

Improvements in the Teaching of Separation Process Design through Interactive Computer Graphics

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Several graphical solution techniques have long played a role in separations processes. McCabe-Thiele and Ponchon-Savarit methods for staged distillation design and graphical methods for gas absorption and stripping design remain in use today and similar procedures are employed for extraction and other less frequently encountered processes. These methods are typically employed due to their conceptually simpler formulation compared to numerically solved processes. However, manual construction of graphics and investigation of the effect of different design parameters on the resulting column are time consuming and tedious procedures. Computer-aided instruction offers solutions to these problems by removing the burden of computational effort while preserving the simple graphical representation. The benefits of introducing state of the art computing technology into the coursework are numerous. With the increased computational speed, a large number of problems can be solved in a fraction of the time one solution would otherwise take. This ability allows students to have a greater exposure to a wide range of complex problem types. Also, the tedious preparation of engineering diagrams and repetitive calculations can easily be done on the computer, which frees the student to concentrate on the interplay of equations and problem specifications.

The aim of this study is to show the applicability of interactive computer programming for solving staged-process design problems.^[1-5] Two computer programs were developed for this purpose. The first program, WDISTIL, was developed to find stage requirements and column operating parameters of a multicomponent and binary distillation tower given feed stream information and desired product purities. WDISTIL, utilizing McCabe-Thiele and Ponchon Savarit graphical solution techniques for binary distillation, was used in a senior level chemical engineering course and proved to be a very successful learning tool. WDISTIL uses the extension of McCabe-Thiele diagram to columns containing multiple feeds, multiple side products, and multiple points of heat removal or addition for complex multicomponent distillation. Distillation columns having multiple feeds, one or more side products, one or more points of heat removal and heat addition or combination of these features can be handled by this graphical procedure. The program was designed to be self explanatory, easy to use and simple to understand. The input routines are completely unstructured to allow the user total freedom of problem specification. Solutions to the problems are generated very rapidly to allow the exploration of various parametric dependencies.

The second program, WGASABS, computes the packed tower height and number of trays for gas absorption or stripping columns. WGASABS was developed for absorption of concentrated mixtures in packed towers under isothermal conditions in the case of diffusion of A through stagnant B in order to calculate the tower height using the numerical and graphical capabilities of personal computers.

Binary Distillation

Several graphical solution techniques used in chemical engineering can be applied directly to a computer graphic screen. ^[1-5] McCabe-Thiele and Ponchon-Savarit diagrams are the most common graphical solution techniques taught in a separation course and details of the method need not be repeated here. Assuming a total condenser is used, the distillate composition is equal to the vapor composition leaving the top tray. With the additional assumptions of constant relative volatility and constant molar overflow, one can easily construct component balance (operating) lines and equilibrium curves.

In the parameter entry section of the program the parameters, including the relative volatility (α), the reflux ratio (R), the feed flow rate (F), the feed composition (XF), the feed quality (q), the distillate (XD) and bottom (XW) compositions are entered into the boxes next to the appropriate symbols. As the cursor passes over an object, information about that object appears in the field at the very bottom of the window. The variable q is used as a measure of the feed condition. The boxes of the feed condition field contain the thermal feed condition data. This variable can be changed to reflect any phase condition from subcooled liquid to superheated vapor. In the equilibrium line entry field, the first option is a relative volatility box. For instructional use, this is the fastest and least troublesome way to specify an equilibrium line. There are several forms of phase equilibrium equations that can be used to analytically solve for the equilibrium line. The simplest form of equilibrium information is the case of constant relative volatility. Using the relative volatility, the equilibrium line is found from a simple one-parameter equation. After the relative volatility is entered through the keyboard, the appropriate equilibrium line appears on the diagram. The second option is a user defined equilibrium line. Individual points of the desired line are entered using the mouse. With the mouse, the user moves cursor over the displayed table.

