

Interactive Matlab Program for Design of Multicomponent Distillation Column using FUG Method

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Abstract— A MATLAB based GUI program is made on most popular shortcut method called FUG for design of multicomponent distillation column. The paper presents the various examples solved from the literature that has been run on this program, with detail justification for each result, along with real towers case studies. The paper also presents the various basic concepts of tray towers and their variations with changing parameters as governed by the equations.

Keywords— FUG, MATLAB, Distillation Column, Shortcut Method, Separating Columns

NOMENCLATURE

α_{LK} = Average relative volatility of light key component with respect to heavy key
 $(x_{LK}, x_{HK})_d$ = Mole fraction of light key and heavy key in distillate
 $(x_{LK}, x_{HK})_b$ = Mole fraction of light key and heavy key in residue
 $\alpha_{LK, feed}$ relative volatility of light key with respect to heavy key at the bubble point of feed
 α_i = relative volatility of specie 'i' with respect to heavy key component
 x_{id} = mole fraction of component 'i' in liquid phase in distillate
 x_{if} = mole fraction of component 'i' in liquid phase in feed
 v = Underwood's equations roots
 R_m = minimum reflux ratio
 q = feed condition
 N = Number of stages
 N_m = minimum number of stages
 N_r = Number of stages in Rectifying section
 N_s = Number of stages in Enriching Section
 F = Feed Flow Rate in kmol/h
 D = Distillate Flow Rate in kmol/h
 B, W = Bottom Flow Rate in kmol/h
 HK = Heavy Key
 LK = Light Key
 $MATLAB$ = Matrix Laboratory
 GUI = Graphical User Interface
 LEF = Light Ended Fractionation
 LPG = Liquefied Petroleum Gas
 f = feed
 d = distillate
 b, w = bottom

I. INTRODUCTION

FUG stands for Fenske-Underwood-Gilliland's method and it is the most widely method used short cut method for determining number of equilibrium stages for multicomponent distillation. The Fenske's equation is used to find the minimum number of theoretical stages required for the desired separation.

Fenske's equation[1]

$$N_m = \frac{\log \left(\frac{x_{LK,d}}{x_{HK,d}} \right) \alpha_{LK}}{\log \alpha_{LK}}$$

Where,

$$\alpha_{LK} = (\alpha_{LK, top} * \alpha_{LK, bottom})^{1/2}$$

If there is a wide difference in the values of α_{LK} at the top most temperature and the bottom most temperature, the use of above equation in the Fenske's equation gives lesser values of N_m required, in such case it is recommended to find α_{LK} by the following equation.

$$\alpha_{LK} = (\alpha_{LK, top} * \alpha_{LK, feed} * \alpha_{LK, bottom})^{1/3}$$

In Underwood's method R_m is determined by solving the following two equations.[2]

$$\sum \frac{x_{id}}{\alpha_i - v} = R_m + 1 \text{ and}$$

$$\sum \frac{\alpha_i x_{if}}{\alpha_i - v} = 1 - q$$

Here, q implies the type of feed.

The correct value of 'v' belongs to the interval starting from 1 to the value of α_{LK} .

The Gilliland [6] correlation or Gilliland plot correlates the reflux ratio and the number of theoretical stages for a distillation column if,

$$X = \frac{R - R_m}{R + 1} \text{ and } Y = \frac{N - N_m}{N + 1},$$

Given minimum reflux ratio R_{min} is calculated and the minimum number of stages N_{min} by Fenskey's method.

The resulting curve stretches form (0,1) coordinate at minimum reflux to (1,0) at total reflux.

One of the most used expressions is that of Molokanov:

$$y = 1 - \frac{1 - R_{min} \cdot x}{1 + R_{min} \cdot x}$$

For higher precision, alternative relations being that of Eduljee:

$$y = 0.75(1 - x^{0.8888})$$

and Rusche:

$$y = 0.1256 \cdot x - 0.8744 \cdot x^{0.291}$$

Lastly to determine the feed tray location Kirkbride's Equation is used:

$$\log\left(\frac{W}{V}\right) = 0.206 \log\left[\left(\frac{W}{D}\right) \left(\frac{D_{HK}}{D_{LK}}\right) \left(\frac{D_{HK}}{D_{LK}}\right)^2\right]$$

1.1 Advantages of this method

The foremost advantage of this method is well established and popular for preliminary design of distillation column for multi-component system. The co-relations are being used since long time and are well applicable for real time columns. Secondly, it gives really precise and accurate results, in very short span of time and with minimal efforts. Lastly the set of equations employed are very simple and can easily be coded.

