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## Computer Aided Investigation of the Effect Changes in Some Parameters on Unsteady State Binary Distillation (Ethanol-Water System)

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**Abstract** The detailed dynamic modelling, and simulation of a continuous binary distillation column is presented. The dynamic behavior was also represented in mathematical form. Given the model equations, MATLAB codes were written for the dynamic simulation of the column. The model considers a mixture of two (2) components (ethanol and water) separated in a 14 trays column. The effects of changes in relative volatility, feed concentration and reflux ratio on the column were monitored with MATLAB. When the relative volatility was decreased by 40% the product purity were badly affected with concentration value of about  $0.7\text{mol/dm}^3$  and the bottom product increased to about  $0.3\text{mol/dm}^3$ . Upon examining the effect of change in reflux ratio on the system. It shows that change in reflux ratio affect the rectifying section more than the stripping section of the column. The decrease in reflux reduces the purity of the top product with little or no effect on the bottom.

**Keywords** MATLAB, Feed Concentration, Reflux ratio, Relative Volatility

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### Introduction

While the use of distillation dates back in recorded history to about 50 B.C., the first truly industrial exploitation of this separation process did not occur until the 12<sup>th</sup> century when it was used in the production of alcoholic beverages. By the 16<sup>th</sup> century, distillation also was being used in the manufacture of vinegar, perfumes, oils and other products. As recently as two hundred years ago, distillation stills were small, of the batch type, and usually operated with little or no reflux. With experience, however, came new developments. Tray columns appeared on the scene in the 1820s along with feed preheating and the use of internal reflux. By the latter part of that century, considerable progress had been made. Germany's Hausbrand and France's Sorel developed mathematical relations that turned distillation from an art into a well-defined technology [1].

Today, distillation is a widely used operation in the petroleum, chemical, petrochemical, beverage and pharmaceutical industries. It is important not only for the development of new products, but also for the recovery and reuse of volatile liquids. For example, pharmaceutical manufacturers use large quantities of solvents, most of which can be recovered by distillation with substantial savings in cost and pollution reduction. While distillation is one of the most important unit operations, it is also one of the most energy intensive operations. It is easily the largest consumer of energy in petroleum and petrochemical processing, and so, must be approached with conservation in mind. Distillation is a specialized technology, and the correct design of equipment is not always a simple task [2].

Distillation, sometimes referred to as fractionation or rectification, is a process for the separating of two or more liquids. The process utilizes the difference of the vapor pressures to produce the separation. Distillation is one of the oldest unit operations. While the first technical publication was developed in 1597, distillation already had been practiced for many centuries — specifically, for the concentration of ethyl alcohol for beverages. Today,



distillation is one of the most used unit operations and is the largest consumer of energy in the process industries.

When a mixture of two or more liquids is heated and boiled, the vapor has a different composition than the liquid. For example, if a 10% mixture of ethanol in water is boiled, the vapor will contain over 50% ethanol. The vapor can be condensed and boiled again, which will result in an even higher concentration of ethanol. Distillation operates on this principle. Clearly, repeated boiling and condensing is a clumsy process, however, this can be done as a continuous process in a distillation column. In the column, rising vapors will strip out the more volatile component, which will be gradually concentrated as the vapor climbs up the column [3].

Distillation is the most common class of separation processes and one of the better understood unit operations. It is an energy-separating-agent equilibrium process that uses the difference in relative volatility, or differences in boiling points, of the components to be separated. It is the most widely used method of separation in the process industries [4]. The distillation process will most often be the choice of separation unless the following conditions exist:

- Thermal damage can occur to the product.
- A separation factor is too close to unity.
- Extreme conditions of temperature or pressure are needed.
- Economic value of products is low relative to energy costs.

According to Lanny, [5] control involves the manipulation of the material and energy balances in the distillation equipment to affect product composition and purity. Difficulties arise because of the multitude of potential variable interactions and disturbances that can exist in single column fractionators and in the process that the column is a part of. Even seemingly identical columns will exhibit great diversity of operation in the field.

In distillation (fractionation), a feed mixture of two or more components is separated into two or more products, including, and often limited to, an overhead distillate and a bottoms, whose compositions differ from that of the feed. Most often, the feed is a liquid or a vapour-liquid mixture. The bottoms product is almost always a liquid, but the distillate may be a liquid or a vapour or both.

