Computer Aided Design of a Multi-Component Distillation Column-Using the Fenske-Underwood-Gilliland Short-Cut Method

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Abstract: Most design calculations in multi-component distillation column are tedious and time consuming, thus the need for the Engineer to embrace the applications of computer for the design of multi-component distillation columns design. At the same time the need for accurate design in engineering cannot be over emphasize, 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 multi-component distillation columns to avoid such errors. The objective of this work is to develop a module that uses Fenske-Underwood-Gilliland (FUG) shortcut method in the design of a multi-component distillation column. The FUG shortcut method for multi-component distillation column design uses the Fenske equations for minimum number stages, the Underwood equations for minimum reflux and the Gilliland correlation for the number of stages for a given reflux. The scope of this design is basically development of software that could be used for the calculations involved in the design of multi-component distillation columns. The package developed however utilizes only the FUG shortcut method. The package is built on the Visual Basic 6++ programming language, which is a user friendly and object oriented program.

Keywords: Computer Aided Design, Multi-Component, Distillation Column, Visual Basic, Short-cut Method

1. Introduction

It is obvious that good design requires good data-especially so, with multi-component calculations. In this section, some basic relations and sources of data are considered.

The reason for such a limited treatment, quite simply, is that the estimation/prediction/extrapolation/interpolation of equilibrium data is an immense problem with difficult method of solution (Makama, 2001).

1.1. Equilibrium Data in Multi-Component Distillation

For multi-component systems, which can be considered ideal, Raoult's law can be used to determine the composition of the vapour in equilibrium with the liquid.

$$p_i = P_i x_i \qquad (1.1)$$

Where p_i is the partial pressure of component i in the vapour in Pa (atm). p_i is the vapour pressure of pure i in Pa (atm) and x_i is the mole fraction of i in the liquid. In

hydrocarbon systems, because of non-idealities, the equilibrium data are often represented by:

$$y_i = K_i x_i \qquad (1.2)$$

Where K_i is the vapour-liquid equilibrium constant or distribution co-efficient for component i

These K- values for light hydrocarbon system (methane to decane) have been determined semi empirically and each K is a function of temperature and pressure. It should be noted that for ideal system;

$$K_i = \frac{P_i}{P} \qquad (1.3)$$

The relative volatility a_i for each individual component in a multi-component mixture can be defined in a manner similar to that for a binary mixture. If component C in a mixture of A, B, C and D is selected as the base component;

$$\alpha_i = \frac{k_i}{k_c} , \alpha_A = \frac{k_A}{k_C} , \alpha_B = \frac{k_B}{k_C}, \alpha_C = \frac{k_C}{k_C} = 1.0, \alpha_D = \frac{k_D}{k_C} \ (1.4)$$

The values of k_i will be a stronger function of temperature than the α_i values, since the k_i values in the database increase with temperature in a similar manner.

1.2. Boiling Point and Dew Point in Multi-Component Distillation Boiling Point

At specified pressure, the boiling point or bubble point of a given multi-component mixture should satisfy the relation:

$$\sum y_i = 1.0$$

For a mixture of A, B, C and D, with C as the base component.

$$\sum y_i = \sum K_i x_i = K_c \sum \alpha_i x_i = 1.0 \qquad (1.5)$$

The calculation is trial and error process as follows:
- First, a temperature is assumed and the values of α_i are calculated from the values of k_i at this temperature.
- Then, the value of k_c is calculated from:

$$k_c = \frac{1.0}{\sum \alpha_i x_{i\ i}} \qquad (1.6)$$

- The temperature corresponding to the calculated value of k_c is compared to the assumed temperature.
- If the values differ, the calculated temperature is used for the next iteration.
- After the final temperature is known, the vapour composition is calculated from;

$$y_i = \frac{\alpha_i x_{i\ i}}{\sum (\alpha_i x_i)} \qquad (1.7)$$

1.3. Dew Point

For the dew point calculation, which is also trial and error:

$$\sum x_i = \sum \left(\frac{y_i}{k_i}\right) = \left(\frac{1}{k_c}\right) \sum \left(\frac{y_i}{\alpha_i}\right) = 1.0 \qquad (1.8)$$

The value of k_c is calculated from;

$$k_c = \sum \left(\frac{y_i}{\alpha_i}\right) \qquad (1.9)$$

After the final temperature is known, the liquid composition is calculated from:

$$x_i = \frac{y_i/\alpha_i}{\sum (y_i/\alpha_i)} \qquad (1.10)$$

1.4. Key Components in Multi-Component Distillation

The component separated are called the *light key,* which is the more volatile (identified by the subscript LK), and the *heavy key* (HK). (Geankoplis 1997).

The components more volatile than the light key are called *light components* and will be present in the bottoms in small amounts. The components less volatile than the heavy keys are called *heavy components* and are present in the distillate in small amounts. The two keys components are present in significant amount in both the distillate and bottoms. (Geankoplis 1997).

1.5. Total Reflux for Multi-Component Distillation: Fenske's Equation for Minimum Stages at Total Reflux

Just as in binary distillation, the minimum number of theoretical stages or steps, N_m, can be determined for multi-component distillation for total reflux. (Geankoplis, 1997).