1.2 Limitations of this method

It presumes the most basic assumptions that are generally made while designing that is constant molar flow of components, i.e., for each stage, molar latent heat of vaporization of liquid phase is equal to molar latent heat of condensation of vapour phase. Hence moles of liquid vaporized over each theoretical stage are equal to moles of vapour condensed on that stage. This implies that, molar flow rate of liquid and vapours in enriching section (L and V) and also in stripping section (\tilde{L} and \tilde{V}) remains constant.

It also assumes that the physical properties of components remain constant throughout the column.

It assumes system to be non-foaming, non-corrosive, non-azeotropic and well thermally insulated, i.e., no heat loss.

It does not accounts for side streams and multiple feed.

1.3 MATLAB – Matrix Laboratory[7]

MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and fourth-generation

programming language. A proprietary programming language developed by MathWorks. MATLAB® is the easiest and most productive software for engineers and scientists, for analyzing data, developing algorithms, or creating models. MATLAB provides an environment that invites exploration and discovery. It combines a high-level language with a desktop environment tuned for iterative engineering and scientific workflows.

The programming is done in MATLAB R2013a version for 64-bit, windows OS.

1.4 Key Features of MATLAB

- High-level language for scientific and engineering computing
- Desktop environment tuned for iterative exploration, design, and problem-solving
- Graphics for visualizing data and tools for creating custom plots
- Apps for curve fitting, data classification, signal analysis, and many other domain-specific tasks
- Add-on toolboxes for a wide range of engineering and scientific applications
- Tools for building applications with custom user interfaces
- Interfaces to C/C++, Java®, .NET, Python®, SQL, Hadoop®, and Microsoft® Excel®
- Royalty-free deployment options for sharing MATLAB programs with end users

MATLAB automates the entire path from research through production. One can:

- Build and package custom MATLAB apps and toolboxes to share with other MATLAB users.
- Create standalone executables to share with others who do not have MATLAB.
- Integrate with C/C++, Java, .NET, and Python. Call those languages directly from MATLAB, or package MATLAB algorithms and applications for deployment within web, enterprise, and production systems.
- Convert MATLAB algorithms to C, HDL, and PLC code to run on embedded devices.
- Deploy MATLAB code to run on production Hadoop system

MATLAB is both an application as well as programming software; it facilitates almost all possible mathematical or engineering computation.

A graphical user interface (GUI) is a graphical display in one or more windows containing controls, called components that enable a user to perform interactive tasks. The user of the GUI does not have to create a script or type commands at the command line to accomplish the tasks. Unlike coding programs to accomplish tasks, the user of a GUI need not understand the details of how the tasks are performed. GUIs created using MATLAB® tools can also perform any type of computation, read and write data files, communicate with other GUIs, and display data as tables or as plots.

II. CASE STUDIES

2.1 From Literature

2.1.1 Case Study - 1[5]

A large butane-pentane splitter is to be shut down for repairs. Some of its feed will be diverted temporarily to an available small column, which has 11 trays plus a partial reboiler. The feed enters on the middle tray. Past experience on similar feeds indicates that the 11 trays plus the reboiler are roughly equivalent to 10 equilibrium stages and that the column has a maximum top – vapour capacity of 1.75 times the feed rate on a mole basis. The column will operate at a condenser pressure of 827.4 kPa (120psia). The feed will be at its bubble point ($q = 1.0$) at the feed-tray conditions and has the following composition on the basis of 0.0126(kg.mol)/s [100(lb.mol)/h]:

Component	F_{X_F}
C₃	5
i – C₄	15
n – C₄	25
i – C₅	20
n – C₅	35
Total	100

The original column normally has less than 7 mol percent i-C₅ in the overhead and less than 3 mol percent n-C₄ in the bottoms product when operating at a distillate rate of D/F = 0.489. Can these product purities be produced on the smaller column at D/F = 0.489?

Solution given in text

Component	x _F	α	αx _F	θ = 1.36		θ = 1.365		x _D	αx _D / α-θ
				α-θ	αx _F / α-θ	α-θ	αx _F / α-θ		
C ₃	0.05	4.99	0.2495	3.63	0.0687	3.625	0.0688	0.102	0.1404
i – C ₄	0.15	2.62	0.3930	1.26	0.3119	1.255	0.3131	0.301	0.6282
n – C ₄	0.25	2.02	0.5050	0.66	0.7651	0.655	0.7710	0.473	1.4581
i – C ₅	0.20	1.00	0.2000	-0.36	-0.5556	-0.365	-0.5479	0.0069	-0.1892
n – C ₅	0.35	0.864	0.3024	-0.496	-0.6097	-0.501	-0.6036	0.055	-0.0949
Total	1.00				-0.0196		+0.0014	1.000	1.9426

