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Comparative Analysis of the Simulation of Unsteady State Binary Distillation Column

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Abstract: The dynamic behavior was 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 12, 14 and 16 trays column. A comparison between ASPEN HYSYS and MATLAB simulated cases were made in terms of liquid distribution in the column and temperature profile of the column. The simulation shows the uneven distribution of the temperature across the distillation column with a difference of 15°C between the top and the bottom for MATLAB case and 14°C for HYSYS case, which is reasonably close to each other. The simulation show the dynamics at start up and the steady state and it was also used to find the best feed tray for the separation which is located to be the seventh tray, with the concentration of feed (0.44mol/dm^3), the top product is at 0.9mol/dm^3 and bottom product is about 0.1mol/dm^3. Further investigation shows that ASPEN HYSYS case cannot attain 94% ethanol purity probably due to its ability to form azeotrope while 98% purity of benzene is achieved with benzene-toluene mixture with the same software. Conclusively, it's advisable and more professional to use ASPEN HYSYS for the simulation of a binary solution which can form azeotrope at certain composition.
Keywords: MATLAB, ASPEN HYSYS, Azeotrope, Concentration, Temperature

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 12th century when it was used in the production of alcoholic beverages. By the 16th 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 a10% 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, [6], 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 compare them in some area of application to ascertain which is more accurate in that specific application to enhance our knowledge. These necessitate the research work to compare the analysis of the unsteady state distillation column of a binary system. In this work the two proven commercial software used are MATLAB and ASPEN HYSYS. Let me state it categorically that it is not meant to condemn one software for the other but to study their relative capabilities.

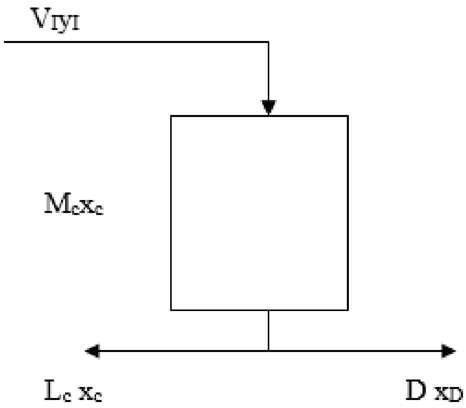
MATERIALS AND METHOD

Materials

- Aspen hysys software
- Mat lab

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.



Fig–1: Material Balance around the Condenser

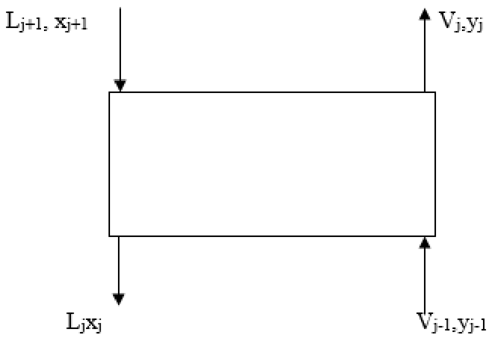
Consideration of the condenser system shows that the governing equations derived from balances are:

Overall Material Balance

$$\frac{dM_c}{dt} = V_I - L_c - D \qquad (2.1)$$

MVC material Balance

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



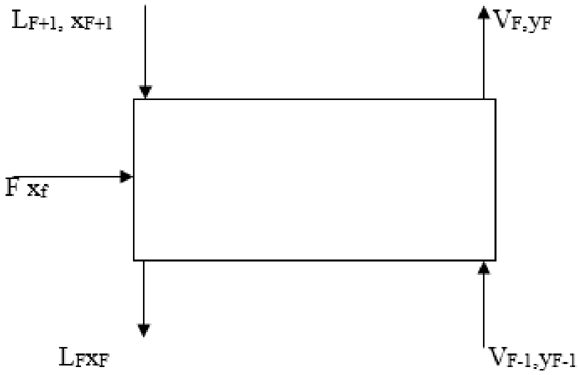
Fig–2: Material Balance around the Rectifying Sections

