Simulation of Distillation Column using DWSIM and ASPEN Plus: A Comparative Study

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***Abstract*- In the present study, a distillation process to separate methanol water was simulated. The work employed NRTL activity coefficients model to describe vapor liquid equilibrium of methanol – water system. The main extractive column took mixture of methanol and water as feed and separated methanol as distillate and water as bottoms product. The simulations were performed on DWSIM and ASPEN Plus version 8.6, thus, this is a comparative study with the prime focus to gain an insight of the obstacles faced in simulations carried out on an open source software. The initial work consisted of simulation of the process using shortcut method, so as to obtain basic sizing of the columns based on the purity required and to obtain data to study variation of reflux ratio with number of stages and thus, to finalize actual number of stages required and reflux ratio for rigorous model. Further, rigorous models were employed so as to get more accurate results using the values obtained earlier. A distillate of substantially pure methanol stream with minimal water was obtained using the above model. Finally, variation of composition of methanol and water with the stages of distillation column were plotted and also, T-x-y and P-x-y plots were generated.**

***Keywords*—Distillation, Aspen Plus, DWSIM, Methanol, Water**

I. INTRODUCTION

Distillation is a process to separate a mixture of two or more components into high purity products based on the difference in their boiling points. It consists of boiling the mixture followed by rapid condensation of the pure vapors. Distillation dates back to 1200 BC where it was used in perfumery operations [1]. Generally, in a distillation column, the distillate is vapor or liquid or both, while, the bottoms product is liquid. Modern distillation units employed stages or trays thus, helping the industry to achieve far greater purity than traditional distillation setups. Moreover, the refining industry has utilized the staged distillation columns extensively, thus, being able to deliver fuels of higher purity and in turn enhancing the recovery of lighter fractions to a much greater extent than it could have been possible with earlier distillation setups.

Distillation is an energy-intensive process and possess the capability to escalate and destroy the refinery's or distillery's profits. Plus, capital involved in setting up new columns and its operating costs can be manipulated to a great extent by the designer, designing the distillation column. With simulation of processes like distillation, designing, optimization and cost estimation of such processes has eliminated the human chances of human error and further, helped industries conserve capital and energy costs.

Distillation differs from absorption and stripping in that the second fluid phase is usually created by thermal means rather than by the introduction of a second phase that may contain an additional component or components not present in the feed mixture [2]. Methanol and water as a mixture can be effectively separated employing staged distillation. The study consisted on simulation of distillation column, but, in turn focused on the various pros and cons of open source softwares like DWSIM in comparison to paid packages like ASPEN Plus.

II. METHODOLOGY

The study initiated with an extensive literature review. Further, the methanol and water distillation was studied in two parts on both the softwares.

A. Shortcut Column or DSTWU

The shortcut column in DWSIM and DSTWU in ASPEN plus, both are shortcut methods to predict the values of variables like - minimum reflux ratio, actual reflux ratio, minimum number of stages, number of actual stages, feed stage position and distillate rate using Winn–Underwood-Gilliland method, which were useful in simulation of rigorous models to get actual composition of the distillate and bottoms streams. The model operates on assumptions of constant molar overflow and constant relative volatility. Also, the feed to the column was saturated liquid. Further, a plot of reflux ratio v/s theoretical stages further proved the number of required stages and the reflux ratio required for the distillation column. The plot was used to determine a reflux ratio for which the number of stages do not go too high also the reflux ratio did not go too high because a excessively high number of trays would add exorbitantly to the capital cost and a high reflux ratio will although reduce the number of trays required but would make the operations more expensive. Thus, higher the reflux ration, more vapor liquid contact will occur, higher will be the purity of distillate, slower will be the distillate collection rate and thus, higher will be the operating costs. Finally, an optimal ground between the two options was required. The Fig. 1 below shows the shortcut column setup in DWSIM.

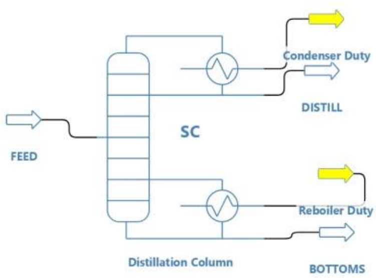

Fig. 1. Shortcut Column

B. Rigorous Model or RadFrac

Rigorous model is further employed to get more accurate results using the values obtained from the shortcut method. Post the simulation of the rigorous model, a plot depicting the composition variation of methanol and water in liquid phase with the number of stage was obtained. Rigorous models like RadFrac differentially simulate column of trays. Also, T-x-y and P-x-y plots for the methanol water distillation system were obtained. Fig. 2 below shows the DWSIM diagram for the rigorous model.