### Statement of Problem

Recently much knowledge has been developed concerning the new trends in engineering education and practice; the most important of them is computer development. The increasing power and speed of computers allow the calculation of complex variable problems. In chemical engineering for example the need for simulation cannot be overemphasized especially in the areas of molecular simulation, microscopic simulations of fluid flow, heat transfer, mass transfer, kinetics, thermodynamics, molecular dynamics, neural networks, dynamics modeling, and others. In this way, commercial simulators are becoming very important in both the academic and professional environments. Simulation helps the students and engineer to develop the skills of analysis, synthesis and evaluation that are very important to the engineers. Simulation in design projects brings sense of reality and design engineering becomes more active and interested.

Each of these commercial simulators in chemical Engineering has their capabilities and limitations even though they are proven to be good. It is therefore necessary to study the effect of some important parameters with the aid of proven software like MATLAB for the purpose of knowledge and see it affect distillation in a binary system.

### Materials and Method

#### Materials

##### *Matlab*

The dynamic modeling of the liquid composition as a function of time for selected stages such as Condenser, Rectifying trays, Feed tray, Stripping trays, and the Reboiler will be studied.

For light components, the change in the liquid composition with time is given. We will derive one model only for this situation and which will include variable hold-ups. The column which we shall consider will be of simple top and bottom product, feed type.



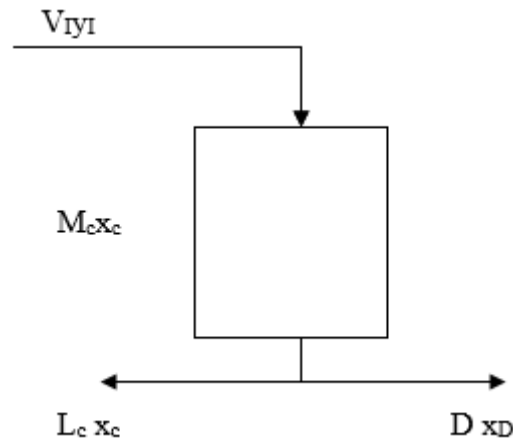


Figure 1: Material Balance around the Condenser

Consideration of the condenser system shows that the governing equations derived from balances are:

Overall Material Balance

$$\frac{dM_c}{dt} = V_I - L_R - D \tag{2.1}$$

MVC material Balance

$$\frac{d(M_c x_c)}{dt} = V_I y_I - L_R x_C - D x_D \tag{2.2}$$

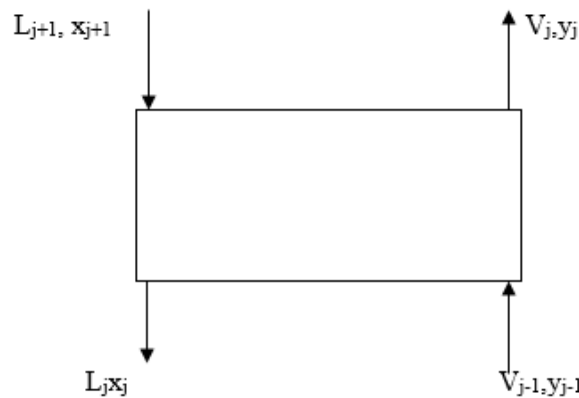


Figure 2: Material Balance around the Rectifying Sections

Overall MB

$$\frac{dM_j}{dt} = V_{j-1} - V_j + L_{j+1} - L_j \tag{2.3}$$

MVC material Balance

$$\frac{d(M_j x_j)}{dt} = V_{j-1} y_{j+1} - V_j y_j + L_{j+1} x_{j+1} - L_j x_j \tag{2.4}$$