Overall MB

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

MVC material Balance

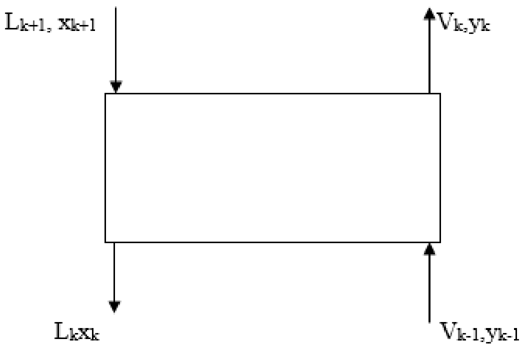
$$\frac{d(M_j x_j)}{dt} = V_{j-1}\ y_{j+1} - V_j y_j + L_{j+1}\ x_{j+1} - L_j x_j \qquad (2.4)$$



Fig–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

Fig–4: Material Balance around the Stripping Sections

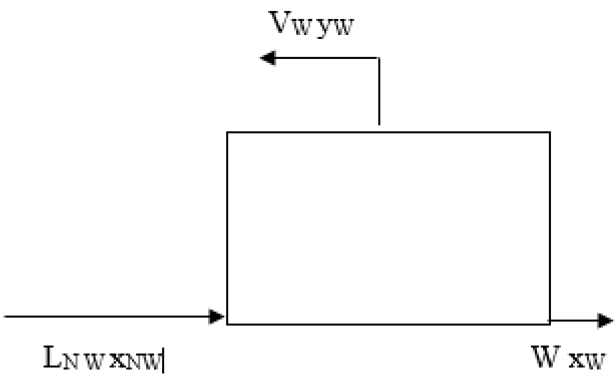
$$\frac{d(M_F x_F)}{dt} = V_{F-1}\, y_{F-1} - V_F y_F + L_{F+1}\, x_{F+1} - L_F x_F + F x_f \quad (2.6)$$

Overall Material Balance

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

MVC material Balance

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



Fig–5: Material Balance around the Reboiler

Overall Material Balance

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

MVC material Balance

$$\frac{d(M_W x_W)}{dt} = L_{N\,W}\, x_{NW} - V_W\, y_W - W\, x_W \quad (2.10)$$

APPLICATION OF THE DEVELOPED MODEL

A continuous distillation column is to be designed to separate 3.78kg/s of a mixture of ethanol and water containing 60mol% 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 10mol% of Ethanol. It is proposed to operate the unit with a reflux ratio of 3kmol/kmol product. The reflux ratio of 3.0kmol/kmol product.

Table-1: Feed Concentration

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: [5]

X –molfraction of ethanol in liquid

Y – mol fraction of ethanol in vapour

Matlab program will only be 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

Given the model equations, Matlab codes were written for the simulation of the column. The codes also show the values of the parameters used for simulation. The calculation of the number of plates required for the given separation was done with the aid of the software. The simulations were performed to obtain 14 trays and the feed is introduced at the 7th tray. The figure 6 below shows the ethanol distribution on the plate at any point in time.

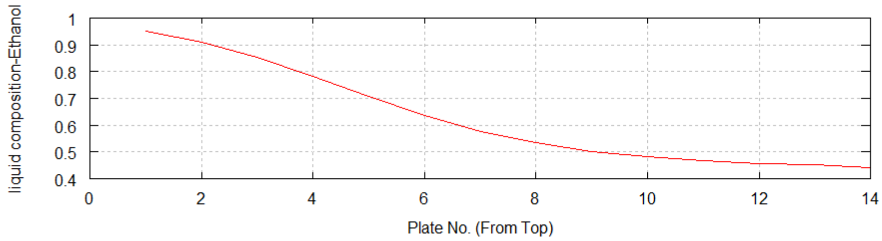


Fig-6: Liquid Composition of the ethanol against plate from HYSYS case

The figure 6 above shows that the liquid compositions at the top plates have higher concentration of ethanol than those at the bottom plates which represent the behavior of the system to some extent. Logically one would expect much liquid in the base of the distillation column but with low ethanol concentration. The figure also shows uneven distribution of liquid across the column.