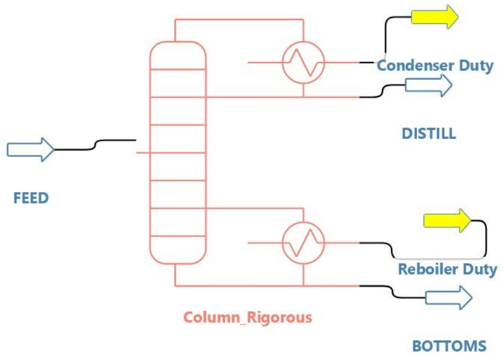

Fig. 2. Rigorous Model

III. SIMULATION AND RESULTS

The distillation column was simulated by two models: shortcut and rigorous.

A. Shortcut Column or DSTWU

The shortcut column gave the estimate parameters to apply in the rigorous model. The parameters are given in Table. 1.

TABLE 1
SHORTCUT METHOD ANALYSIS

Property	**Reading obtained from Shortcut Method**
Minimum reflux ratio:	0.749392379
Actual reflux ratio:	0.974210093
Minimum number of stages:	9.50606537
Number of actual stages:	19.2898529
Feed stage:	15.2252259
Number of actual stages above feed:	14.2252259
Reboiler heating required:	60946880 (Btu/hr)
Condenser cooling required:	60599229.6 (Btu/hr)
Distillate temperature:	148.203992 F
Bottom temperature:	209.859033 F
Distillate to feed fraction:	0.3966

From the parameters, the reflux ration of 0.75 was used for rigorous model. Also, the number of stages used was 20. Feed stage was taken as 15 and distillate rate was 2015.57 lbmol/hr.

The reflux ratio v/s theoretical stages plot was plotted and is shown in Fig. 3.

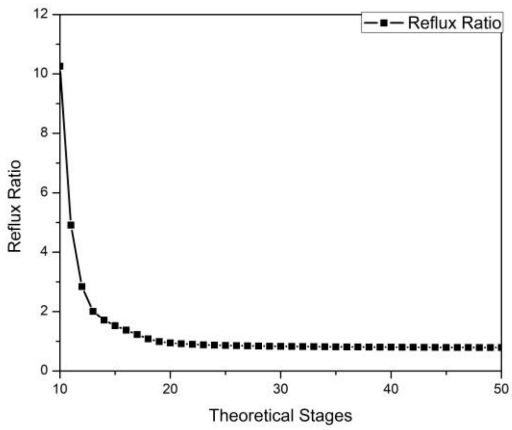

Fig. 3. Reflux ratio v/s Theoretical stages

From Fig. 3 it was concluded that the number of stages should be 20 since, at the number of stages to be 20, the column exhibits a reflux ratio which appears to be optimum and increasing the number of stages beyond 20 does not decrease the reflux ratio to a great extent, thus, the capital cost will not go extremely high and operations will also be economic, following the above model.

B. Rigorous Model or RadFrac

Using the data in Table. 1., the rigorous model was simulated. The simulations gave far more accurate results, than the shortcut method displayed.

A comparative study of the hourly molar flow rate of methanol and water in feed, distillate and bottoms calculated by shortcut and rigorous models is given in Table. 2.

TABLE 2
COMPARATIVE STUDY

	STREAM	**WATER**	**METHANOL**
Shortcut Model	FEED	3053.889	2035.926
	DISTILLATE	3.054	2015.567
	BOTTOMS	3050.835	20.359
Rigorous Model		**WATER**	**METHANOL**
	FEED	3053.889	2035.926
	DISTILLATE	90.37	1928.251
	BOTTOMS	2963.519	107.676

As it can be seen in Table. 2 employing the shortcut method the molar flow rate of water in distillate and methanol in bottoms is quite low and taking these values as a standard for a column to be built might lead to deviation in product by this column. Thus, rigorous analysis displays more accurate values that will be in great coherence with the actual output the column might give and thus, results of shortcut method should not be treated as final results.

Further, a plot of variation of composition of methanol and water in liquid phase with stage number was generated and is shown in Fig. 4.

This in turn helped to prove the validity of simulation results as the composition of methanol in liquid increased from bottoms i.e. stage 20 to the distillate i.e. stage 1 and the composition of water in liquid increased from stage 3 where it was zero to 0.95 at stage 20. It is also clear from this plot that, the higher methanol in liquid in the upper stages of the column is because of reflux which is extremely high in methanol composition and the high water composition in liquid on stage 20 may account for higher water content of the bottoms product.

