CC-Dynamic Column
a new feature of Chemstations

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Recently the process simulation program CHEMCAD has been extended with the addition of a new product, CC-Dynamic Column. With this new program, processes dependent on time can be simulated. Simulation of mass and energy balances in a distillation column has been part of CHEMCAD for more than 10 years; the new dynamic model CC-Dynamic Column allows the investigation of the control responses and column stability under upset conditions. With this tool field tests are no longer necessary, due to the fact that during plant design the best strategy can be found and tested. Moreover previous jobs can be simulated and optimised. Therefore, the CC-Dynamic Column represents an optimisation tool in order to achieve the utmost best results with the lowest amount of effort. The danger of producing off specification material is reduced.

The following example deals with the dynamic simulation of a distillation column. In order to simulate the entire time behaviour a simulation of the column alone is inadequate. The controller, controlling valves and dynamic vessel are also required for the total simulation. Figure 1 shows such a distillation column consisting of the systems

- condenser
- distillate receiver
- distillate pump
- reflux drum
- reboiler system
- side stream draw-off
- bottom draw-off
- condenser pressure control
- distillate draw-off control
- side stream draw-off control
- reboiler heating control
- product draw-off control

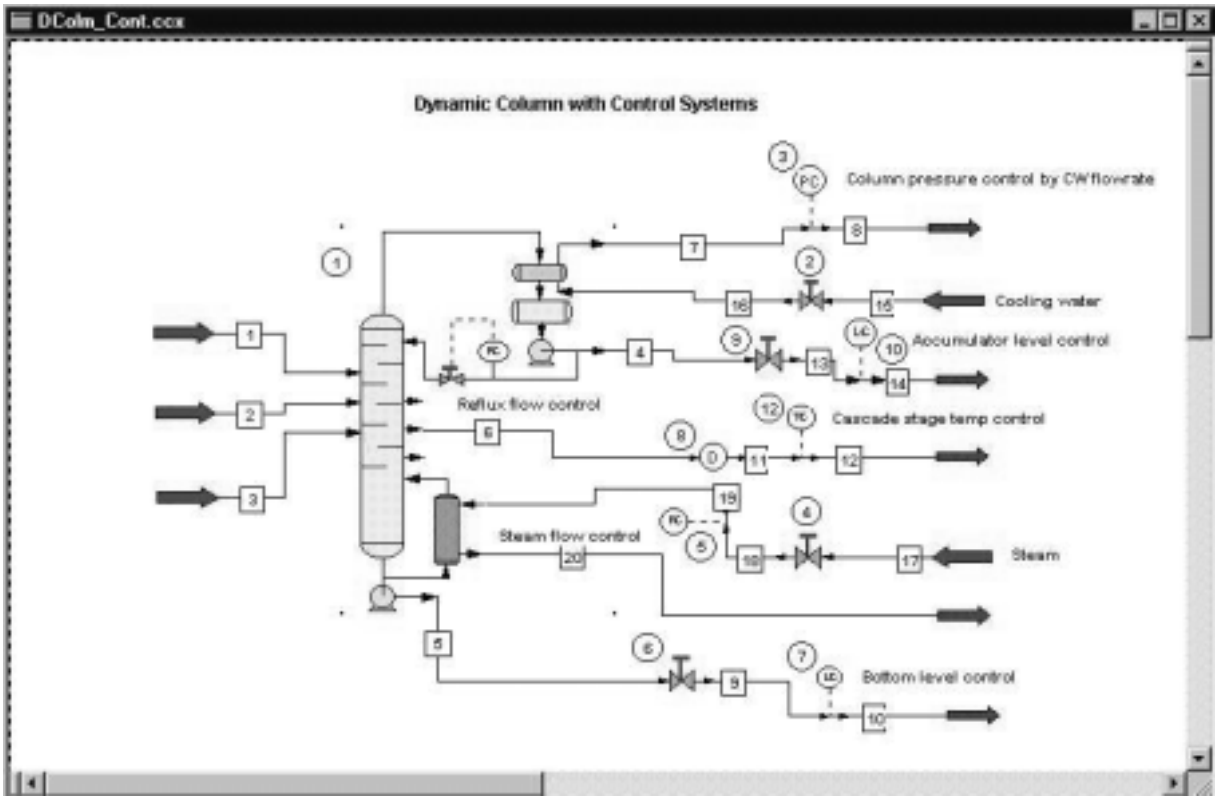


Figure 1
Flowsheet of a dynamically simulated column

The user can create this flowsheet easily, using the mouse. From the symbol palette the appropriate unit operations can be selected and then connected with lines, which represent the streams. Thus the complete column set up can be modelled. Changes can be made, swiftly and easily at any time. The subsequent specification of the individual unit operations and the feed streams as well as the choice of the thermodynamic model complete the preparations for the simulation. Mathematical inputs such as differential equations are not necessary.

