed Level 0.5
XF : Feed Tray 0.5
S : Heat Quantity 0
XB : Stripping Value 0.1625
miu : Relative Viscousit 0.00037
alpha : Relative Volatilit 2.1
gamma : R coeficient 1.7117

Rmin	1.7617	Efficiency	0.5259
Nminimum	4.7962	Ntheory	8.0835
Nactual	2.8430	NMacCab	8

The Column Height = 1.9357

Figure 1: Screen shot of Software

The model was used by supplying the input and the level of simulation was provided which gives an output that translated to the plotting of the McCabe-Thiele graph.The report is generated and displayed. Parameters such as RR, R_{Coeff}, x_D, x_B, x_F, Viscosity, q were varied in the programme to obtain the Number of trays. The values obtained from the software were verified by comparing to values obtained from mathematical computation. To obtain the optimum design parameters for use in mechanical design, a central composite experimental design was used.

McCabe-Thiele Theoretical Analysis

The McCabe-Thiele method uses the equilibrium curve diagram to determine the number of theoretical stages (trays) required to achieve a desired degree of separation. It is a very useful tool for the understanding of distillation operation [8].The VLE data is available at the operating pressure of the column. Information required were the feed condition (temperature, composition), distillate and bottom compositions; and the reflux ratio (R) is defined as the ratio of reflux liquid over the distillate product. The feed has a concentration of x_F (mole fraction) of the more volatile component, and a distillate having a concentration of X_D of the more volatile component and a bottom having a concentration of x_B was desired.The method involves the plotting on the equilibrium diagram, 3 straight lines: the rectifying section operating line (ROL), the feed line (also known as the q-line) and the stripping section operating line (SOL). Each of these lines passes through the points representing the mole fractions of the more volatile component in the distillate, bottoms and feed (x_D, x_B and x_F) respectively. These lines represent the relationship between the concentrations in the vapour phase (y) and the liquid phase (x). The number of theoretical stages required for a given separation was then the number of triangles that can be drawn between these operating lines and the equilibrium curve. The last triangle on the diagram represents the reboiler.

In the simplest case, the McCabe-Thiele Method to determine the number of theoretical stages followed the steps below:

- Analysis of the Rectifying section, and determining the ROL using x_D and R
- Analysis of the Feed section, and determining the feed condition (q)
- Determination of the feed line (q-line) using x_F and q
- Locate the intersection point between ROL and q-line
- Analysis of the Stripping Section, and determining the SOL using, ROL, q line and x_B

The plates are numbered serially from the top and the plate under consideration is the n-th plate from the top.The plate immediately above this plate is plate (n-1) and the plate immediately below this plate is plate (n+1).

The Operating Line Equation for the rectifying section under constant molal flow is given as:

$$y_{n+1} = \frac{R}{(R+1)} x_n + \frac{1}{(R+1)} x_D \qquad 1$$

Usually the subscripts "n+1" and "n" are not known, so that equation 1 can be put together in the form equation 2

$$y = \frac{R}{(R+1)} x + \frac{1}{(R+1)} x_D \qquad 2$$

The feed operating line equation is given as:

$$y = -\frac{q}{(1+q)} x + \frac{1}{(1-q)} x_F \qquad 3$$

The stripping operating line (SOL) equation is given as:

$$y = \frac{L'}{(L'-B)} x - \frac{B}{(L'-B)} x_B \qquad 4$$

Total Reflux

The Fenske Equation was also used to determine the minimum number of trays required for a given separation using eqn. 5.

$$N_{\min} = \frac{\ln\left(\frac{x_D\left(1-x_B\right)}{x_B\left(1-x_D\right)}\right)}{\ln\left(\alpha_{AB}\right)} - 1 \qquad 5$$

Minimum Reflux

The minimum reflux rate was determined mathematically from the endpoints of the rectifying line at minimum reflux -- the overhead product composition point (x_D,x_D) and the point of intersection of the feed line and equilibrium curve (x', y').