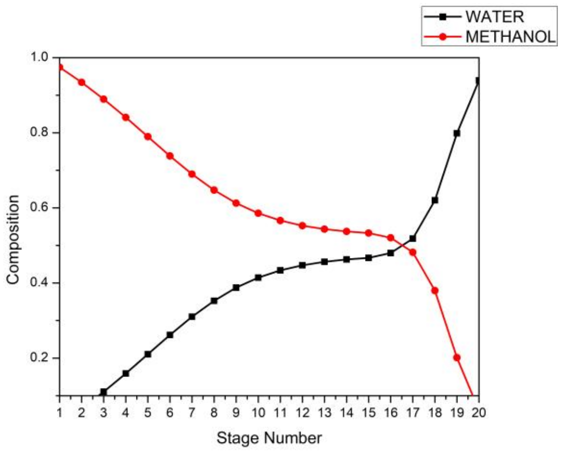

Fig. 4. Variation of composition of methanol and water in liquid phase v/s stage number

Further, Fig. 5 below shows T-x-y plot for ethanol/water. Here the pressure is constant. The bubble point and dew point at varied compositions can be found using Fig. 5.

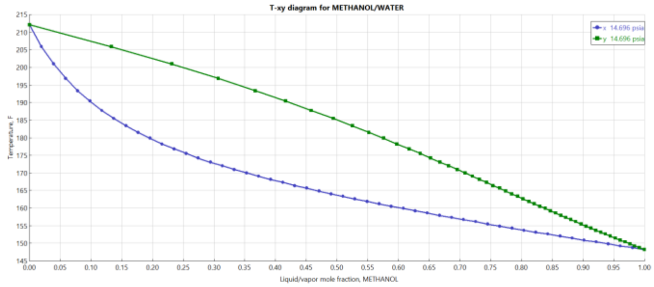

Fig. 5. T-x-y

Also, Fig. 6 shows the P-x-y plot for ethanol/water. Here the temperature is constant. The bubble point and dew point at varied compositions can be found using Fig. 6.

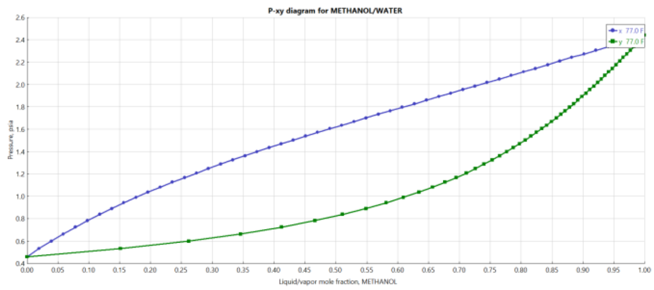

Fig. 6. P-x-y

C. *Differences in simulating using DWSIM and ASPEN Plus*

- Graphical interface –

  Graphical interface of ASPEN Plus is far more aesthetic and appealing than DWSIM's graphical interface.

- User interface –

  The user interface of ASPEN Plus is easy to be used and get used to. For instance, while connecting streams to distillation column in ASPEN Plus, one has to just click and drag the arrows indicating streams to the column, which seems to be quite easy, whereas, in DWSIM one has to specify the material or energy streams for the column by choosing each and every stream for the particular port on the column and thus, making connections.

- Restriction of Units

  In ASPEN Plus, if a user wants to use a unit for a quantity, which is not the default system of unit, using different units for different quantities within a single project is possible. Even, the results obtained can be viewed in various units available. On the contrary, in DWSIM if once a system of units is chosen by the user, the user cannot modify the units for a single quantity, either, he or she has to convert the quantity or change the unit of measurement for the whole project.

  Since, a project can consist of quantities in various units of measurement, the restrictions in DWSIM can create extra work for many users.

- Results

  Results can be better viewed and comprehended in ASPEN Plus, which shows it in tabular form, in comparison to DWSIM which shows the results in a pdf listed one after the other.

- Post result analysis

  ASPEN plus provides options for various analysis like binary analysis, reflux ratio with stages variation, composition with stages variation analysis, by default in its package while, DWSIM lacks such options.

- Lack of literature and Solved cases

  DWSIM being newer simulation software than ASPEN plus, lacks resources such as literature and video lectures.

- Lower application

  ASPEN Plus has been in market far longer than DWSIM and has thus, created a brand value. Industries prefer to implement a well-known and tested tool rather than a newer one. This problem further enhances as these industries tend to employ candidates proficient in software packages like ASPEN and thus, again adding to lower application of open-source softwares like DWSIM.

- Stability

  Open-source softwares like DWSIM tend to be less stable in operation in comparison to paid software packages like ASPEN Plus. For instance, a computer was running DWSIM V 5.2 update 1 and the user facing many stability issues, although, post an update these issues were resolved.

IV. Conclusion

From the present study, it was concluded that the number of trays for the distillation column should be 20 and reflux ratio should be 0.75. Plus, optimum location for feed was stage 15. Boiling point and dew point at various compositions could be found out using P-x-y and T-x-y plots. Finally, variation of composition of methanol and water in liquid with stage number was quantified by the plot. Lastly, it can be concluded that although DWSIM has limitations and flaws, but being a open-source software it is at par with paid packages like ASPEN Plus and at the staggering rate at which it is improving one day it might even DWSIM might even supersede paid software packages like ASPEN Plus.

Acknowledgment

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