Interpolation gives θ = 1.3647

$$R_{m+1} = 1.9426$$

$$R_m = 0.9426$$

$$R = 2.713 \cdot R_m \text{ is taken.}$$

Top Section	Bottom Section
D = 48.9 (lb.mol)/h	B = 51.1 (lb.mol)/h
V = 175 (lb.mol)/h	V' = 175 (lb.mol)/h
L = 126.1 (lb.mol)/h	L' = 226.1
V/L = 1.388	V'/L' = 0.7739
L/L' = 126.1/226.1 = 0.5577	
R = 126.1/48.9 = 2.579	

Given that Number of trays = 11 (including the Reboiler) and Feed tray location as 6th from top.

Solution from Program Run

The acceptable value of Underwood's root = 1.3770

The minimum value of reflux ratio at infinite plates = 0.7434

Here, it is evident from the two results given that the value of Underwood's root creates significant change in the value of R_m.

Although, theoretically this value may not present a dramatic difference but when considered further for flow rates calculation one will find that on long term basis it incurs a heavy duty on condenser and reboiler duties and

thus the operating cost. It is really clear that the proportionality chain goes as follows:

$$R_m \rightarrow R \rightarrow V \text{ and } L \rightarrow \text{Heat duty required} \rightarrow \text{Operating Cost}$$

Also, looking into the computational aspects of Underwood's Roots, the method given in the book is long, tedious and inherits obvious errors because of rough judgement of relative volatilities from the graph as well as the error incorporated in the method of interpolation. Furthermore, the need of convergence or adjustment required to be done to retrofit the data directly affects the results, whereas these all considerations are not required while working on the computer. Given below are three output windows on FUG's module, the first two are run models for reflux values given in the text, on the other hand the third one is for the value obtained by Underwood's module.

There is marginally any difference in the values of reflux ratios taken, approximately about 0.03 to bring down the vapour flow rate at top to value of 179.81, which is still higher than the predicted value of 175 (lb.mol)/s, for no change in the number of trays.

For the minimum reflux ratio values that the program has given, the value of vapour flow rate at the top is coming to 154.797, which is even lower than the predicted value, for the same number of trays. Also, the distillate and the bottom lcompositions remain the same, hence the system is not compromising with the product qualities too.

Result Summary			
	Interpolation Method	Adjusted Value	Program Results
R_m	0.9426	0.9782	0.7434
R	2.557	2.6557	2.0295
N_m	8.24939	8.24939	8.24939
N	12	12	12
N_r	5	5	5
N_s	7	7	7
F_t	6	6	6
V_{top}	182.583	186.793	154.797
L_{top}	131.487	135.697	103.700
V_{bot}	182.583	186.793	154.797
L_{bot}	231.487	235.697	203.700
D	51.0965	51.0965	51.0965
W	48.9035	48.9035	48.9035

2.1.2 Case Study – 2 [6]

In this case study a distillation column is to separate 4750 ml/h of feed composed of 37% n – butane, 32% i – pentane, 21% n – pentane and 10% n – hexane. The column operates at an average pressure of 2 atm and will produce a distillate product containing 95% n – butane and 5% i – pentane. The bottom product is allowed to contain no more than 570mol/h of n – butane. Use Underwood's method to determine the minimum reflux for the required separation. Feed is 25% vapour by mole. Assume ideal vapour – liquid equilibrium. All compositions are mole%.

Specie	Feed		Distillate		Residue	
	mol%	mol/h	mol%	mol/h	mol%	mol/h
n – butane	37	1757.5	95	1187.5	16.3	570
i – pentane	32	1520.0	5	62.5	41.6	1457.5
n – pentane	21	997.5	-	-	28.5	997.5
n – hexane	10	475.0	-	-	13.6	475.0
Total	100	4750.0	100	1250	100	3500

Component	α_{22}	α_{47}	α_{avg}
n – butane	2.7125	2.43	2.567
i – pentane	1	1	1
n – pentane	0.75	0.774	0.762
n – hexane	0.216	0.258	0.236

In-text Result

Underwood's Root $\theta = 1.6045$

Minimum Reflux Ratio $R_m = 1.45095$

We get results exactly the same as text, that is $N_m = 4.11713$ and $N = 6$ with $N_r = 4$ and $N_s = 2$. Besides that as the program uses Eduljee's equation in place of Malokanov's equation to validate this particular part, several values of R (same as text), has been tested and the result summary is produced:

R	N (text)	N (program)	N _r (program)	N _s (program)
1.7	10.67	11	7	4
2.0	8.75	9	6	3
2.5	7.27	7	5	2
3.0	6.52	6	4	2
3.5	6.07	6	4	2
4	5.76	6	4	2

2.1.3 Case study – 3 [3]

In this case, heavy alkanes like Hexane, Heptane and Octane are considered.