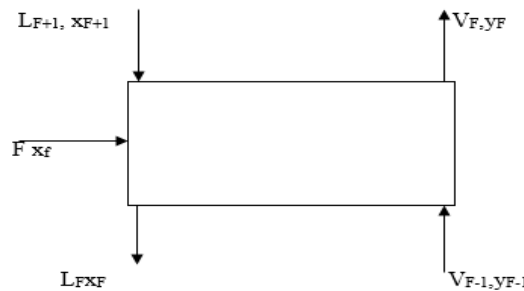


Figure 3: Material Balance around the Around Feed Plate

Overall Material Balance

$$\frac{dM_F}{dt} = V_{F-1} - V_F + L_{F+1} - L_F + F \quad (2.5)$$

MVC material Balance

$$\frac{d(M_F x_F)}{dt} = V_{F-1} y_{F-1} - V_F y_F + L_{F+1} x_{F+1} - L_F x_F + F x_F \quad (2.6)$$

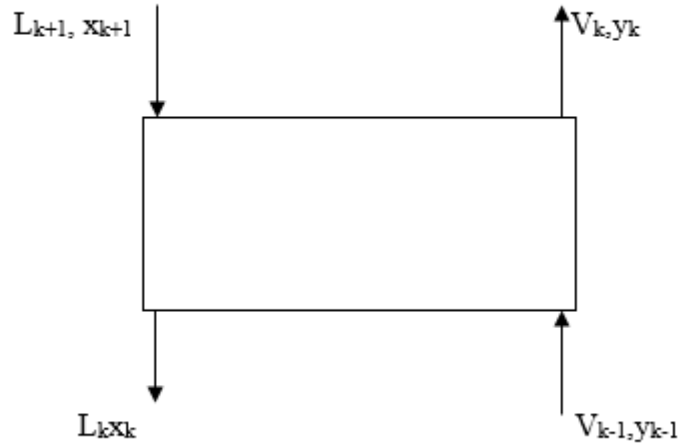


Figure 4: Material Balance around the Stripping Sections

Overall Material Balance

$$\frac{dM_k}{dt} = V_{k-1} - V_k + L_{k+1} - L_k \quad (2.7)$$

MVC material Balance

$$\frac{d(M_k x_k)}{dt} = V_{k-1} y_{k-1} - V_k y_k + L_{k+1} x_{k+1} - L_k x_k \quad (2.8)$$

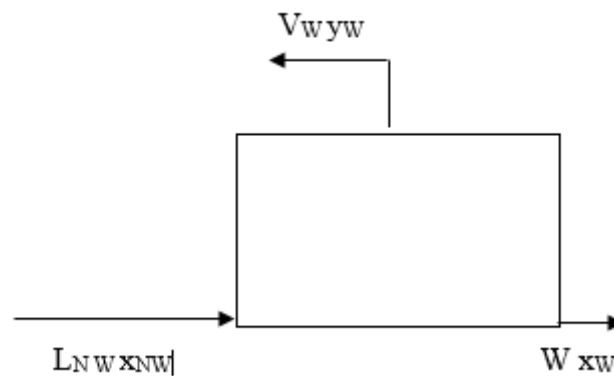


Figure 5: Material Balance around the Reboiler

Overall Material Balance

$$\frac{dM_W}{dt} = L_N - V_w - W \quad (2.9)$$

MVC material Balance

$$\frac{d(M_W x_W)}{dt} = L_{NW} x_{NW} - V_w y_w - W x_w \quad (2.10)$$

### Application of the Developed Model

A continuous distillation column is to be designed to separate 3.78 kg/s of a mixture of ethanol and water containing 60 mol% of ethanol to be separated to give a product of 90 mol% of ethanol at the top and a bottom product of not more than 10 mol% of Ethanol. It is proposed to operate the unit with a reflux ratio of 3 kmol/kmol product. The reflux ratio of 3.0 kmol/kmol product.



**Table 1:** Feed Concentration [6]

x	0	0.38	0.6	0.8	0.9	1.0
y	0	0.2	0.4	0.6	0.8	1.0

(Source: Ikezue, E.N., 2012)

X –molfraction of ethanol in liquid

Y – mol fraction of ethanol in vapour

Matlab program was only written for the dynamics of the rectifying and stripping trays only and also to solve for the numbers of theoretical plates required for the separation.