The Fenske equation (1932) also applies to any two components in a multi-component system. When applied to the heavy key HK and light key LK, it becomes;

$$N_m = \frac{\log[(\alpha_{LD} D/x_{HD}D)(x_{HW}W/x_{LW}W)]}{\log(\alpha_{L,av})} \qquad (1.11)$$

Where x_{LD} = mole fraction of light key in distillate.
x_{LW} = Mole fraction of the light component in bottoms.
x_{HD} = Mole fraction of heavy component in bottoms.
The average value α_L (α is the relative volatility) of the light key is calculated form the α_{LD} at the top temperature (dew point) of the tower and α_{LW} at the bottoms temperature:

$$\alpha_{L,av} = \sqrt{\alpha_{LD} \alpha_{LW}} \qquad (1.12)$$

Note that, the distillate dew point and bottoms boiling-point estimation is partially trial and error, since the distribution of the other components in the distillate and bottoms is known and can affect these values.

1.6. Distribution of Other Components

To determine the distribution or concentration of other components in the distillate and the bottoms at total reflux, Equation (1.12) can be rearranged and written for any other component i as follows. (Geankoplis, 1997).

$$\frac{x_{iD}D}{x_{iw}W} = (\alpha_{L,av})^{N_m} \frac{x_{HD}D}{x_{HW}W} \qquad (1.13)$$

1.7. Minimum Reflux Ratio for Multi-Component Distillation

As in the case for binary distillation, the minimum reflux ratio R_m is that reflux ratio that will require an infinite number of trays for the given separation of the key components (Geankoplis, 1997).

For binary distillation only one "pinch point" occurs where the number of steps become infinite, and this is usually at the feed tray. For multi-component distillation, two pinch points or zones of constant composition occur; one in the section above the feed plate and another below the feed tray. The rigorous plate-by-plate stepwise procedure to calculate R_m is trial and error and can be extremely tedious for hand calculations.

1.8. Underwood's Shortcut Method to Calculate Minimum Reflux R_m

The Underwood (1948) shortcut method to calculate R_m uses constant average α values and also assumes constant flows in both sections of the tower. This method provides a reasonably accurate value. The two equations to be solved to determine the minimum reflux ratio are:

$$1\text{-}q = \sum \frac{\alpha_i x_{iF}}{\alpha_i - \theta} \tag{1.14}$$

$$R_m + 1 = \sum \frac{\alpha_i x_{iD}}{\alpha_i - \theta} \tag{1.15}$$

The values of x_{iD} for each component in the distillate in Equation (1.15) are supposed to be the values at the minimum reflux (Geankoplis, 1997).

However, as an approximation, the values obtained using the Fenske total reflux equation are used. Since each α_i may vary with temperature, the average value of α_i to use in the proceeding equations is approximated by using α_i at the average α which is used in the Fenske equation or the α at the entering feed temperature. To solve for R_m, the value of θ in Equation (1.15) is first obtained by trial and error. This value of θ lies between the α value of the light key and α of the heavy key, which is 1.0 using this value of θ in Equation (1.15), the value R_m is obtained directly.

1.9. Number of Stages (Theoretical) at Operating Reflux Ratio Number of Stages at Operating Reflux Ration

The determination of the minimum number of stages for total reflux and the minimum reflux ratio as discussed subsequently are useful for setting the allowable ranges of number of stages and flow conditions. These ranges are helpful for selecting the particular operating conditions for a design calculation.

1.10. Gilliland Shortcut Method for Number of Stage Operating Reflux Ratio

Gilliland's (1940) shortcut method, which is developed into an equation by Molokanov (1972), is an empirical correction considered as an approximation method. It is utilized at the operating reflux ratio R (for flow rates at the column top) is correlated with the minimum R_m obtained using the Underwood method, the minimum number of stages N_m

obtained by the Fenske method, and the number of stages N at the operating R, given by (Perry and Green, 1999);

$$\frac{N-N_m}{N+1} = 1\text{-}\exp\left\{\left(\frac{1+54.4\psi}{11+117.2\psi}\right)\left(\frac{\psi-1}{\psi^{0.5}}\right)\right\} \tag{1.16}$$

Where $\psi = \left(\frac{R-R_m}{R+1}\right)$

1.11. Estimation of Feed Plate Location

Kirkbride has devised an approximate method to estimate the number of theoretical stages above and below the feed, which can be used to estimate the feed stage location. This empirical relation is as follows:

$$\log \frac{N_e}{N_s} = 0.206 \log\left[\left(\frac{x_{HF}}{x_{LF}}\right)\frac{W}{D}\left(\frac{x_{LW}}{x_{HD}}\right)^2\right] \tag{1.17}$$

Where N_e is the number of theoretical stages above the feed plate and N_s the number of theoretical stages below the feed-plate. The feed point is N_e tray above the fed point.