The pictorial representation of the screen fields in the work place is shown in Figure 1. This screen displays the current status of the McCabe-Thiele diagram under construction. The latest equilibrium and operating lines along with the most recent solution are shown here. In the left portion of the screen is the largest of the fields, the Diagram Field. This is where the McCabe-Thiele diagram construction takes place. The master object displayed consists of a McCabe-Thiele plot with appropriate equilibrium and operating lines and the ladder of stages. The program finds the number of theoretical trays for the desired separation by stepping off the trays like a stairway between the equilibrium and operating lines as shown in the Figure 1. The tray numbers can be specified using a top to bottom numbering convention. If a mouse is used, the option will be given to alternate graphical modes involving zoomed displays of the stage-by-stage details for selected regions of the tower. In the upper right corner of the screen lies the result of the construction. Changing any of the design parameters is easily accomplished and produces an almost instantaneous response in recomputing the McCabe-Thiele plot, redisplaying them on the monitor. These interactions are designed so those qualitative trends in column design resulting from parameter changes are viewed continuously if desired. The user alters operating parameters by selecting appropriate spin buttons for the reflux ratio (R) and q values. Pressing the mouse alters their respective values with immediate response from the programs, producing altered images for the McCabe-Thiele plot. For example, a first problem solution can ask for the number of trays necessary to achieve a desired separation at a chosen operating conditions. After the number of trays has been solved for, the reflux ratio or q value can be changed. In this way, a range of

solutions with varying reflux ratios and q values can be generated quickly and easily. M_p is the Murphree plate efficiency based on the vapor phase. By clicking on the M_p button at the top of the diagram the user can see the dashed curve for actual exit phase compositions, which replace the thermodynamic equilibrium curves for a particular set of operating lines. The “default” box sets all the flowrates and operating parameters back to their initial preset values.

The operation of all columns, theoretical and real, lies between two limiting operational conditions. These limiting conditions are the minimum number of stages and the minimum internal reflux ratio. The limiting condition of minimum stages requires an infinite (or total) reflux ratio and the condition of minimum internal reflux requires an infinite number of stages. The box marked as “ R_m ” allows the user to determine the minimum value of the reflux ratio and “ N_m ” gives the minimum number of theoretical stages. One can slowly decrease the reflux ratio until a pinch-point occurs to visually calculate the minimum reflux ratio, or increase the reflux ratio to show that the operating lines collapse to the $y=x$ line. The printer button triggers the production of a paper copy of the current screen contents. The disk button allows the user to copy the graphic. The user may select a particular option by moving the mouse until the cursor lies within the required area (or button) designated for this option. Pressing the mouse activates the button to perform a specific task.

The second part of the program is based on the Ponchon-Savarit method as seen in Figure 2. In the McCabe-Thiele construction, material balance equations are plotted on a x - y phase equilibrium diagram, the stages being calculated by alternate use of the material balance and equilibrium relationships. The Ponchon diagram embodies both enthalpy and material balance relationships as well as phase equilibrium conditions. Since it is unnecessary to assume constant molal overflow, the calculations can be done on a per mole or per mass basis. Any set of consistent units may be used. In the data entry screen the equilibrium line points and enthalpy values are entered through the keyboard or with the mouse. On the right side of the screen, the options of the three different feed conditions are given: saturated vapor, saturated liquid and general case. This field is also used for variable specification. In the six boxes of the field, the defining diagram information is found. If a mouse is in use, the option will be given during every variable specification to use the mouse to point at values directly on the table. Distillate (X_D), feed (X_F) and bottom (X_W) compositions, reflux ratio (R), and feed flow rate (F) can be selected by using the mouse to “point and pick”. The last box (H_F) contains the feed enthalpy information. If a specified enthalpy is being used for the column, the enthalpy values will be displayed in this box. The H_f button shown below these boxes can be clicked at any time using the mouse to calculate feed enthalpy by using heat capacity values. By clicking on the R box, the reflux can be calculated by using q_c (heat removed in the condenser) and q_r (reboiler heat) values. After the desired working conditions are chosen, the program enters the work place screen to begin diagram constructions. The number of ideal stages can be computed by graphical construction as shown in the Figure 2. To the right of the diagram, the numerical values of all of the results are shown. The number of trays, feed tray location, feed (F), distillate (D) and bottom (W) product flow rates are displayed in this field.