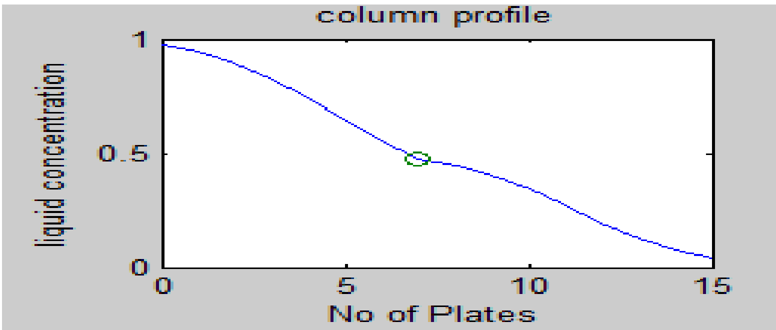


Fig-7: MATLAB Column Profile showing Liquid composition and feed position

The simulation can also be used to find a better feed plate for the distillation as shown by the column profile figure 7, the feed plate is best at plate number seven (7). The concentration of feed is 0.44mol/dm^3, the top product is at 0.9mol/dm^3 and bottom product is about 0.1mol/dm^3.

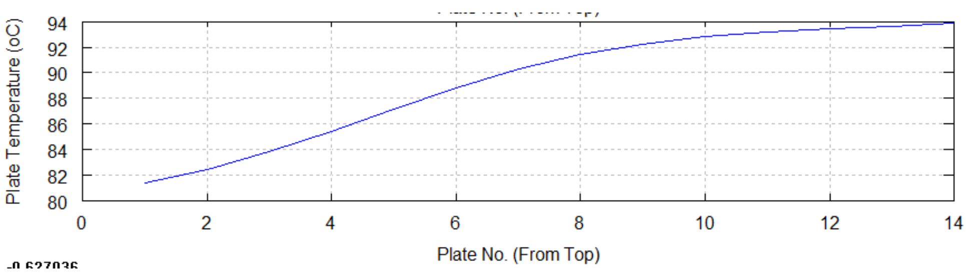


Fig-8: Temperature Profile across the Column from HYSYS

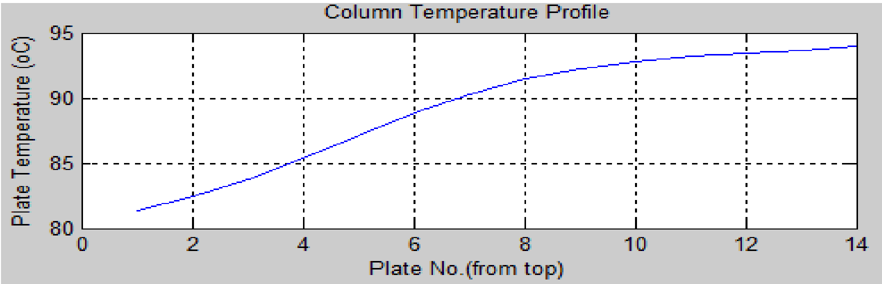


Fig-9: Temperature Profile across the Column from Matlab

The plots (figure 8 and 9) show the uneven distribution of the temperature across the distillation column with a difference of 15°C between the top and the bottom for MATLAB case and 14°C for HYSYS case.

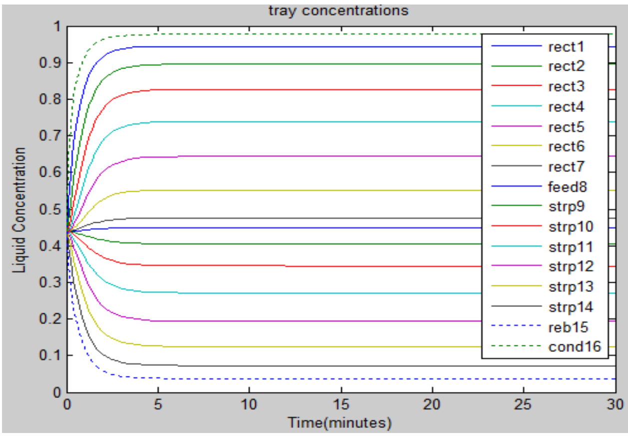


Fig-10: Tray Dynamics at Start up

The figure 10, show 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 many changes, it is relatively stable over the period of start up as the graph is approximately straight.