Component	Feed		Distillate		Bottoms	
	F	x _F	D	x _D	B	x _B
Hexane	40	0.40	40	0.534	0	0
Heptane	35	0.35	34	0.453	1	0.04
Octane	25	0.25	1	0.013	24	0.96

Feed is liquid at its boiling point. $R_m = 0.83$.

Solution:

R	N (text)	N (program)	N _r (program)	N _s (program)
1	19	21	11	10
2	11.8	13	7	6
5	9.1	10	5	5
10	8.2	9	5	4

2.1.4 Case Study – 4[4]

Here a finishing column is required to produce 99.9% (vol.) trichlorethylene purity from 10,000lb/hour of a feed of 40% (wt.) trichlorethylene and 60% (wt.) perchlorethylene. Only 1% (vol.) of the trichlorethylene can be accepted in the bottoms. Because the process system that will receive vents from this condensing system is operating at 5 psig, allow 5 psi pressure drop to ensure positive venting and set top of tower pressure at 10 psig.

Feed (158 ^o F)	Wt%	Mol. Wt.	Moles	Mole Fraction
Trichlorethylene	40	131.4	0.00304	0.456
Perchlorethylene	60	165.9	0.00362	0.544
Total	100		0.00666	1.000

The results generated by program are tabulated as follows:

Quantity	Text Results	Program Results
Distillate Flow Rate	30.05	30.0791
Bottom Flow Rate	36.65	36.6209
Minimum Number of trays	11.18	11.171
Number of trays	40	39
Number of trays (Rectifying)	30	29
Number of trays (Stripping)	10	10

2.2 Real Columns Data Validation

2.2.1 LEF Column

Data Given:	
Feed Flow Rate	2433 kmol/hr
Feed Condition	1
Pressure (in psi)	405
Light Key Fraction in Feed	0.4685
Heavy Key Fraction in Feed	0.0045
Light Key Fraction in Top	0.705
Heavy Key Fraction in Top	0.0001 \approx 0
Light Key Fraction in Bottom	0.0001 \approx 0
Heavy Key Fraction in Bottom	0.0134
Reflux	0.74

	Company Data	Output Obtained
Vapour Flow Rate at the Top		2813.07 kmol/hr
Liquid Flow Rate at the Bottom		3629.36 kmol/hr
Distillate Flow Rate	1620 kmol/hr	1616.71 kmol/hr
Bottom Flow Rate	813.4 kmol/hr	816.292 kmol/hr
Minimum Number of Trays		10
Actual Number of Trays	42	41
Feed Tray Location	9	10
Number of trays in Enriching Section		9
Number of trays in Stripping Section		32

The results generated by program are almost same as that of real column, although there is a negligible difference in flow rates which can be justified by the fact that presence of non-condensable gases are not taken into account while designing with shortcut method, also the actual number of trays in column is 1 more than the calculated, this extra tray accounts for better product consistency which would otherwise vary because of dynamic disturbances and higher safety considerations as products are highly volatile and easily inflammable.

2.2.2 LPG Column

Data Given:	
Feed Flow Rate	830 kmol/hr
Feed Condition	1
Pressure (in torr)	11782
Light Key Fraction in Feed	0.6056
Heavy Key Fraction in Feed	0.0132
Light Key Fraction in Top	0.657
Heavy Key Fraction in Top	0.0001 \approx 0
Light Key Fraction in Bottom	0.0001 \approx 0
Heavy Key Fraction in Bottom	0.1676
Reflux	0.35

	Company Data	Output Obtained
Vapour Flow Rate at the Top kmol/hr		1032.83
Liquid Flow Rate at the Bottom kmol/hr		1097.77
Distillate Flow Rate kmol/h	764	765.056
Bottom Flow Rate kmol/h	65	64.944
Minimum Number of Trays		22
Actual Number of Trays	52	51
Feed Tray Location		12
Number of trays in Enriching Section		11
Number of trays in Stripping Section		40

The results generated by the program are exactly the same as the real column.

III. CONCLUSION

The program is extremely robust and suitable for most of the conventional distillation systems. The interactive GUI window makes it more user-friendly. The program can be used by researchers and design engineers to estimate rough design of columns, academicians for teaching purpose and by students for learning.

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