The operating parameters lie directly below the results section. Access to this field is made by selecting the desired box. The first box contains the reflux ratio (R) and the second box contains the feed enthalpy (H_f) values. Pressing the mouse changes the values with immediate response

from the program. The minimum number of plates, N_m , and the minimum reflux ratio, R_m , are calculated here. By choosing the “default” button, the program returns to initial preset values. The second and third options are the print and save buttons. From here all the file manipulations and diagram printing takes place. As in the case of McCabe-Thiele, information about the object appears at the bottom of the window when the cursor passes over an object. This feature helps students use the program with little or no training.

Complex Multicomponent Distillation

Distillation systems can add up to a significant amount of the total energy requirements of a processing scheme and efforts to reduce plant utility costs can lead to energy integration requiring heat addition/removal at locations other than the main reboiler/condenser. There are many techniques that can be used to reduce energy consumption. These features such as interreboilers, intercondensers or intercoolers and multiple feed and side product arrangements have saved energy at the expense of greater column complexity. These features have made column design and performance evaluation calculations more difficult. There are high-tech simulation programs, recently made available for personal computers. Even though they are very powerful tools for the process engineer, they can be frustrating for a newcomer to use and usually require long hours of studying technical manuals. Moreover, these programs are cost-prohibitive for most students and faculty members. Because of the computational complexity inherent in the multicomponent multistage separation problem, approximate calculation methods are widely used for preliminary design. Kister extended the McCabe-Thiele diagram to columns having multiple feeds, multiple side products, multiple points of heat removal or addition (e.g., intercondensers or interreboilers), and any combination of these features.^[3] To plan the design roughly on a McCabe-Thiele diagram is a great help in obtaining a swift convergence of the simulation program. Hence, this type of problem is of value in making students consider the McCabe-Thiele construction as a flexible tool rather than a rigid routine. This simplified graphical procedure is suitable for making initial design estimates of columns. For the preliminary design, this method is very useful to provide an approximate solution for analyzing column design and performance. The number of trays that it predicts is close to that given by the rigorous calculation technique over a wide range of conditions.^[6-7]

This program computes the tray requirements, location of feeds, sideproducts, interreboiler or intercondenser, the reflux ratio and the product stream compositions of a multicomponent distillation tower. To begin the problem solution procedure, a material balance is obtained by first making an initial estimate of side-stream composition. To get this estimate, a preliminary reflux ratio must be assumed. The two key components must be selected for multicomponent feed mixtures. The key components are those that the distillation process is designed to separate. The theoretical goal of the distillation column is to have all of the light key and more volatile components leave through the top of the column. Constant molar overflow, except at the points of heat addition and removal, is assumed in this procedure, as in the McCabe-Thiele method. Reflux and stage requirements are determined by means of a McCabe-Thiele diagram. A multicomponent system is reduced to an equivalent binary one made up of the key components. Nonkey components are assumed to be present in the liquid and vapor of each section, at their respective limiting flowrates for the section. Limiting flowrates are estimated by Jenny's method.^[8] The minimum refluxes computed for each section are compared with each other in a manner similar to

that suggested by Yaws.^[9] The highest calculated equivalent binary reflux ratio of the keys (R_e) is dominant and considered the equivalent minimum reflux ratio for the column. The corresponding minimum liquid flow in the section is calculated. This liquid flow can be multiplied by a certain factor; commonly between 1.05 and 1.3, to give the optimum liquid flow. The actual reflux ratio was calculated using optimum liquid flow. The intercept of each operating line on the y-axis can now be calculated using actual reflux ratio and the number of stages can be found graphically by the usual stepping procedure. The actual flows and side stream composition are calculated in the column. These values can then be compared to the initial estimate of the side stream composition. If the values differ by an amount less than the set tolerance, the loop is exited.