1.12. Computer Aided Design

CAD is an acronym for Computer Aided Design, and it is a technology concerned with the use of computer to perform certain functions in Design, production, and manufacture, CAD may also be defined as the use of Computer system to assist in the creation, modification, analysis or the optimization of a design (Oguntoyinbo, 1993).

The evolution of Computer Aided Design has been largely related to the developments in the Computer Graphics, and Interactive Computer Graphics (ICG) form the essential technological foundation of Computer Aided Design (Oguntoyinbo, 1993).

The CAD set-up consists of the hardware and software to perform the specialized design functions required by the particular user, institution or firm. The hardware includes but is not limited to the computer, Graphic Display terminals, keyboards and other peripherals like plotters, printers, e.t.c, whereas the software consists of computer programs to implement computer graphics on the systems plus application programs to facilitate Engineering functions of a particular job (Oguntoyinbo, 1993).

As the system is a user-oriented system, the user is the designer who communicates data and commands to the computer through an input device (keyboard) and the computer communicates with the user via the monitor (CRT) (Oguntoyinbo, 1993).

2. Design Methodology

A successful program cost less to produce than the sales or savings it generates from an industrial point of view. Naturally, to have the best chance of generating savings, or sales, a program should have the four qualifications as listed below:
- To be correct.
- Efficient
- Useful
- And easy to use

To these four qualifications, a good program must be cost-effective; conversely, it also follows that a good programmer must be cost-effective (Cannon, 1997).

2.1. Design Method

The source code was developed in visual basic programming language and it is given in Appendix B.

The package is based on the following assumptions:

- Constant molar overflow
- Phase equilibrium between an existing vapor and single existing liquid phase is achieved at each stage.
- Neither of the existing phases entrains the other phase.
- No chemical reaction occurs.
- Total condenser.
- Single feed point.

2.2. Development of the Module

A data bank of the physical and thermodynamic properties (K-value) of some 20 different hydrocarbons (Geankoplis, 1997 and Schweitzer, 1979) was created. The constants were used to evaluate relative volatility and K-value of each component, at a temperature, particularly, the light and heavy keys respectively.

2.3. Coding Language

The design program was developed using *visual basic*, because of its advanced features that are well suited for modular programming (Onifade, 1999).

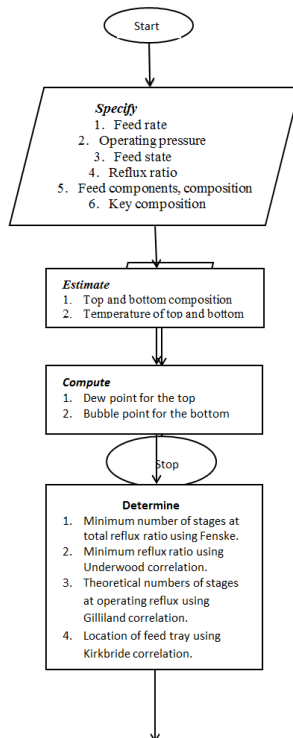The file or module name used for the simulation is "MULTICAD 1.0".

2.4. Flow Chart

Figure 1. *Process flow chart.*

The flow for this source code is as shown below; it is a menu oriented and user-friendly programming language. There is an executable form of MULTICAD 1.0, which can be run DOS environment.

The program draws data from the *"equilibrium K-value data bank"*. At constant pressure.

2.5. Program Run

To operate the package successfully, the following steps should be applied: it should be mentioned here that a visual aid of the package is introduced to aid understanding of the program:

Step 1: Insert the package (soft copy) into the CD drive of your system.

Step 2: From the start menu, scroll up to my computer (this can also be done directly from the desk top. And then click. A box appears, displaying the drives and then click (double) on CD-Drive.

Step 3: The program installs itself "auto run".

Step 4: Click on the start icon on the desk top, a fly-out appears, scroll up to multi-component distillation column and click on the name (icon).

Step 5: A splash page appears as shown in Figure 2. Click on "next".

Step 6: Another information page appears showing a typical distillation column with single feed location, on the right side of the page are the introductory note of the program and assumptions made, as shown in Figure 2. Click on "next".
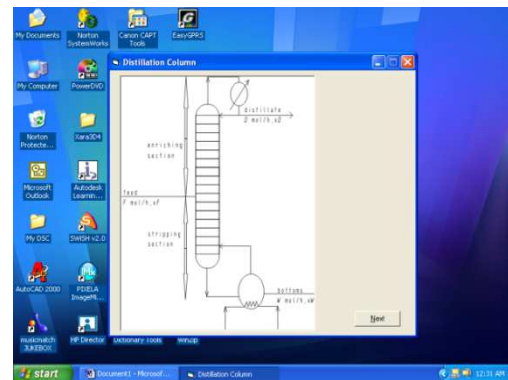

Figure 2. *Display of feed rate data.*

Step 7: A page appears showing the program interface. Begin by entering the feed rate as shown in Figure 2 above.
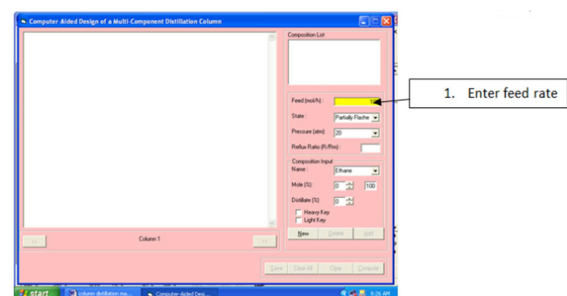

