

# Comparison of Determination of Theoretical Number of Stages Calculated Manually by MATLAB Software in Distillation Columns

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Publishing Date: October 22, 2016

## Abstract

In this study the numbers of theoretical stages for four systems in a sieve tray column were calculated manually by McCabe-Thiele method. The same were determined using MATLAB software developed by Gasmeelseed and Kamal. The number of the theoretical stages is important for the column design coupled with the overall stage efficiency to obtain the actual number of stages; this is combined with tray spacing to determine the height of the column. The method developed from MATLAB software superseded the difficult Mc-Thiel plot and make things much easier. It is recommended that to develop a full software program using MATLAB for complete design of the distillation column, in fact this work is in progress.

**Keywords:** Distillation Columns, MATLAB, Fractional Distillation.

## Introduction and Literature Review

Computer Aided Process Engineering is one sector in the field of Process Engineering defining all what is process related and computer assisted. It starts from the molecular modeling and passes through computation of physical or chemical properties, mathematical modeling and simulation, computer control, optimization and integrated process design. It is very applied engineering and nowadays the name is redundant because there is no physically existent process or product in elaboration which is not helped by computer if it is to be considered in the light of sustainable development or to be valued on the market<sup>[1]</sup>.

Distillation is a commonly used method for purifying liquids and separating mixtures of liquids into their individual components. Familiar examples include the distillation of crude fermentation broths into alcoholic spirits such fuel gasoline and heating oil. In the organic lab, distillation is used for purifying solvents and liquid

reaction products. To understand distillation, first consider what happens upon heating a liquid. At any temperature, some molecules of a liquid possess enough kinetic energy to escape into the vapor phase (evaporation) and some of the molecules in the vapor phase return to the liquid (Condensation) equilibrium are set up, with molecules going back and forth between liquid and vapor. At higher temperatures, more molecules possess enough kinetic energy to escape, which results in a greater number of molecules being present in the vapor phase.

The separation of liquid mixtures into their various components is one of the major operations in the process industries, and distillation, the most widely used method of achieving this end, is the key operation in any oil refinery. In processing, the demand for purer products, coupled with the need for greater efficiency, has promoted continued research into the techniques of distillation. In engineering terms, distillation columns have to be designed with a larger range in capacity than any other types of processing equipment, with single columns 0.3–10 m in diameter and 3–75 m in height. Designers are required to achieve the desired product quality at minimum cost and also to provide constant purity of product even though there may be variations in feed composition. A distillation unit should be considered together with its associated control system, and it is often operated in association with several other separate units. The vertical cylindrical column provides, in a compact form and with the minimum of ground requirements, a large number of separate stages of vaporization and condensation. The basic problems of design are considered and it may be seen that not only the physical and chemical properties, but also the fluid dynamics inside the unit, determine the number of stages required and the overall layout of the unit. The separation of benzene from a mixture

with toluene, for example, requires only a simple single unit as shown in Figure (1), and virtually pure products may be obtained. A more complex arrangement is shown in Figure (2) where the columns for the purification of crude styrene formed by the dehydrogenation of ethyl benzene are shown. It may be seen that, in this case, several columns are required and that it is necessary to recycle some of the streams to the reactor. In this study consideration is given to the theory of the process, methods of distillation and calculation of the number of stages required for both binary and multicomponent systems, discussion on design methods is included for plate and packed columns<sup>[2]</sup>.

**Distillation**, process involving the transfer of a liquid into vapor that is subsequently condensed back to liquid form. It is exemplified at its simplest when steam from a kettle becomes deposited as drops of distilled water on a cold surface. Distillation is used to separate liquids from

nonvolatile solids, as in the separation of alcoholic liquors from fermented materials, or in the separation of two or more liquids having different boiling points, as in the separation of gasoline, kerosene, and lubricating oil from crude oil. Other industrial applications include the processing of such chemical products as formaldehyde and phenol and the desalination of seawater<sup>[3]</sup>.