The complex multicomponent distillation example, which is based on a problem presented by King^[10], involves depropanizing three feed mixtures. In this example, a single column involving three feed streams and one-side streams of a multicomponent mixture of C_1 , C_2 , C_3 , C_4 , C_5 , and C_6 of components is considered. A side-stream of liquid product containing 80% propane is to be drawn off at the rate of 100 lb-mol/h. The top product is recovered as a vapor that must not contain more than 0.5 % C_4 . Propane in the bottoms must not exceed 1%. The low-pressure steam is available for interreboilers. The best place for interreboiling is where the ratio of C_4 to C_3 in the liquid is 4:1. The column is designed to operate at an L/V ratio 25% above the minimum.

During the development of the program, care was taken to make the input routines as easy to use and as self-explanatory as possible. Titles are placed on the top of every box directing the user to enter the requested information at each step of the input procedure. A list of feed and operating variables must be given to start the computational method. Flow rates of each stream and the thermal conditions of feeds are requested as an input data,. Figure 3 and Figure 4 illustrate the screen design construction for the multicomponent distillation. On the first screen, the computer-generated scale diagram of the distillation column is presented; the feed and product stream compositions and operating conditions are shown numerically. The information about the current values of the various operating parameters such as feed and side stream compositions, total feed flow rates (lb-mol/h) and representation of the feed stream thermal conditions (q values) are displayed near the distillation column. The values are entered by placing the mouse at some point within the box. The upward and downward arrow buttons at the bottom of the screen allow the user to add or subtract the value of the stream compositions. The identification and desired splits of the light and heavy key components are entered into the "Products" button. The two adjacent keys are chosen together. The desired percentage of the light key recovered and allowed percentage of the heavy key contaminant in the distillate stream is then specified. When the "next" button is selected the program calculates minimum reflux and then D and B values are calculated by making mass balance.

In the equilibrium line entry window, there are two options. The first option allows users to construct an equilibrium diagram by using the relative volatility of the equivalent keys if we can make an assumption that there is no major variation in relative volatility. The vapor-liquid equilibrium of multicomponent mixtures, however, is not ideal and is instead best represented by tabulated equilibrium data. Using tabulated data in this program is quite simple. An easier technique involves programming the entered equilibrium data to generate a least-squares quartic polynomial to fit the data and then use this equation to draw the equilibrium line and to design the

system. If the fit obtained by this method is unsatisfactory, additional data points can be added to improve the fit or a higher order curve can be used.

The boxes at the bottom of the column in Figure 3 show the user prompts which can be chosen to add a feed, intercondenser, interboiler and side product to different points of the distillation column. In the upper left corner of the screen the file option allows the user to enter the name of the data file. The program checks if the file exists, and if so, clears the screen, opens the file, reads the data. At the right bottom corner of the screen is a help button that identifies and explains the functions of each of the boxes on the screen as the cursor is moved across the boxes.

The second screen displays the tray requirements, the feed (F), side product (P), interboiler (Boi) or intercondenser (Con) location. The graphical construction of the diagram can be performed using the computer as shown in Figure 4. The diagram shows that 25 theoretical stages are required including reboiler and partial condenser. The side product (P1) drawoff is at Stage 4, and feeds enter Stages 7 (F2), 10 (F3), 14 (F4). The interboiler (Boi5) is located at Stage 20. The users can change any operating conditions and immediately see the impact of such a change on the diagram, thus facilitating his or her understanding of the cause and effect relationship in the problem.

The two screens of results can be flipped back and forth by using left arrow key in the right bottom corner of the screen. Use of the printer button shows the flow profile of the example column. By clicking on the disk icon the user can save the file on the disk. The next button allows the user to save the file on clipboard.