Figure 3. *Display of feed rate selected.*

Step 8: Select feed state by clicking on arrow on the "state" portion of the interface, a fly out appears as shown in Figure 3. Then chose your feed state.By clicking on the desired feed state.
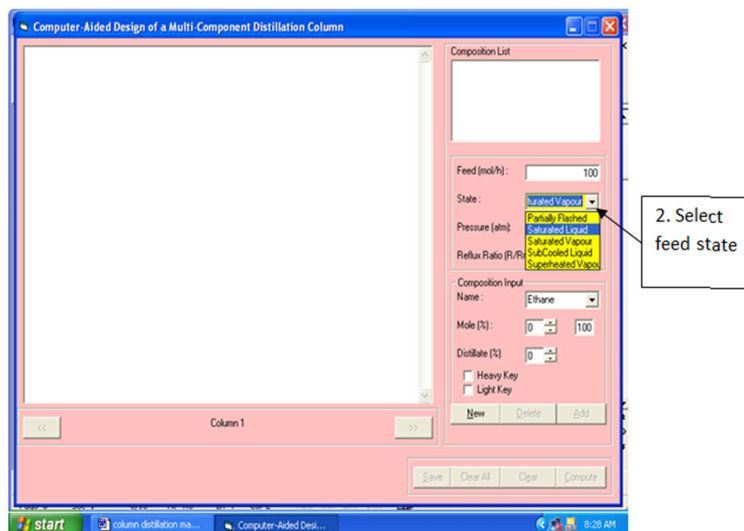

Figure 4. Display of feed state selected.

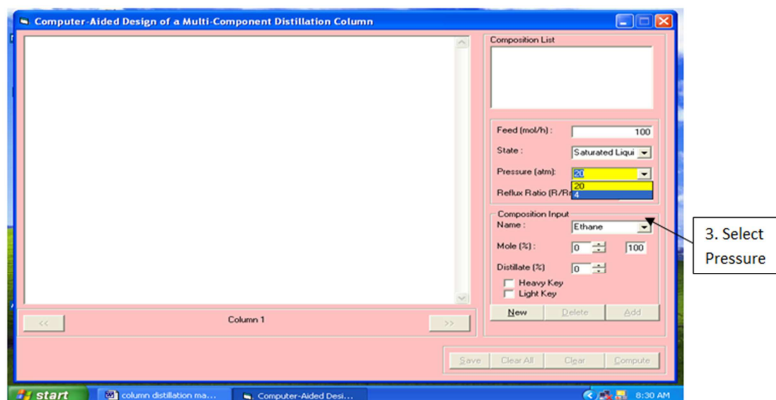Step 9: Similarly, select operating pressure, a process similar to Step 9, as shown in figure 4 above.

Figure 5. Display of selected pressure.

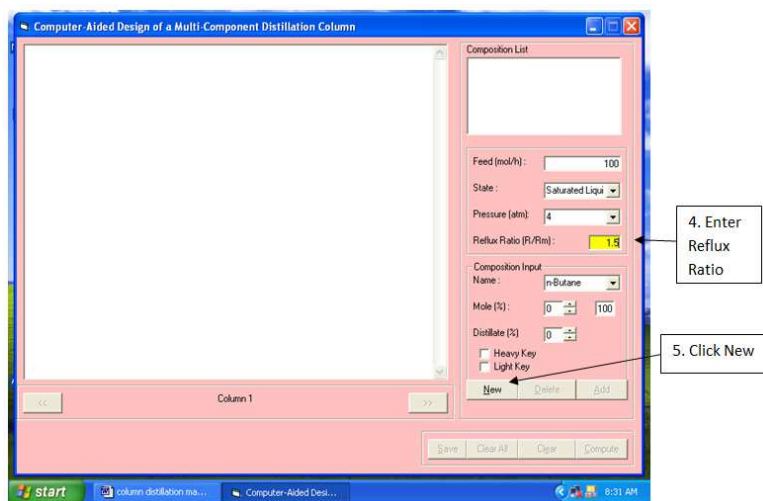Step 10: Enter reflux ratio and then click on "New" as shown in Figure 5 above.
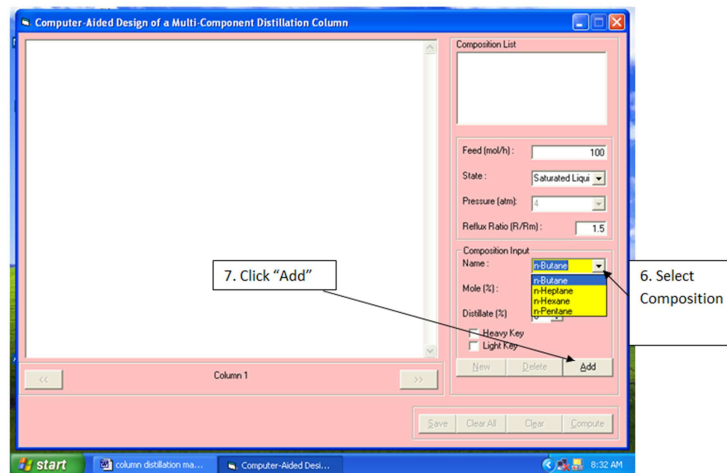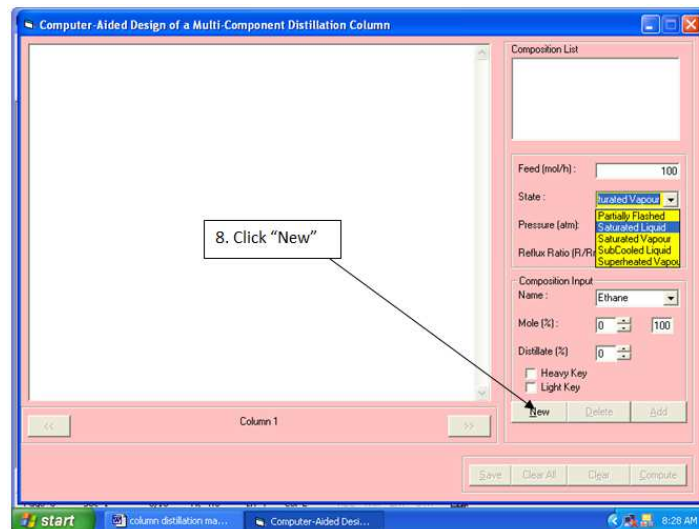