Distillation may be carried out by either of two principle methods. The first method is based on the production of a vapor by boiling the liquid mixture to be separated and condensing the vapors without allowing any liquid to return to the still. there is then no result. The second method is based on the return of part of condensate to the still under such conditions that this returning liquid is brought into intimate contact with the vapors on their way to the condenser. Either of these methods may be conducted as a continuous or as a batch process<sup>[4]</sup>.

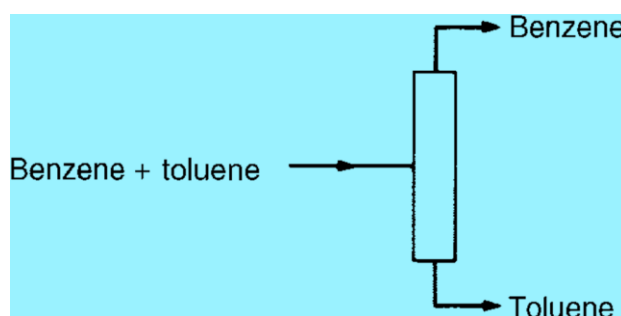


Figure 1: Separation of a binary mixture

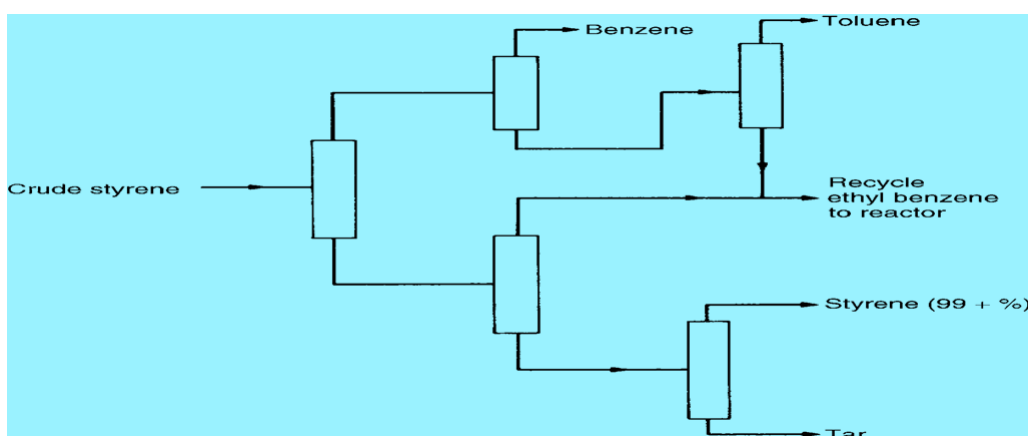


Figure 2: Multicomponent separation

A method called fractional distillation, or differential distillation, has been developed for certain applications, such as petroleum refining, because simple distillation is not efficient for separating liquids whose boiling points lie close to one another. In this operation the vapors from a distillation are repeatedly condensed and revaporized in an insulated vertical column especially important in this connection are the still heads, fractionating columns, and condensers that permit the return of some of the condensed vapor toward the still. The objective is to achieve the closest possible contact between rising vapor and descending liquid so as to allow only the most volatile material to proceed in the form of vapor to the receiver while returning the less volatile material as liquid toward the still. The purification of the more volatile component by contact between such countercurrent streams of vapor and liquid is referred to as rectification, or enrichment.

More than 80 years ago. McCabe and Thiele developed a creative graphical solution technique based on Lewis's assumption of constant mol over flow (CMO) for the rational design of distillation column. The McCabe- Thiele diagram enabled decades of effective design and operational

analysis of distillation column and has been used to teach several generations of chemical engineers to design and trouble shoot distillation and other cascaded processes<sup>[5]</sup>.