Gas Absorption

Most absorption operations are carried out in countercurrent flow processes, in which the gas phase is introduced in the bottom of the absorber and the liquid solvent is introduced in the top of the tower. Packed towers are used for continuous countercurrent contacting of gas and liquid in absorption. A large area of intimate contact between the liquid and the gas is provided by the packing. The process of absorption may be regarded as the diffusion of a soluble gas A into liquid. The molecules of A have to diffuse through a gas film and then through a stagnant liquid film before entering the main bulk of liquid. The absorption of a gas consisting of a soluble component A and an insoluble component B is a problem of mass transfer through a stationary gas.

In the case of dilute gases in packed towers when the mole fractions in the gas and liquid streams are less than about 10%, there are simplified design methods. Straight operating lines and approximately straight equilibrium lines are obtained. In the case of concentrated gas mixtures, the operating line and usually the equilibrium line will be substantially curved and mass transfer coefficients k_x' and k_y' may vary with total flows. In addition, in most cases, only experimental data are available for the equilibrium lines instead of representative equations. If there is no equilibrium line equation available and for the case of diffusion of A through stagnant B, determination of interface compositions can be carried out with combined graphical and numerical trial and error methods. WGASABS was developed based upon the method of designing for absorption of concentrated mixtures in packed towers under isothermal conditions in order to calculate the tower height using numerical and graphical capabilities of the personal computers. The obvious benefits

of the program to the user are the savings of hours of hand calculation and the ability to run through a wide variety of design or operating 'what-ifs' in minutes.

The information, which is submitted to the program as input data, is shown in the data entry screen (Figure 5). Inlet gas flow, composition, and molecular weight, inlet liquid composition and molecular weight, minimum liquid flow to gas flow ratio, requested outlet composition, mass transfer coefficients or predicted using empirical correlation, number of packing increments or maximum number of overall iterations are entered through keyboard or desired absorption system data is loaded from the disk

The second screen is where the computational time is spent for constructing and solving the problems. The equilibrium and operating lines along with the most recent solution are shown here. WGASABS performs these calculations for a continuous absorption column and the graphical solution of problem is shown in the results screen. Figure 6 shows the implementation of this technique that calculates the column height necessary for a particular gas absorption system. The spin button for the Simpson's interval allows the user to change values of intervals and study the resulting effects on column height.

References

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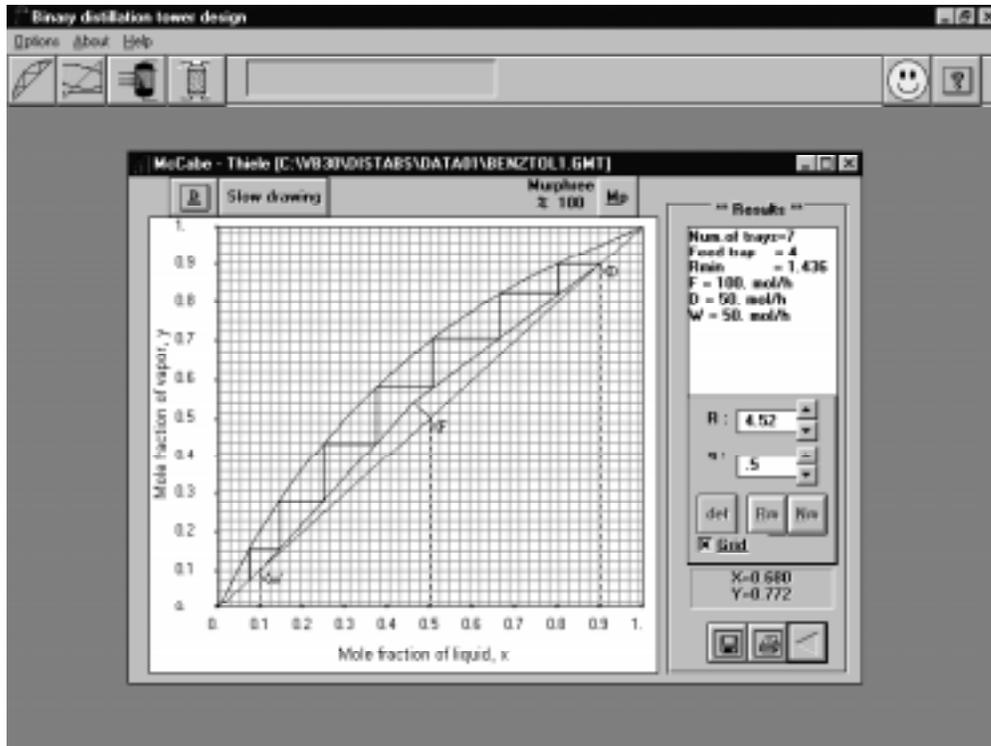