Figure 6. Display of selection for composition.

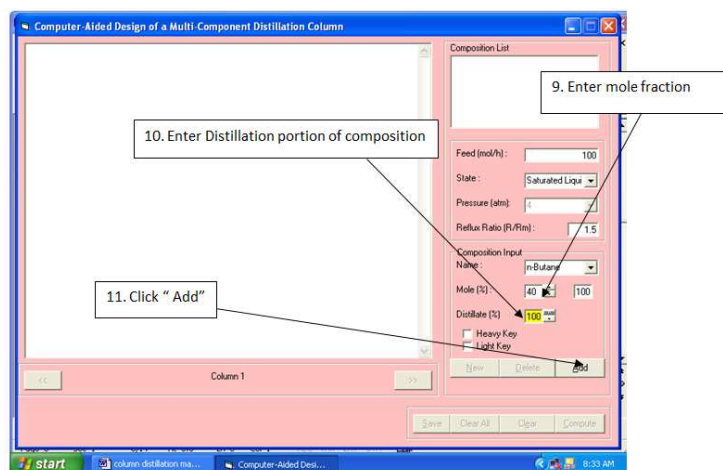Step 11: Select composition as shown in Figure 6 above.

Figure 7. *Display of the selected composition.*

Step 12: enter mole fraction of the selected composition, click on "Add" as shown in Figure 7 above.

Figure 8. *Display of selection for new data input.*

Step 13: then click on "New" as shown in Figure 8 above.

Figure 9. *Display for input of more constituents.*

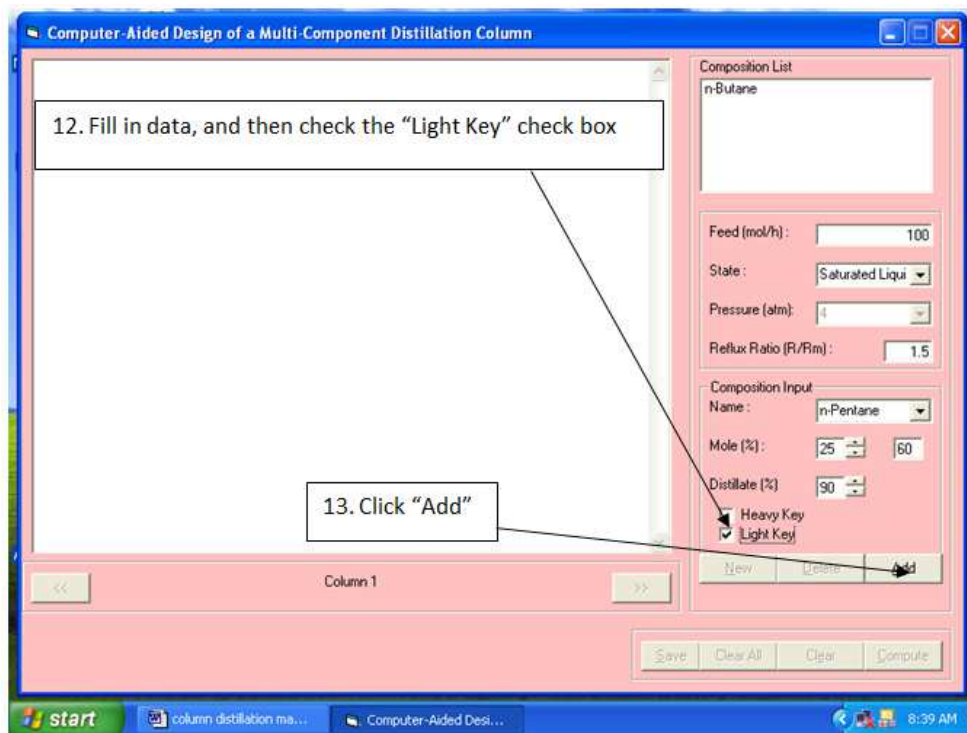Step 14: Fill in data for more constituents. Select light key and click on "Add" as shown in Figure 9 above.