### Design Procedure and Feed Conditions

- ✚ Starting with VLE data and draw an equilibrium x-y diagram
  - ✚ Determination of the three operating lines and draw them on the x-y diagram
  - ✚ Using the rectifying operating line and the equilibrium curve draw steps from the distillate composition to the feed point
  - ✚ Counting the number of steps. Each one equals an equilibrium or theoretical stage
  - ✚ Using the stripping operating line and the equilibrium curve draw steps from the bottoms composition to the feed point
  - ✚ Adding the number of steps to the previous to give the total number of theoretical stages
  - ✚ Converting this to a number of actual plates by dividing by the plate efficiency.
- Design Illustrated

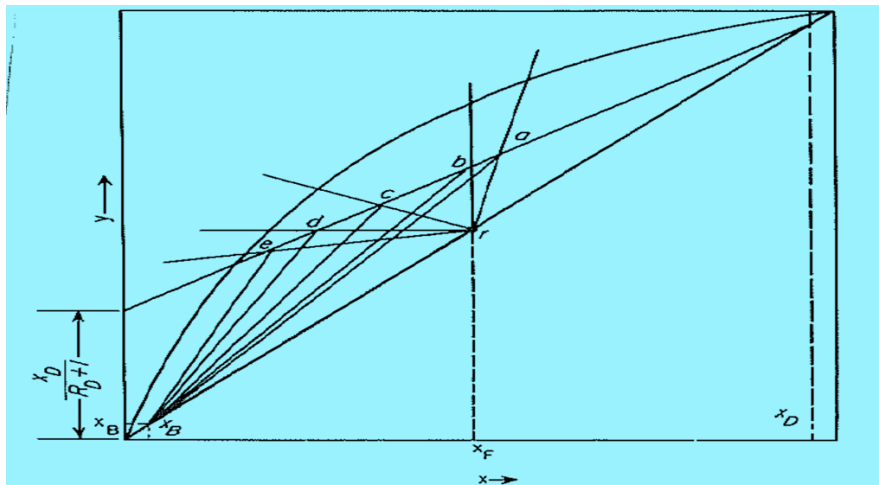


Figure 3: Effect of feed conditions on feed line, that is: ra, feed is cold liquid; rb, feed saturated liquid; rc, feed partially vaporized; rd, feed saturated vapor; re, feed superheated vapor<sup>[3]</sup>

### Tables, Figures and Method

Methodology of determination the number of the theoretical stages by using MATLAB<sup>[6]</sup>.

Open the MATLAB and do the following:

```
>> kml
```

type 1 and press enter for given relative volatility alpha ,R ,xD , xB , xf ,

type 2 and press enter for given relative volatility alpha , xD , xB , xf ,

type 3 and press enter for putting x,y mole fraction manually, xD , xB , xf ,

type 4 and press enter for putting x,y mole fraction manually, Reflux R,  $x_D$ ,  $x_B$ ,  $x_F$

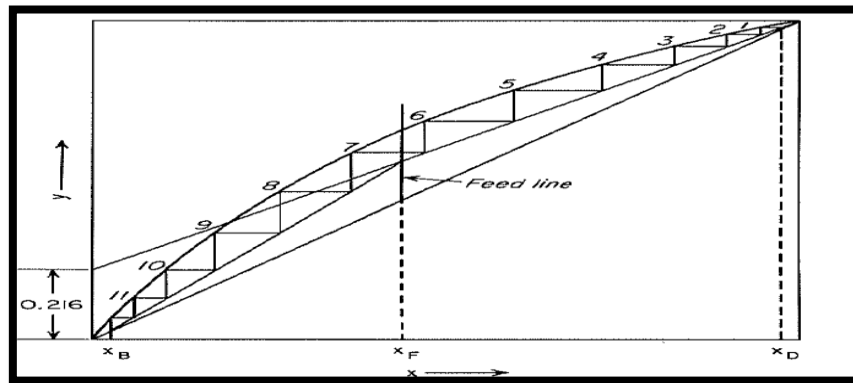
Remark: kml= a subroutine file in MATLAB software developed by<sup>[6]</sup>.