$$R_{\min} = \frac{x_D - y'}{y' - x'} \qquad 6$$

III. RESULTS AND DISCUSSION

The results of the effect of Reflux Ratio and relative volatility on number of trays obtained using the developed software at constant temperature is shown in Figures 2 and 3 respectively. It was observed that increase in reflux ratio and relative volatility led to decrease in the value of number of trays. This is not unexpected as high refluxration during distillation process reqired less number of trays. [10] in a research on ethanol productivity from cassava reported similar observation in his study. The variation in relative volatility showed corresponding number of trays of distillation column that would give the highest purity of ethanol. The obtained values from the developed software and the predicted values from central composite design are also shown in Table 1. A correlation coefficient of 0.97 was obtained for the two results indicating that the developed software can adequately provide the expected output within the input range considered. A model was obtained relating the various experimental variables to the outputs; Number of Trays using Fenske and McCabe, as well as the Column height and Efficiency of distillation column. The model was then used to establish the optimum variable parameters for the distillation process. Model Optimization result obtained from the central composite design is shown in Table 2.

Table 1. Comparison of results obtained from the Developed Software (DS) and predicted result from Central Composite Design (CCD) model at various input levels

Std	RR	X_D	X_B	RV	RCoeff	McCabe No of Trays		Fenske No of Trays		Column Height(m)		Efficiency
						Software (DS)	Predicted (CCD)	Software (DS)	Predicted (CCD)	Software (DS)	Predicted (CCD)	%
1	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.47	53.2
2	7.06	0.59	0.16	1.58	1.2	3	3.21	4	4.27	2.04	2.1	56.2
3	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.47	53.2
4	4.24	0.8	0.16	2.42	1.2	3	2.89	6	6.06	1.95	1.89	50.9
5	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.47	53.2
6	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.47	53.2
7	4.24	0.8	0.32	1.58	1.5	3	2.59	4	3.72	2.02	1.96	57.1
8	4.24	0.59	0.32	1.58	1.5	2	1.71	2	2.04	1.34	1.36	57.1
9	4.24	0.8	0.16	2.42	1.5	2	2.21	6	6.06	1.66	1.56	50.9