Figure 10. *Display on how to add in more components.*

Step 15: Click on "New" and select the heavy key as is done in Step 13, then click on "Add" as shown in Figure 10.
Step 16: Add more constituent(s) as shown in Figure 8 above and click on "Add".
Step 17: On reaching the specified data for a particular problem, click "Compute" or "Alt+C" as shown in Figure 11.
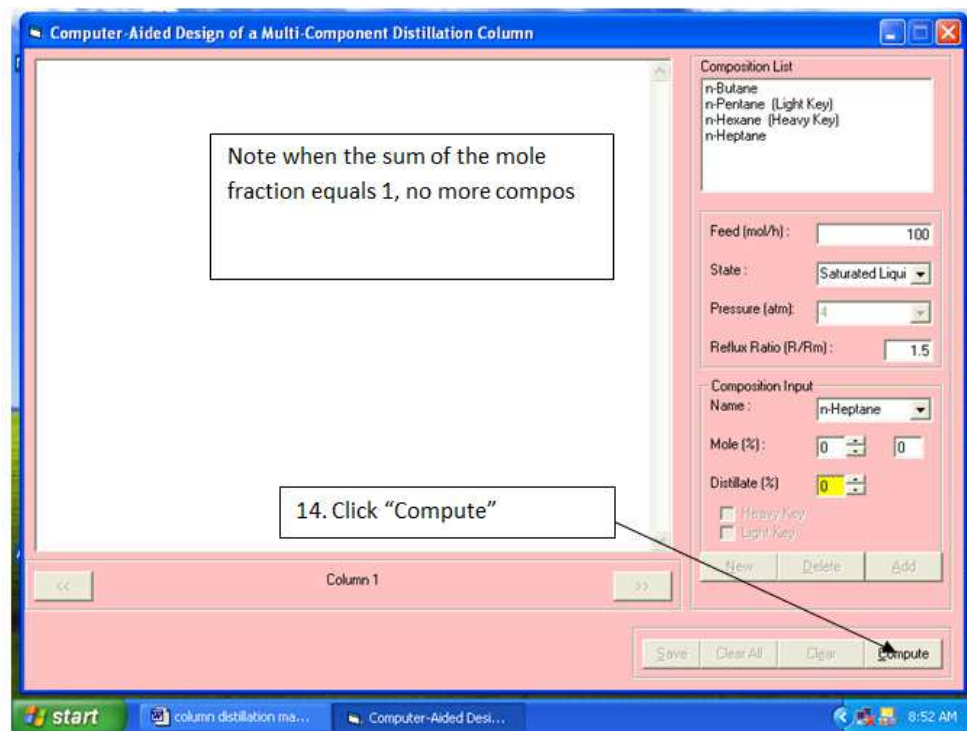

Figure 11. *Display on how to compute data inputted.*

Step 18: The results are then displayed as shown in figure 12 after a few seconds.
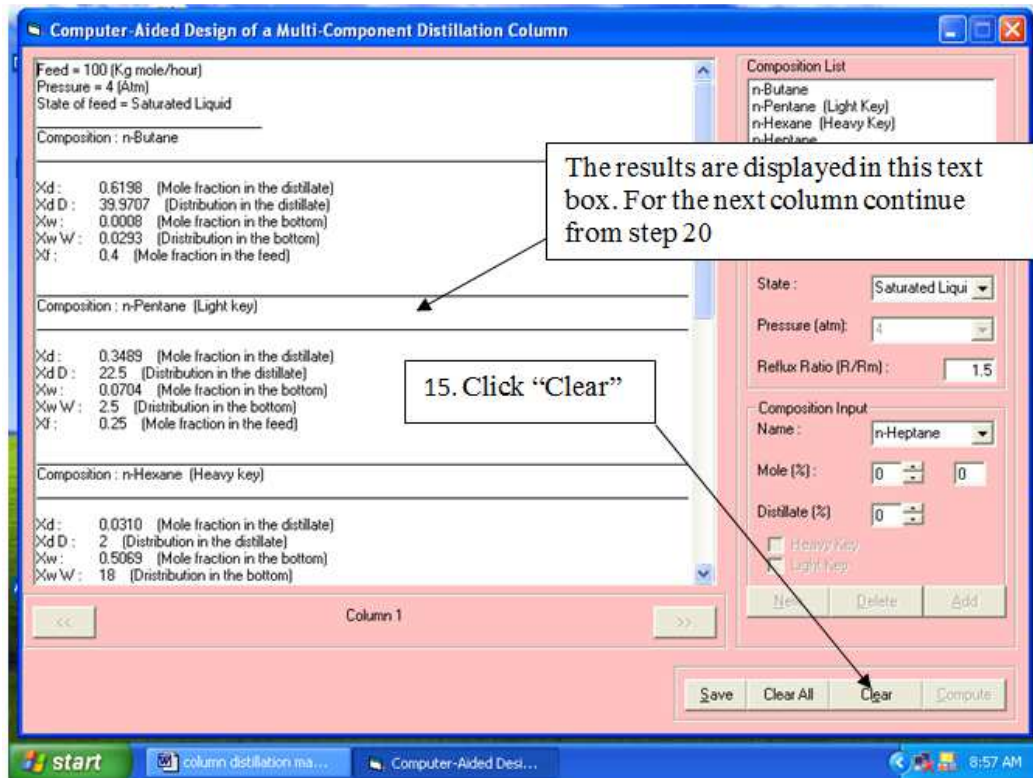
Figure 12. Display of the calculated result.