## Results and Discussions

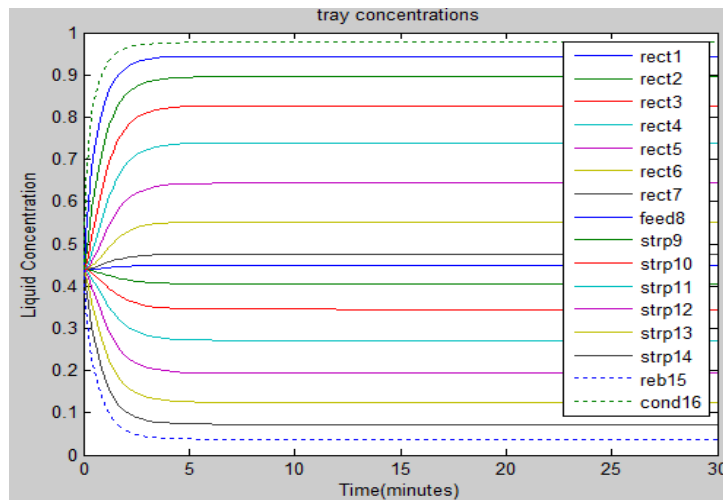


Figure 6: Tray Dynamics at Start up

The figure 6 shows the dynamics of the trays, reboiler and condenser at start up. It shows that it takes about five (5) minutes for the entire column to reach stability but the feed tray does not show much changes, it is relatively stable over the period of start up as the graph is approximately straight.

The effects of change in relative volatility on the separation process was monitored as shown in figures 7 and 8 below. When the relative volatility was decreased by 40% the product purity were badly affected with concentration value of about  $0.7\text{mol/dm}^3$  and the bottom product increased to about  $0.3\text{mol/dm}^3$ . The other effects of the reduction in relative volatility is that the entire tray concentration plot will be too close showing that the more trays would be needed for better separation.

Figure 8 shows the 40% increase in relative volatility, here the purity of the top product is very high with concentration value of approximately  $0.98\text{mol/dm}^3$  and low bottom product of  $0.02\text{mol/dm}^3$ . The figure 8 show a better separation compared to the figure 7.