The PID controller will be used as an example to demonstrate how easy the input of necessary parameters is. A single click on the appropriate symbol opens the menu pages. These pages allow the simulation of the plant to be defined.

All data can be adjusted to every measuring parameter. At any time the user can decide how to enter the pressure, in bar or atm. The integrated database gives evidence about the physical properties used for the single components.

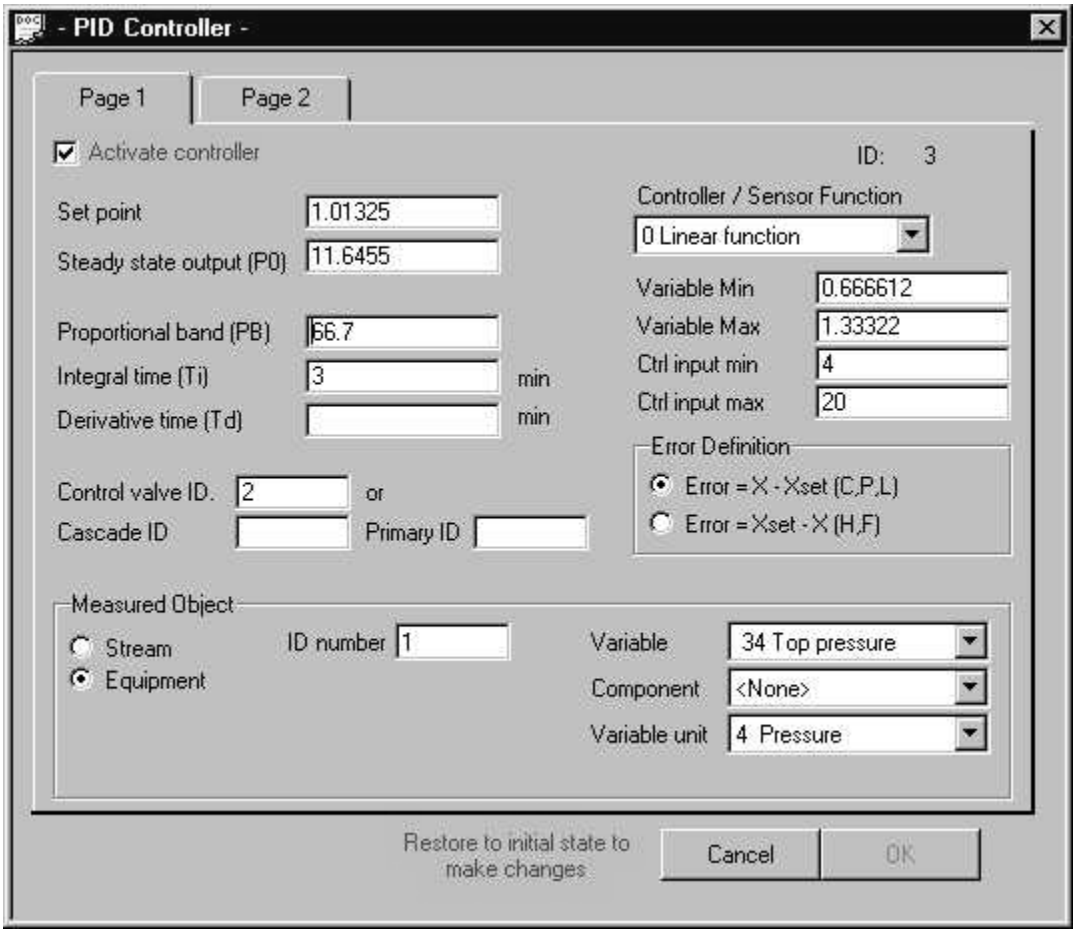
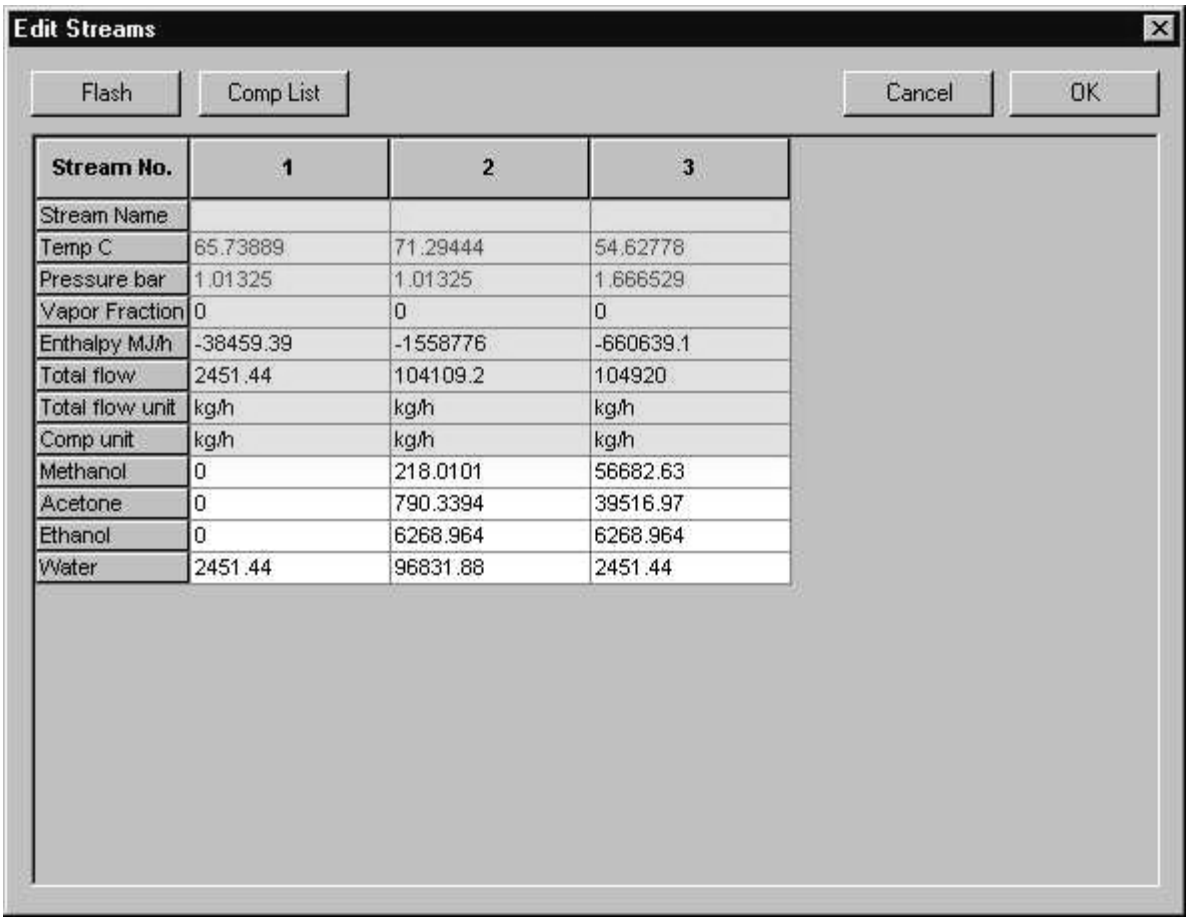


