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# Numerical Procedure for Calculating Minimum Reflux Ratio in Distillation Columns

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**ABSTRACT:** Most design calculations in distillation columns involve a tediously large number of steps, thus computation in engineering becomes a key step in simplifying this process. At the same time the need for accurate design in engineering cannot be over emphasized, meaning that the safety of lives and property so much depend on the accuracy of design calculation, thus, the need for computer packages that will aid the design of distillation columns to avoid such errors. The objective of this work is to provide an alternative numerical method to calculate minimum reflux ratio in distillation columns, which is an alternative to the traditional way of using Underwood equations to evaluate this parameter. The Underwood method also has certain limitations which can be conveniently ignored while using this method. A model was built in excel to computationally prove the validity of the method; also, Visual Basic (VBA) tools were used during this process. The reflux ratio in particular is a key parameter in monitoring performance and controlling product quality in industrial columns. Thus, this article can better help in the design of distillation column as a whole.

**KEYWORDS:** Distillation Column, VBA, Reflux Ratio, Design, Model.

## I. INTRODUCTION

The below paper is an extension of the work done by McCabe WL, Thiele [1] for calculating the number of stages in distillation Column for a binary component mixture. The objective of this paper is to describe a procedure to calculate minimum reflux ratio numerically. A model has also successfully been developed to verify the validity of the procedure. VBA programming has also been used for numerical computation during model verification process. A flowchart has also been given for detailed understanding of the process.

## II. STEPS FOR CALCULATING MINIMUM REFLUX RATIO

Steps for Calculation after plotting McCabe–Thiele [1] diagram:

- Step 1  
Compute the slopes and intercepts of Minimum Reflux line and q line and write in the form  $ax+by+c=0$ , where  $-a/b$  is the slope and  $-c/b$  is the intercept.

- Step 2  
Find point of intersection of the lines by solving two equations simultaneously  $a_1x+b_1y+c_1=0$ , and  $a_2x+b_2y+c_2=0$ . The point  $(x, y)$  satisfies both the equations.

$$(x, y) = \left[ \frac{b_1c_2 - b_2c_1}{a_1b_2 - a_2b_1}, \frac{a_2c_1 - a_1c_2}{a_1b_2 - a_2b_1} \right]$$

- Step 3  
Tabulate Values of liquid mole fraction  $x$  with a selected step size starting from zero to one.



- Step 4  
Calculate the corresponding values of mole fraction of vapor's with VLE relationship or equilibrium data.

$$y = \frac{\alpha x}{1 - (1 - \alpha)x}$$

- Step 5  
Calculate the q line, y values corresponding to the x values calculated in step 1. From the q line equation.

$$y = \left( \frac{q}{q-1} \right) x - \left( \frac{z_f}{q-1} \right)$$

- Step 6  
Calculate the absolute difference of the q line and the equilibrium line y values.

$$|y_1 - y_2|$$

- Step 7  
Locate the minimum value of the absolute difference and locate the corresponding x value.  
The x and y values thus found are the point of intersection of the q line and the equilibrium line at minimum at reflux condition.

- Step 8  
Now we need to find the absolute difference of the y values calculated in step 7 and step 2 and find the absolute difference.

- Step 9  
This absolute value calculated in Step 8 is minimized by varying Rmin, which can be done using excel solver or goal seek by setting the absolute value to zero.

### III. FLOW CHART

The procedure for calculating Rmin and model verification involves a series of steps which is represented in a diagram format. The flowchart also describes McCabe–Thiele [1] method and further proceeds to describe the method of estimation of minimum Reflux Ratio.