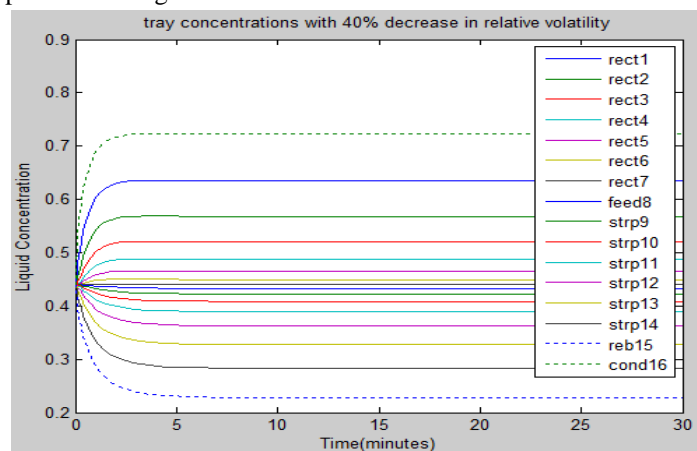


Figure 7: Tray Concentration with 40% decrease in relative volatility



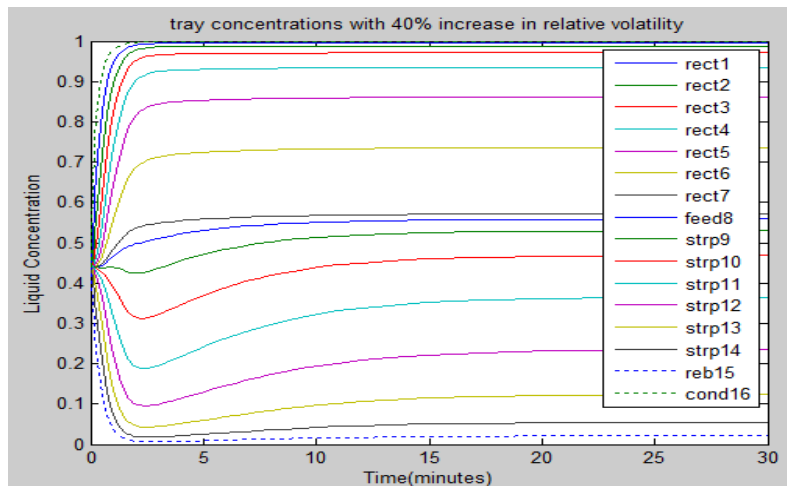


Figure 8: Tray Concentration with 40% increase in relative volatility

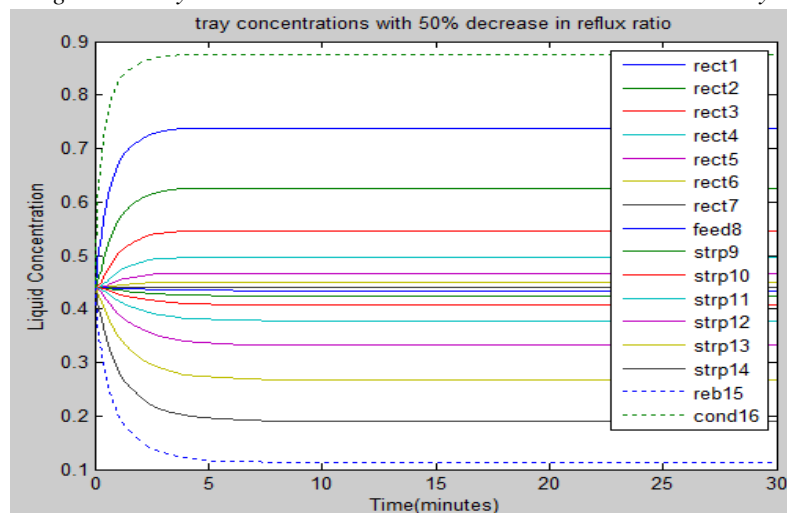


Figure 9: Tray Concentration with 50% decrease in reflux ratio

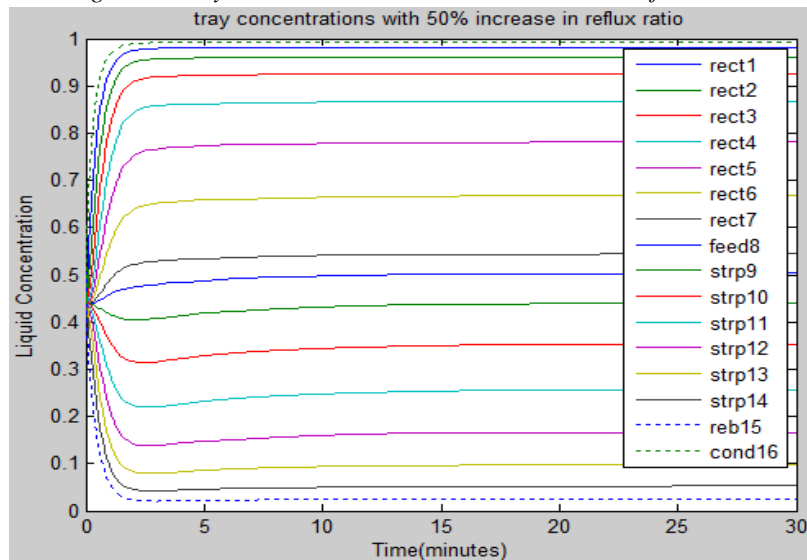


Figure 10: Tray Concentration with 50% increase in reflux ratio

Figure 9 and 10 examined the effect of change in reflux ratio on the system. It shows that change in reflux ratio affect the rectifying section more than the stripping section of the column. The decrease in reflux reduces the purity of the top product with little or no effect on the bottom.

Figure 10 show that the purity of the overhead product is enhanced and the bottom is also not affected by the increase in the reflux ratio.