**Case study #1:** feed is at its boiling point, at  $q=1$ ,

### Manual calculation and Plotting is:

#### Data Required:

1. Equilibrium data or coloration of benzene-toluene
2.  $x_F=0.44$ ,  $x_D=0.974$ ,  $x_W=0.023$ ,
3.  $\alpha = 2.5$



**Figure 4: McCabe-Thiele diagram for distillation of benzene-toluene for case1 (manually)**

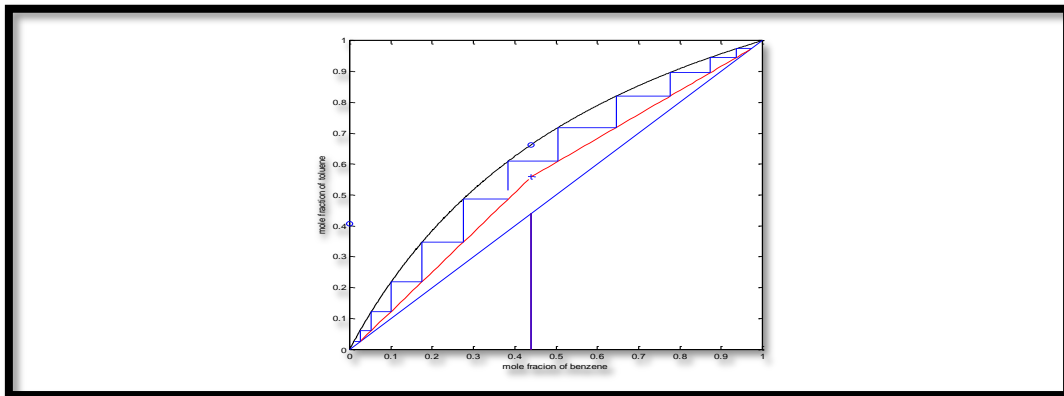
From figure (4) No of theoretical plate = 11

Feed plate location = 7

By using MATLAB software:

#### Data Required:

1.  $\alpha = 2.5$ ,
2.  $x_F=0.44$ ,  $x_D=0.974$ ,  $x_W=0.023$ ,
3.  $R = 3.5$



**Figure 5: McCabe-Thiele diagram for distillation of benzene-toluene for case1 (MATLAB)**

From figure (5) No of theoretical plate = 11

Feed plate location = 7

By using these techniques on the case 2,3 and 4 we the following results are obtained

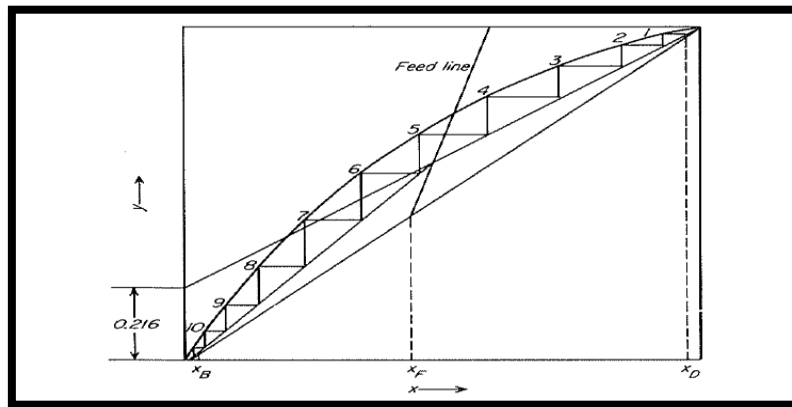


Figure 6: McCabe-Thiele diagram for distillation of benzene-toluene for case 2 (manually)