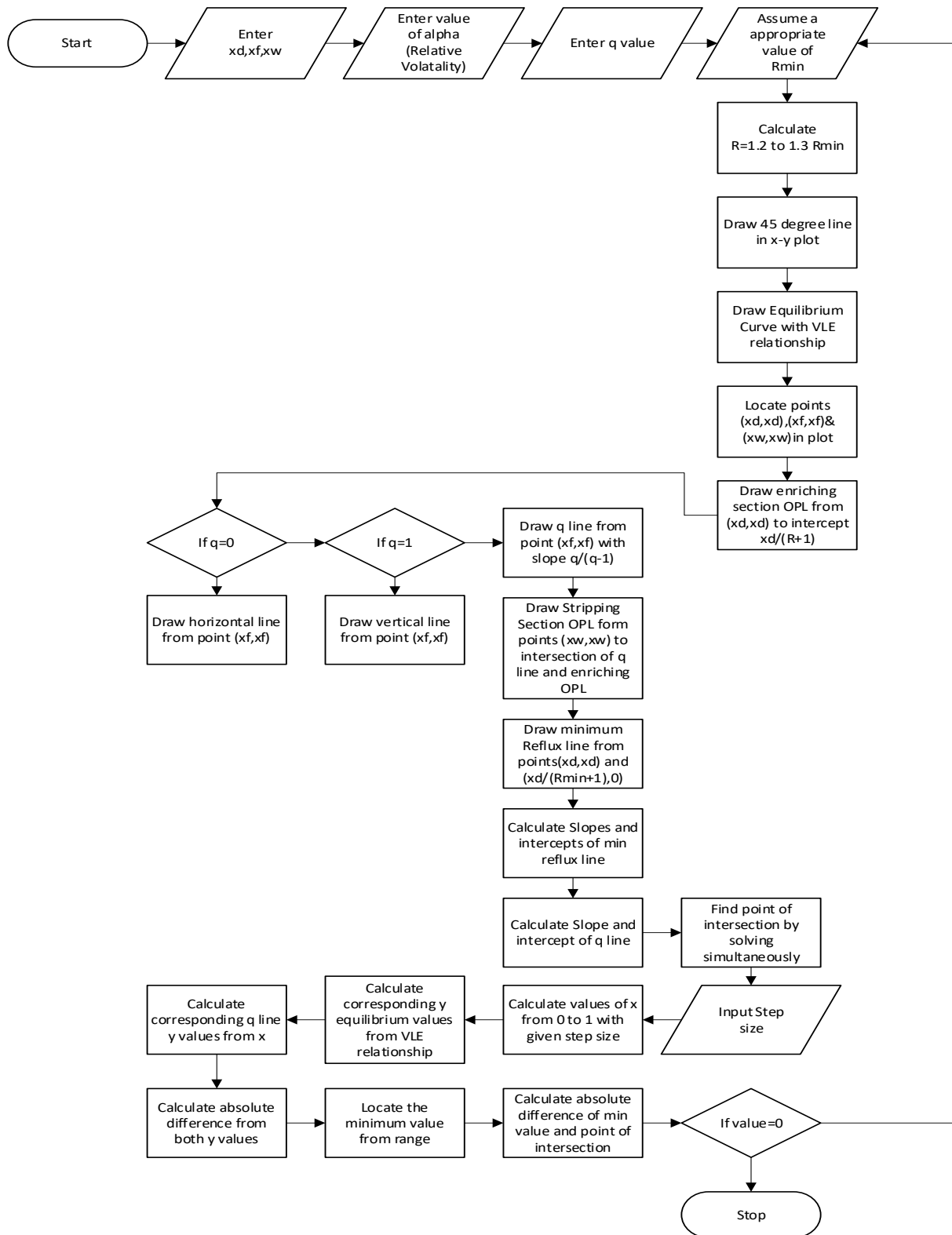


Figure1 Flowchart



IV. MODEL VERIFICATION

Model Initiation

45 line		$x_D$	0.99
x	y	$x_F$	0.45
0	0	$x_W$	0.01
1	1	$\alpha$	3
$y = \frac{\alpha x}{1 - (1 - \alpha)x}$		$R_{min}$	3
		R	3.75
Equilibrium relation		q	0.5
x	y	slope	-1
0	0	q-line	
0.1	0.25	x	y
0.2	0.428571429	0.45	0.45
0.3	0.5625	0.3	0.58
0.4	0.666666667	Top Section	
0.5	0.75	x	y
0.6	0.818181818	0.99	0.99
0.7	0.875	0	0.208421053
0.8	0.923076923	Bottom	
0.9	0.964285714	x	y
1	1	0.01	0.01
Min Reflux Line		0.386470588	0.513529412
x	y		
0.99	0.99		
0	0.2475		