To recalculate in case of inputting data for a particular constituent, click on the constituent in the composition sub-box and click on the "Clear" button.

To calculate for the next column, click on the "Clear" button, repeat Step (8) to (9).

To save results obtained, click on "Save", a dialogue box appears, results are save in note pad, similar to any MS- word

applications. When the work is saved, a dialogue box appears indicating that the work is been saved and then click on "ok" to proceed. Figure 14 displays a typical illustration of how work is save in note pad. The results can also be easily printed out by following the normal procedure of printing any work in MS word package.
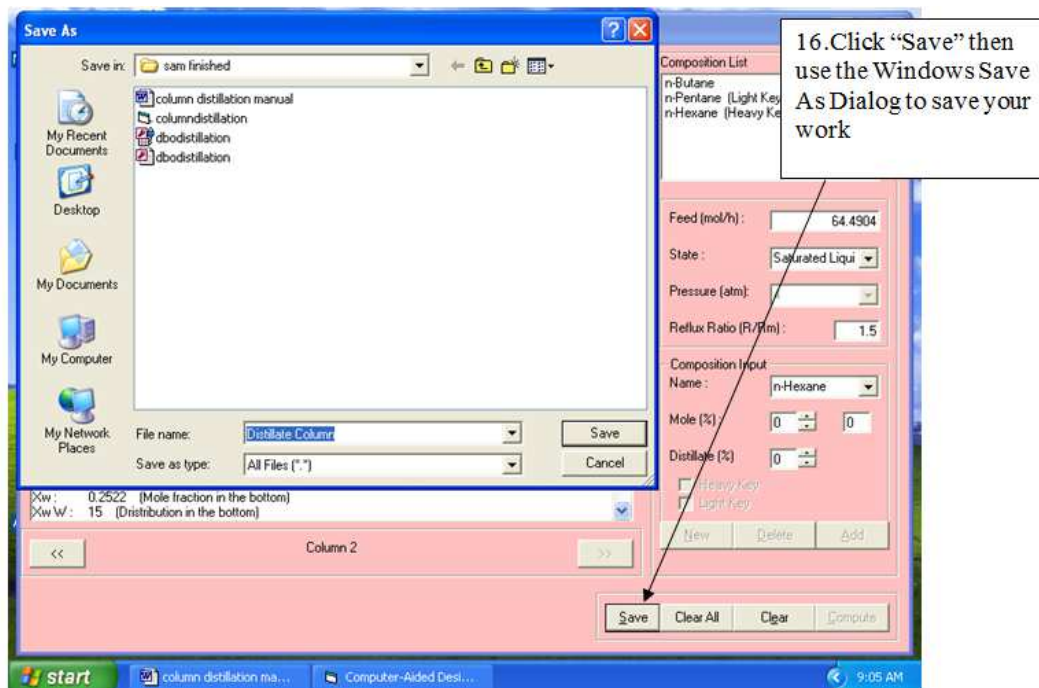

Figure 13. Display on how to save computed result.

3. Results

3.1. Test Problem

A liquid feed at a pressure of *4Atm.* (405.3*KPα*) *abs* is fed to a distillation tower. The composition in mole fractions is a follows:

n-butane ($x_A = 0.40$), n-pentane ($x_B = 0.25$), n-hexane ($x_C = 0.20$), n-heptane ($x_D = 0.15$). the feed is to be fractionated so that 90% of n-pentane (B) is recovered in the distillate and 90% of the n-hexane (C) in the bottom. Calculate:

a. Moles per hour and composition of distillate and bottoms.
b. Top temperature (dew point) of distillate and boiling point of bottoms.
c. Minimum stages for total reflux, using Fenske correlation and distribution of other components in the distillate and bottoms.
d. Minimum reflux ratio, using the Underwood method.
e. Number of theoretical stages at an operating reflux ratio R of $1.5R_m$ using Gilliland correlation.
f. Location of feed tray using the method of Kirkbride. (Geankoplis, 1997).