Table-2: MATLAB Result for Ethanol-Water

No of Plates	Bottom B (kmol/hr)	Bottom liquid Xb (mol/dm^3)	Dist. D (kmol/hr)	Dist. Comp. Xd (mol/dm^3)
12	99.25	0.35	20.75	0.88
14	98.65	0.34	21.35	0.9
16	96.25	0.31	23.75	0.98

Table-3: ASPEN HYSYS Result for Ethanol-Water

No of Plates	Bottom B (kmol/hr)	Bottom liquid copmXb (mol/dm^3)	Dist. D (kmol/hr)	Dist. Comp. Xd (mol/dm^3)
12	99.25	0.001314	20.75	0.9320
14	98.65	0.000305	21.35	0.9330
16	96.25	0.000147	23.75	0.9332
23	96.25	0.000145	23.75	0.9333

Table-4: MATLAB Result for Benzene-Toluene

No of Plates	Bottom B (kg/hr)	Bottom liquid Xb (mol/dm^3)	Dist. D (kmol/hr)	Dist. Comp. Xd (mol/dm^3)
12	82930	0.000543	20.75	0.93338
14	82940	0.000017	21.35	0.93334

16	82950	0.000003	23.75	0.93334

Table−5: ASPEN HYSYS Result for Benzene - Toluene

No of Plates	Bottom B (kg/hr)	Bottom liquid copmXb (mol/dm^3)	Dist. D (kg/hr)	Dist. Comp. Xd (mol/dm^3)
18	82930	0.00006	213400	0.9838
20	82950	0.00014	213400	0.9854
23	82970	0.00000	213400	0.9878

Further investigation shows that ASPEN HYSYS case never go up to 94% ethanol purity probably due its ability to form azeotrope as shown in table 2 to 5 above. Ethanol and water form an azeotrope, or constant boiling solution, of about 95 percent alcohol and five percent water. The five percent water cannot be separated by conventional distillation. This mixture is called hydrous ethanol and can be used as a fuel alone, but unlike anhydrous ethanol, hydrous ethanol is not miscible in all ratios with gasoline, so the water fraction is typically removed in further treatment in order to burn in combination with gasoline in gasoline engines.

But with MATLAB 98% concentration of ethanol can be achieved. The reason for this is not far fetch as MATLAB only run on well written codes while ASPEN HYSYS is specifically design for process simulation with different highly specialized packages that suite different process works.

For this reason it's advisable and more professional to use ASPEN HYSYS for the simulation of a binary solution which can form azeotrope at certain composition. With benzene – toluene mixture ASPEN HYSYS can achieve 95% purity or even purer as shown in table 3.40 above.

CONCLUSION

In this work, ASPEN HYSYS simulator is used and MATLAB program is written to simulate the unsteady state behavior of ethanol-water system with the given sets of models. The steady state occurs after five (5) minutes. Investigation shows that ASPEN HYSYS case cannot attain 94% ethanol purity probably due its ability to form azeotrope. Ethanol and water form an azeotrope, or constant boiling solution, of about 95 percent alcohol and five percent water. The five percent water cannot be separated by conventional distillation. But with MATLAB 98% concentration of ethanol can be achieved. The reason for this is not far fetch as MATLAB only run on well written codes while ASPEN HYSYS is specifically design for process simulation with different highly specialized packages that suite different process works. For this reason it's advisable and more professional to use ASPEN HYSYS for the simulation of a binary solution which can form azeotrope at certain composition. A comparison between ASPEN HYSYS and MATLAB simulated cases were made in terms of liquid distribution in the column and temperature profile of the column. The simulations show the uneven distribution of the temperature across the distillation column with a difference of 14^{o}C between the top and the bottom for MATLAB case and 15^{o}C for HYSYS case, which is reasonably close to each other.

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