Figure 1. The graphical output and the results screen of the McCabe-Thiele solution.

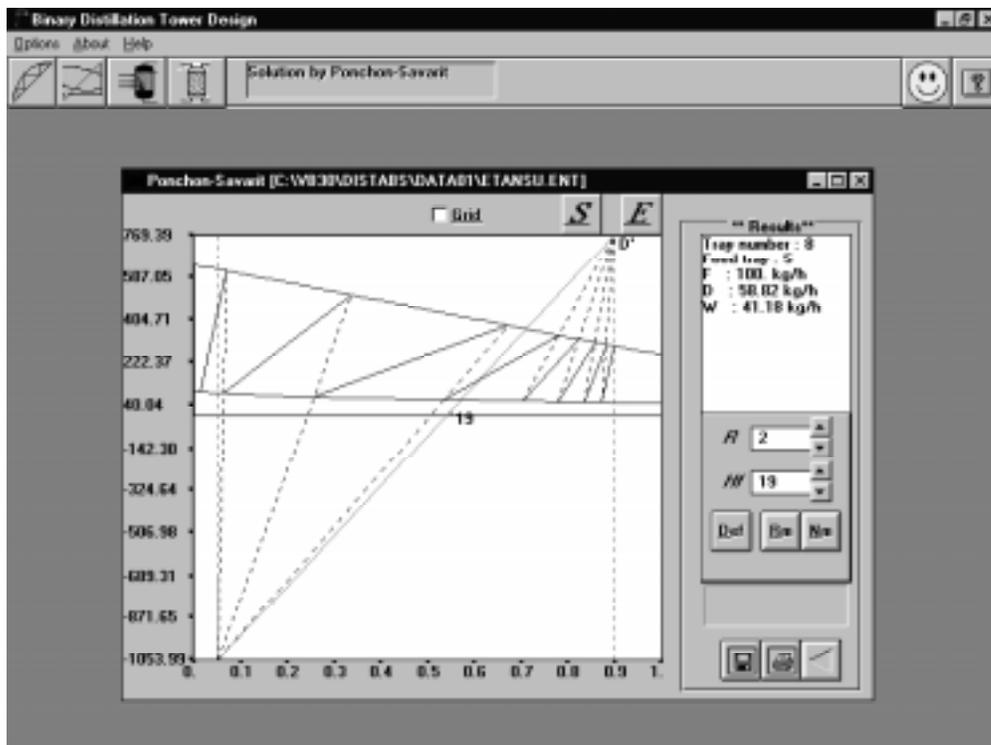


Figure 2. The graphical output and the results screen of the Ponchon-Savarit solution.