3.2. Results from Manual Computation

The temperature (to use for determining the values of α_i is the average between) the top $67\,°C$ and bottom $132\,°C$ temperature.

Table 1. Manually computed results.

Component	Distillate, D		Bottoms, W	
	$y_D = x_D$	$x_D{}^D$	x_w	$x_w{}^W$
A(n-butane)	0.6197	39.9610	0.0011	0.0390
B(n-pentane)	0.3489	22.5000	0.0704	2.5000
C(n-hexane)	0.0310	2.0000	0.5068	18.000
D(n-heptane)	0.0004	0.0230	0.4217	14.9770
	1.0000	D = 64.4840	1.0000	W = 35.5160

3.3. Results from CAD Computation

Feed = 100 mol/hr
Pressure = 4 Atm
State of feed = Saturated Liquid

_____

Composition: n-Butane

_____

Xd: 0.6198
Xd D: 39.9707 (mole fraction in the distillate)
Xw: 0.0008
Xw W: 0.0293 (mole fraction in the bottom)
Xf: 0.4 (mole fraction in the feed)

_____

Composition: n-Pentane (light key)

_____

Xd: 0.3489 (mole fraction in the distillate)
Xd D: 22.5 (amount in the distillate)
Xw: 0.0704 (mole fraction in the bottoms)
Xw W: 2.5 (amount in the bottoms)
Xf: 0.25 (mole fraction in the feed)

_____

Composition: n-Hexane (heavy key)

_____

Xd: 0.0310 (mole fraction in the distillate)
Xd D: 2 (amount in the bottoms)
Xw: 0.5069 (mole fraction in the bottoms)
Xw W: 18 (amount in the bottoms)
Xf: 0.2 (mole fraction in the feed)

_____

Composition: n-Heptane

_____

Xd: 0.0003 (mole fraction in the distillate)
Xd D: 0.0197 (amount in the distillate)
Xw: 0.4219 (mole fraction in the bottoms)
Xw W: 14.9803 (amount in the bottoms)
Xf: 0.15 (mole fraction in the feed)

_____

D = 64.4904 mol/hr

W = 35.5096 mol/hr
Minimum stages at total reflux = 5.655
Minimum Reflux Rm: 0.3954

Actual Number of Trays: 13
Number of trays above feed location, Ne = 7
Number of trays below feed location, Ns = 6
The feed tray is tray from the top of the column = 7
Top temperature = 68 Degree Celsius
Bottom Temperature = 132 Degree Celsius

4. Discussions

Table 2. Results discussion figures.

Component	Distillate, D		Bottoms, W	
	$y_D = x_D$	$x_D{}^D$	x_w	$x_w{}^W$
A(n-butane)	0.6197	39.9610	0.0011	0.0390
A*(n-butane)*				
B(n-pentane)	*0.6197*	*39.9707*	*0.0008*	*0.0293*
B*(n-pentane)*	0.3489	22.5000	0.0704	2.5000
C(n-hexane)	*0.3489*	*22.5*	*0.0704*	*2.5*
C*(n-hexane)*	0.0310	2.0000	0.5068	18.000
D(n-heptane)	*0.0310*	*2.0*	*0.5069*	*18.8*
D*(n-heptane)*	0.0004	0.0230	0.4217	14.9770
	0.0003	*0.0197*	*0.4219*	*14.9803*
Total	1.0000	D = 64.4840	1.0000	W = 35.5160
Total	*1.0000*	*D = 64.4904*	*1.0000*	*W = 35.5096*

Note: The result in bold face is the result of the CAD computation.

From the result in Table 2 above:

1. The top composition for the manual computation is 64.4840 mol/hr and that for the CAD is 64.4904 mol/hr, the variation in the two results is as a result of better computation of value by the CAD result (with a difference in value of 0.0064), which is very close.
2. The top temperature for the manual computation is 67 degrees Celsius and that of the CAD is 68 degrees Celsius. The variation in the two results is the data bank, meaning that more accurate result could be obtained with closely imputed value in the data bank.
3. The bottom temperatures are the same for both computations.
4. For the minimum stages using Fenske correlation the manual computation is 5.404 and that of the CAD is 5.655. This is more accurate in that it the calculation process involves iteration.
5. For the manual computation the minimum stages at total reflux for the minimum reflux ratio using the Underwood correlation, for the manual computation is 0.395 and that of the CAD is 0.3954, also here, the variation is as a result of more accurate computation by the CAD computation the results are very close.
6. Number of theoretical stages at operating reflux, using Gilliland correlation is the same for both computations, as 13.
7. The feed tray location is the same for both computations, as the 7th tray.

5. Conclusion

In conclusion, it can be said that the aim of the research has been achieved, in that the model designed works and more importantly, gives more accurate, time saving and reliable results.

The following have been outlined as room for further studies:

- The Erbar-Maddox chart should be work upon to see if it could give more accurate results that Underwood correlation.
- That a correlation should be generated for the Erbar-Maddox chart as it is for Gilliland.
- The module can be further improved upon with time by increasing more correlation in the source code to compute for other parameters, like the tray spacing, e.t.c.

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