10	7.06	0.59	0.16	2.42	1.5	2	1.33	4	4.27	1.54	1.33	50.9
11	4.24	0.8	0.16	1.58	1.2	5	4.49	6	6.06	3.1	2.9	57.1
12	7.06	0.8	0.32	1.58	1.2	3	2.87	4	3.61	2.12	2.09	56.2
13	7.06	0.8	0.32	2.42	1.5	2	1.52	4	3.61	1.31	1.21	50.9
14	2.3	0.69	0.24	2	1.35	2	2.55	5	4.08	1.56	1.58	53.2
15	5.65	0.69	0.24	3	1.35	1	0.96	4	3.95	1.25	1.32	48.2
16	4.24	0.59	0.32	2.42	1.5	1	0.65	2	2.04	1	0.92	50.9
17	7.06	0.59	0.16	2.42	1.2	2	2	4	4.27	1.49	1.66	50.9
18	7.06	0.59	0.32	2.42	1.5	1	0.64	2	1.93	0.99	0.95	50.9
19	4.24	0.59	0.32	2.42	1.2	1	1.33	2	2.04	1.14	1.25	50.9
20	4.24	0.8	0.32	2.42	1.2	2	2.21	4	3.72	1.58	1.51	50.9
21	7.06	0.8	0.32	1.58	1.5	3	2.2	4	3.61	1.78	1.76	56.2
22	5.65	0.69	0.44	2	1.35	1	1.12	0	1.03	1.1	1.15	53.2
23	5.65	0.69	0.04	2	1.35	4	3.51	8	6.87	2.38	2.39	53.2
24	4.24	0.8	0.32	2.42	1.5	2	1.53	4	3.72	1.35	1.18	50.9
25	7.06	0.59	0.32	2.42	1.2	1	1.32	2	1.93	1.14	1.28	50.9
26	9	0.69	0.24	2	1.35	2	2.08	4	3.82	1.47	1.37	53.2
27	4.24	0.8	0.32	1.58	1.2	4	3.27	4	3.72	2.38	2.29	57.1
28	7.06	0.59	0.32	1.58	1.2	2	1.99	2	1.93	1.44	1.49	56.2
29	4.24	0.59	0.16	2.42	1.2	2	2.01	4	4.38	1.52	1.63	50.9
30	5.65	0.69	0.24	2	1.7	2	1.52	4	3.95	1.32	1.6	53.2
31	5.65	0.69	0.24	1	1.35			4	3.95		1.47	63.1
32	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.47	53.2
33	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	1.59	53.2
34	7.06	0.8	0.16	2.42	1.5	2	2.21	6	5.95	1.62	1.3	50.9
35	4.24	0.59	0.16	2.42	1.5	2	1.33	4	4.38	1.3	2.57	50.9
36	4.24	0.8	0.16	1.58	1.5	4	3.81	6	6.06	2.61	1.77	57.1
37	7.06	0.59	0.16	1.58	1.5	2	2.54	4	4.27	1.73	1.47	56.2
38	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	2.37	53.2
39	7.06	0.8	0.16	1.58	1.5	4	3.42	6	5.95	2.31	1.97	56.2
40	4.24	0.59	0.16	1.58	1.5	3	2.93	4	4.38	1.92	2.7	57.1
41	7.06	0.8	0.16	1.58	1.2	4	4.1	6	5.95	2.75	1.16	56.2
42	7.06	0.59	0.32	1.58	1.5	1	1.31	2	1.93	1.24	1.69	56.2
43	4.24	0.59	0.32	1.58	1.2	2	2.39	2	2.04	1.55	2.01	57.1
44	5.65	0.95	0.24	2	1.35	2	3.4	4	6.03	1.49	1.47	53.2
45	5.65	0.69	0.24	2	1.35	2	2.31	4	3.95	1.49	2.37	53.2
46	5.65	0.69	0.24	2	1	4	3.11	4	3.95	2.56	2.3	53.2
47	4.24	0.59	0.16	1.58	1.2	4	3.61	4	4.38	2.27	1.92	57.1
48	7.06	0.8	0.16	2.42	1.2	3	2.89	6	5.95	1.91	0.96	50.9
49	5.65	0.44	0.24	2	1.35	1	1.27	2	1.95	1.03	1.54	53.2
50	7.06	0.8	0.32	2.42	1.2	2	2.2	4	3.61	1.54		50.9