Figure 2 Initiated Values  
Equilibrium Diagram

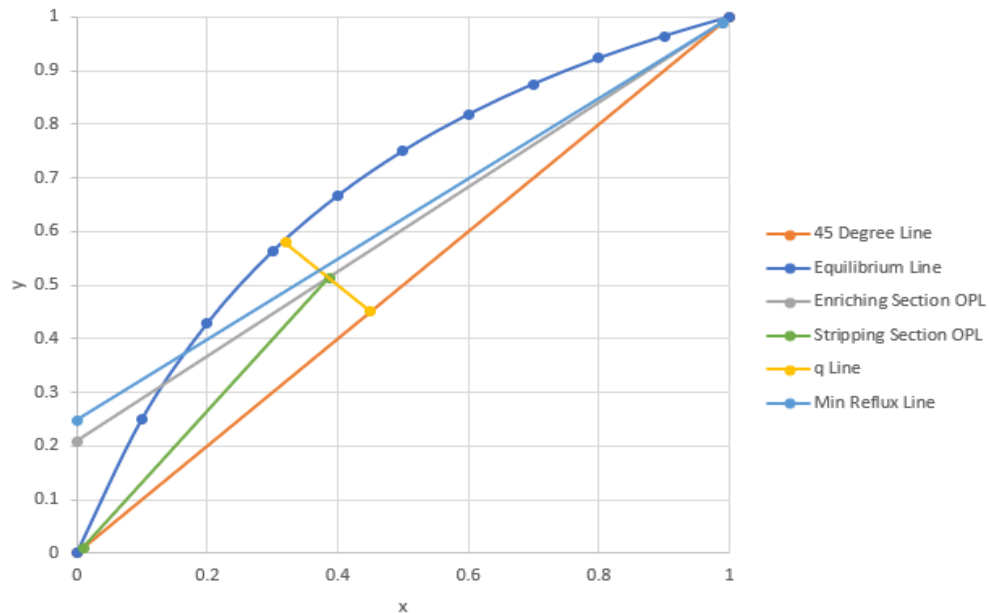


Figure 3 Graph before Model Execution



Model Execution

45 line		$x_D$	0.99
x	y	$x_F$	0.45
0	0	$x_W$	0.01
1	1	$\alpha$	3
$y = \frac{\alpha x}{1 - (1 - \alpha)x}$		$R_{min}$	1.571848265
		R	1.964810332
Equilibrium relation		q	0.5
x	y	slope	-1
0	0	q-line	
0.1	0.25	x	y
0.2	0.428571429	0.45	0.45
0.3	0.5625	0.3	0.58
0.4	0.666666667	Top Section	
0.5	0.75	x	y
0.6	0.818181818	0.99	0.99
0.7	0.875	0	0.333916807
0.8	0.923076923	Bottom	
0.9	0.964285714	x	y
1	1	0.01	0.01
Min Reflux Line		0.340458103	0.559541897
x	y		
0.99	0.99		
0	0.384937173		

Figure 4 Values after Model Execution

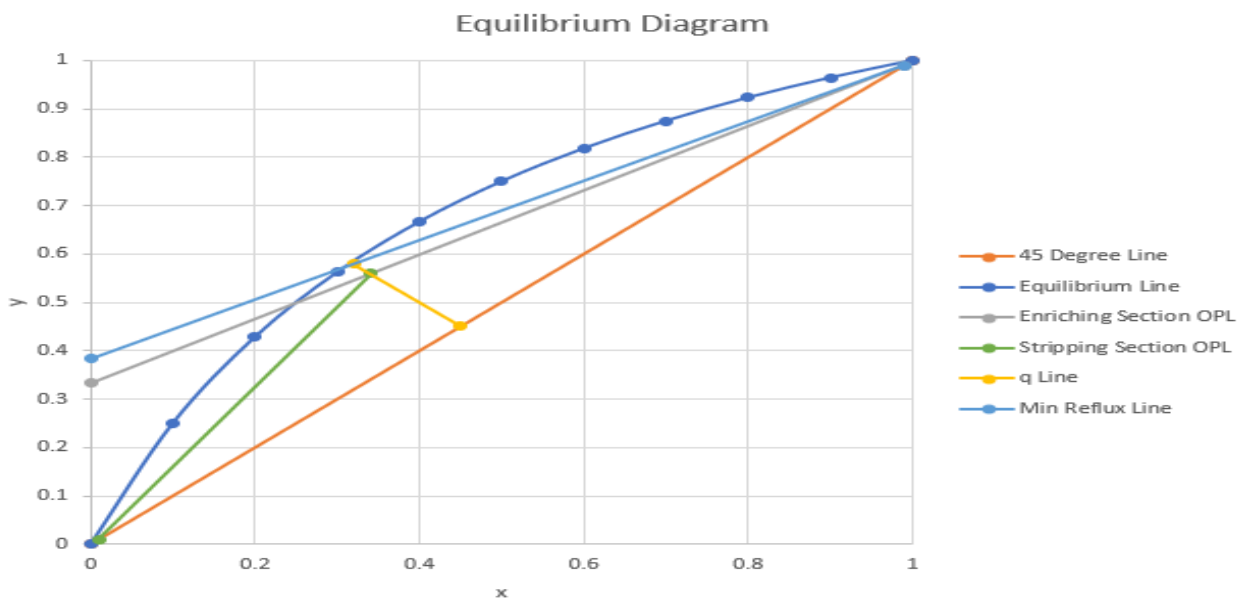


Figure 5 Graph after Model Execution



#### V. CONCLUSION

The described method is numerical method thus is not restricted by assumptions such as constant relative volatility and constant molal overflow, which is an advantage over traditional methods such as Underwood equations. It also facilitates easy and accurate computation; thus, it can be used effectively as model block in various Simulation Software's like Aspen Hysys, Aspen Plus, CHEMCAD, UniSim etc. In addition to the above points, it can be used as a useful tool in shortcut calculations.

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