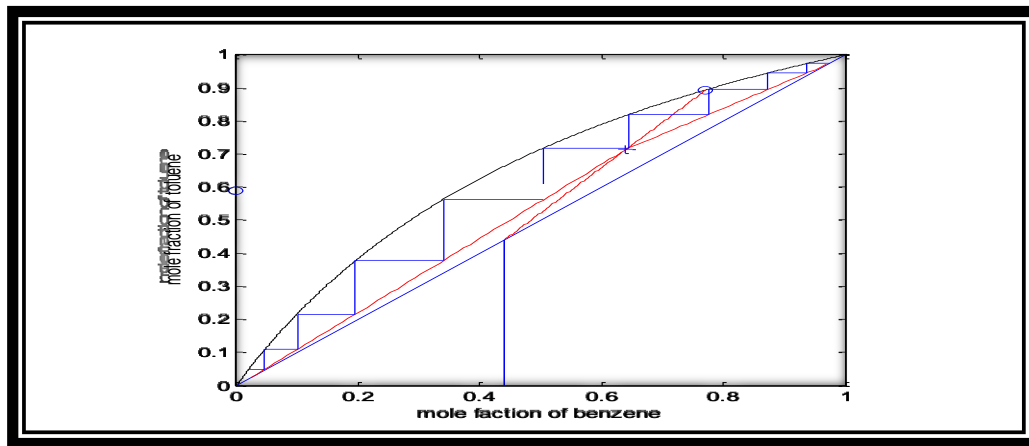


Figure 7: McCabe-Thiele diagram for distillation of benzene-toluene for case 2 (MATLAB)

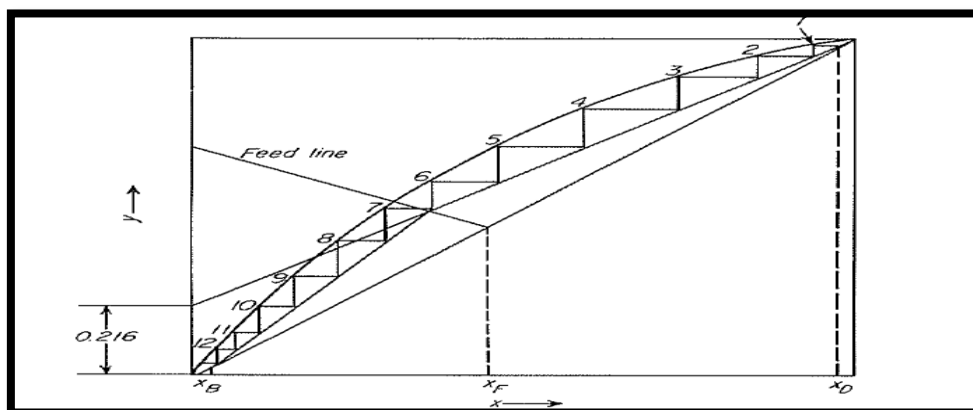


Figure 8: McCabe-Thiele diagram for distillation of benzene-toluene for case3 (manually)

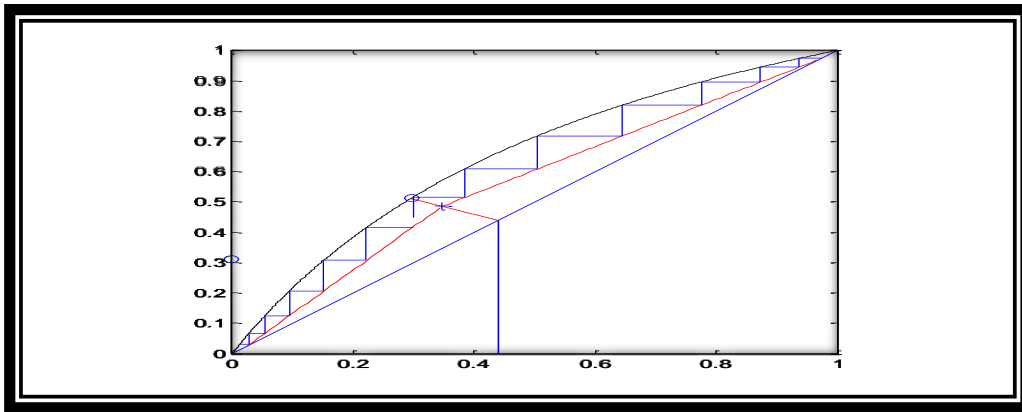


Figure 9: McCabe-Thiele diagram for distillation of benzene-toluene for case3 (MATLAB)