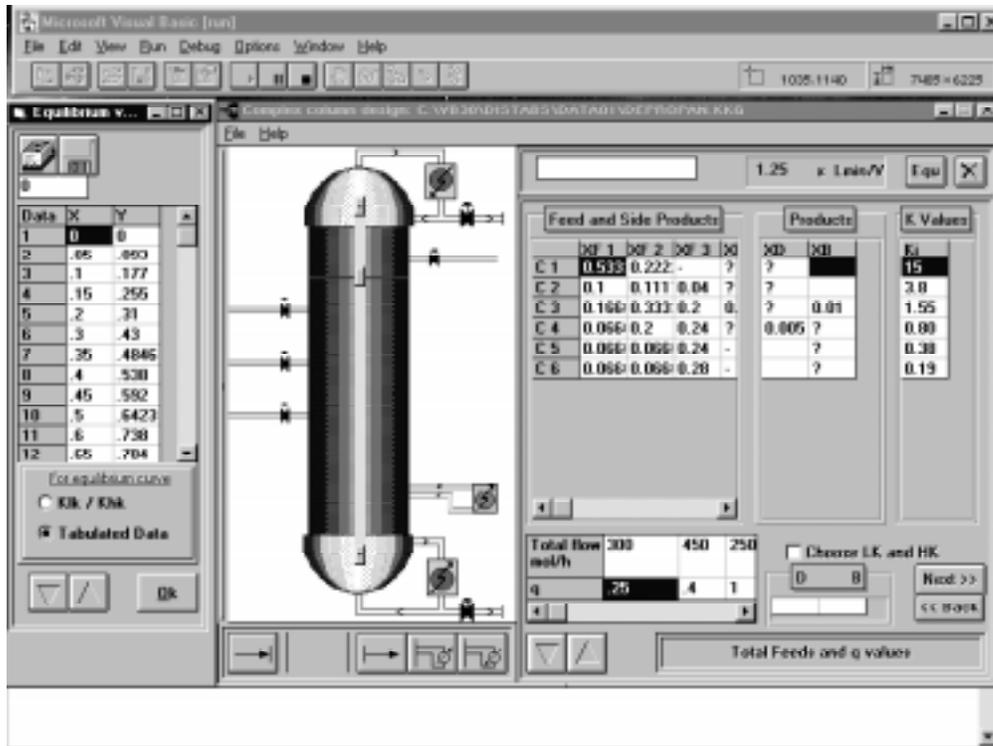


Figure 3. The diagram of the distillation column and information about the operating parameters for multicomponent distillation.

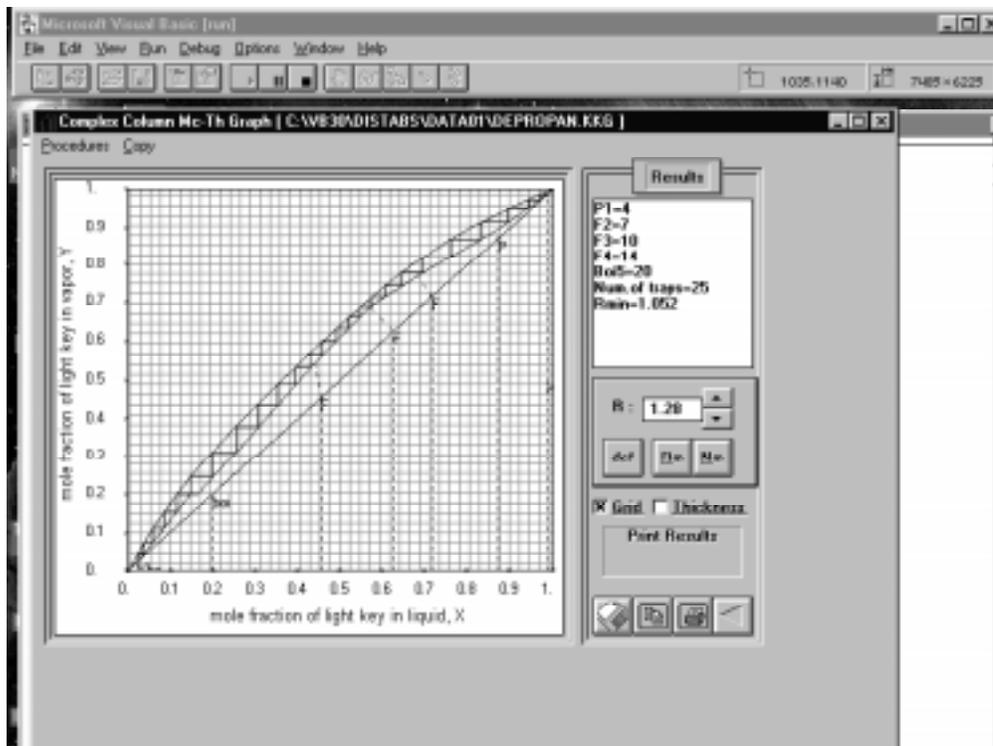


Figure 4. The graphical construction and result screen for the multicomponent distillation.