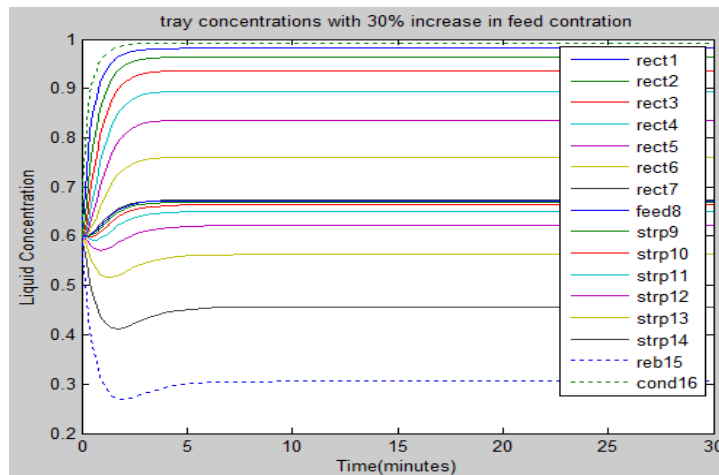


Figure 11: Tray Concentration with 30% increase in feed concentration

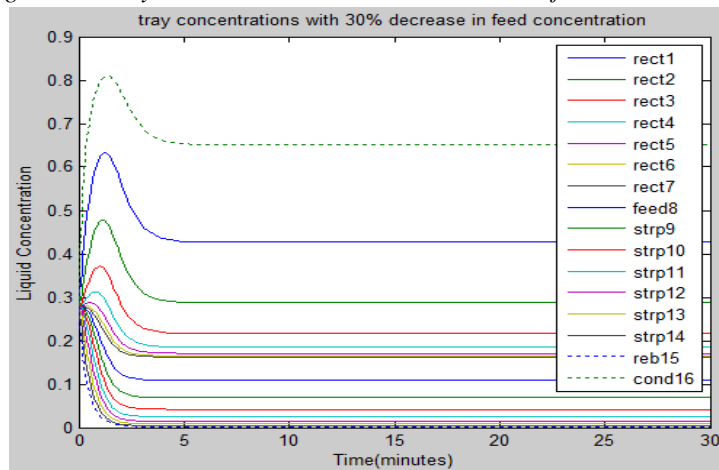


Figure 12: Tray Concentration with 30% decrease in feed concentration

From figure 11 above an increase in the feed concentration will enhance purity of the top product and more ethanol liquid at rectifying section of the column while less liquid will be found at the stripping section.

From figure 12, a decrease in feed concentration reduces the purity of the overhead product and more ethanol liquid will flow to the stripping section of the column.

## Conclusions

MATLAB program is written to simulate the unsteady state behavior of ethanol-water system with the given sets of models. The steady state occur after five (5) minutes and hence other dynamics such as the effects of changes in relative volatility, feed concentration and the effect of reflux ratio were monitored. When the relative volatility was decreased by 40% the product purity were badly affected with concentration value of about  $0.7\text{mol/dm}^3$  and the bottom product increased to about  $0.3\text{mol/dm}^3$ . The other effects of the reduction in relative volatility is that the entire tray concentration plot will be too close showing that the more trays would be needed for better separation. The 40% increase in relative volatility, here the purity of the top product is very high with concentration value of approximately  $0.98\text{mol/dm}^3$  and low bottom product of  $0.02\text{mol/dm}^3$ . Upon examining the effect of change in reflux ratio on the system. It show that change in reflux ratio affect the rectifying section more than the stripping section of the column. The decrease in reflux reduces the purity of the top product with little or no effect on the bottom. An increase in the feed concentration will enhance purity of the top product and more ethanol liquid at rectifying section of the column while less liquid will be found at the stripping section. While a decrease in feed concentration reduces the purity of the overhead product and more ethanol liquid will flow to the stripping section of the column.



**References**

- [1]. Gary, J. H., Handwerk, G. E. (2001). *Petroleum Refining Technology and Economics*, Marcel Dekker Inc., New York, 4th edition, pp. 1 – 66.
- [2]. Harry A. K. and Ross T., (2006). *The ChemSep Book*. Copyrightc 2006 by H.A. Kooijman and R. Taylor.
- [3]. Cardona C.A.A. and O.J. Sanchez T., (2005): Energy consumption analysis of integrated flowsheets for production of fuel ethanol from lignocellulosic biomass.
- [4]. Black C., (1980): *Distillation modeling of ethanol recovery and dehydration processes for ethanol and gasohol*.
- [5]. Lanny Robbins (2011). “*Distillation control And Tuning Fundamentals and strategies*” CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742
- [6]. Ikezue, E.N., (2012). “*Fundamentals of Mathematical Modeling and Analysis*” MIKON PRESS 102 Nike Road, Abakpa Nike, Enugu.