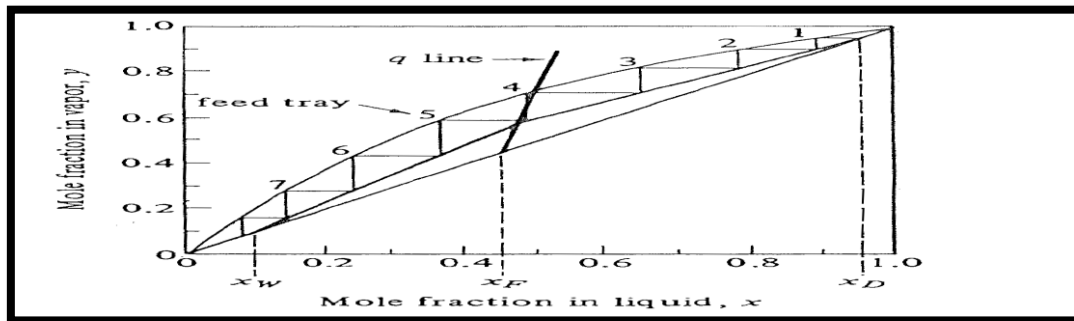


Figure 10: McCabe-Thiele diagram for distillation of benzene-toluene for case 4 (manually)

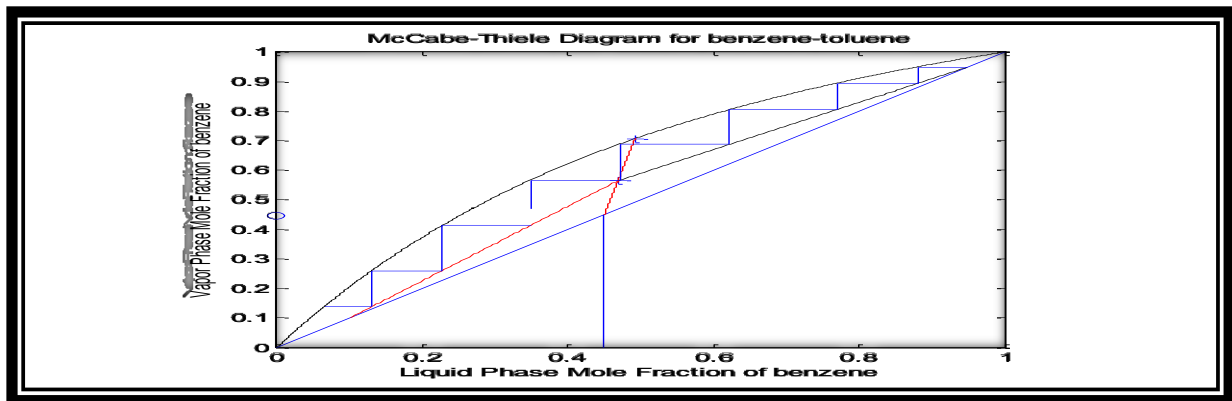


Figure 11: McCabe-Thiele diagram for distillation of benzene-toluene for case4 (MATLAB)

Table 1: Summary of the Results

Case No	q-line	No of theoretical stages		Feed location	
		manual	MATLAB	manual	MATLAB
1	1	11	11	7	6
2	3.7	10	10	5	5
3	-0.5	11	11	7	7
4	1.195	7	7	4	4

## Conclusions

From the results shown in figures (4, 5, 6, 7, 8, 9, 10 and 11) and table (1) it's proved that the manual methods of calculations and the MATLAB software results have shown very good agreement which is considered to be suitable for column design. It's recommended that this software (MATLAB) method has to be generalized for quick design data of a fractionation column. This study is concerned for design of a sieve tray column, but it can be applicable for bubble cap and valve tray columns. Further work has to be carried out for determination of the NTU, HTU and consequently the height of packed distillation column.

## Acknowledgement

The authors which to thank the graduated college of Karry university for giving us the opportunity and sport to complete this work for PhD in chemical engineering , the author also which to thank M.Kamal and Prof Gasmeelseed for allowing the application of their developed MATLAB software for computer calculation of the number of theoretical stages.

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