Table 2. Optimization result obtained from the central composite design

	Optimum Input variable values					Optimum Software Responses				
Optimized parameter	RR	X_D	X_B	RV	RCoeff	McCabe No of Trays	Fenske No of Trays	Column Height	Distillation Column Efficiency	Desireability Value (%)
Mc Cabe no of Plates	4.27	0.8	0.16	1.58	1.5	4	-	-	-	80.0
Fenske no of Plates	4.24	0.8	0.16	1.90	1.5	-	6	-	-	85.0
Column Height(m)	4.43	0.8	0.16	1.58	1.5	-	-	2.58	-	81.0
Efficiency	4.42	0.8	0.29	1.58	1.5	-	-	-	57.0	77.0
All Combined	4.53	0.8	0.16	1.58	1.5	4	6	2.58	57.0	79.0

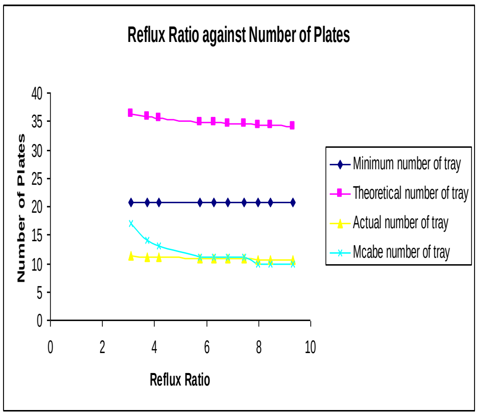


Figure 2: Effect of Reflux Ratio on distillation column height

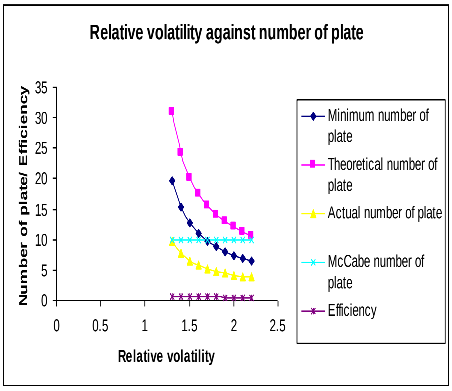


Figure 3: Effect of Relative Volatility on number of plates

A partubation plot also revealed that the optimum values for parameters are close to the centre points. It also showed that R_{coeff} and RV are the two most important variables affecting our desire (Optimization), while Reflux ratio had the least influence (Figure 4).

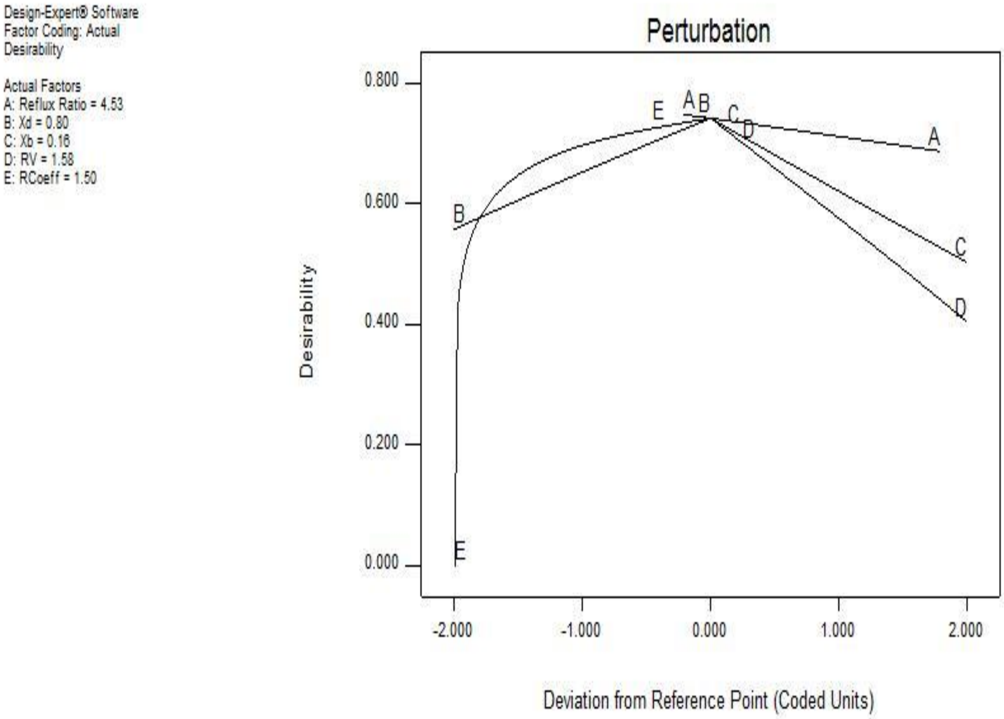


Figure 4: Interactive effects Desirability and deviation from reference point on perturbation

IV. CONCLUSION

The behaviour of thermodynamic properties of ethanol-water system during the distillation process was studied and the parameters that will give the best grade of ethanol with minimal impurities were optimized for effective design of distillation column. The process simulation results show that the reflux ratio, relative volatility increases with increase in temperature at constant pressure and have significant effect on purification of ethanol compared to other parameters.

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