GASABSW- [C:\WB3\ADISTAB\MEVZAT\ACETON.ABS]

File

Equilibrium Data		
	X	Y
1	0	0
2	.0333	.0095
3	.072	.026
4	.117	.11237
5	.171	.1395
6		
7		
8		
9		
10		
11		

Operation conditions

Pressure(atm) Temperature(C)

Cross-sectional area(m²) Tower packing size(m)

Absorbed component Scrubbing solution

Entering gas conditions

Inlet gas flowrate (kmol/s) MW of inert gas

Fraction of absorbed amount MW of absorbed component

Exit gas conditions

Fraction of absorbed amount

Entering Liquid Conditions

Fraction of absorbed amount MW of liquid

Liquid flowrate (kmol/s) x Lmin x 1

Mass Transfer Coefficients

k_{xa}(kmol/s.m³) G_xⁿ G_yⁿ

k_{ya}(kmol/s.m³) G_xⁿ G_yⁿ

<< Back Next >>

Figure 5. Parameter entry section of gas absorption.

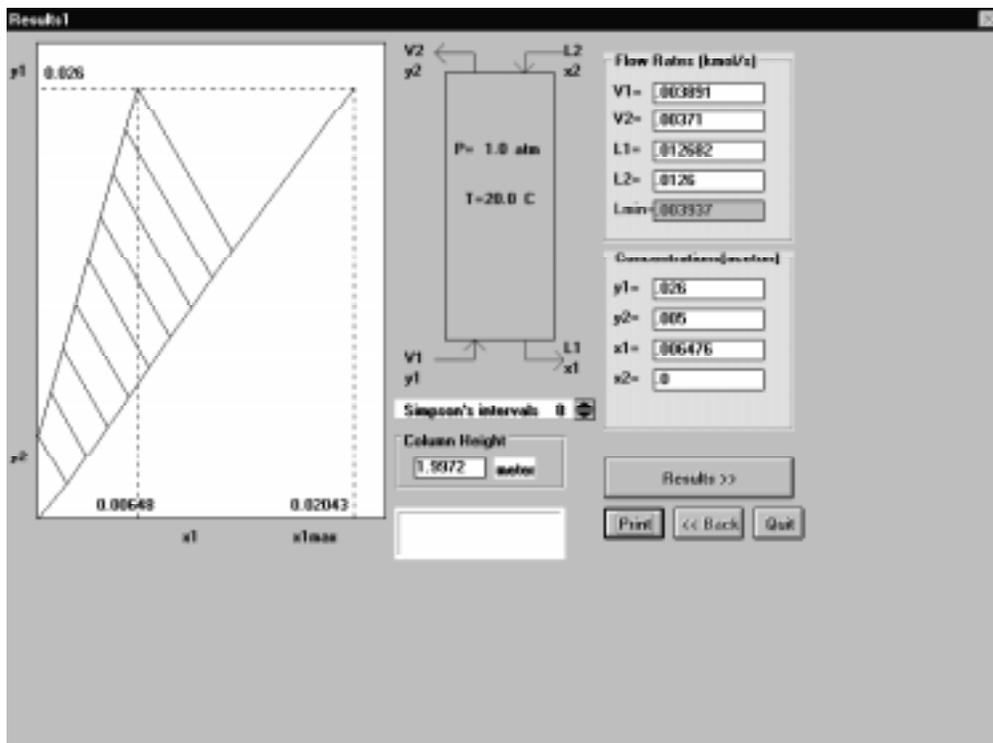


Figure 6. The graphical output section of the continuous packed column absorption.