Figure 2
Input menu of a PID controller

It can be seen that the Proportional band, Integral time and Derivative time values can be entered (66.7, 3 and 0 in this case). The controller sends a 4 – 20mA signal to the control valve no. 2. The controller calculates its output from the difference formed by the pressure in unit operation 1 (column) and the given pressure (1.01325 bar). The signal sent by the controller to the control valve adjusts the valve position according to it's control parameters, thus allowing more or less cooling water to run into the condenser. This influences the pressure in the condenser, thus allowing the system to achieve steady state. In this simulation, 6 control systems are modelled. This, together with the column loading itself, represents a typical set-up used by many companies.

In this example the purpose of the distillation is to separate a mixture consisting of methanol, acetone, ethanol and water. Here the low boiling acetone should exit the system as pure as possible.

The feed mixture is formed from 3 feed streams, which are fed to the column, see fig. 3. The simulation shows the results obtained during 300 minutes, i.e. in 5 hours. The complete simulation time using a typical PC normally takes only minutes. A single simulation of a column needs only seconds.



Stream No.	1	2	3
Stream Name			
Temp C	65.73889	71.29444	54.62778
Pressure bar	1.01325	1.01325	1.666529
Vapor Fraction	0	0	0
Enthalpy MJ/h	-38459.39	-1558776	-660639.1
Total flow	2451.44	104109.2	104920
Total flow unit	kg/h	kg/h	kg/h
Comp unit	kg/h	kg/h	kg/h
Methanol	0	218.0101	56682.63
Acetone	0	790.3394	39516.97
Ethanol	0	6268.964	6268.964
Water	2451.44	96831.88	2451.44

Figure 3 - Composition of column feed streams

For this example a column with 50 theoretical stages is available. NRTL serves as the thermodynamic model, and all binary parameters are available in the CHEMCAD database. There are approximately 20 thermodynamic of which UNIFAC or PSRK could be chosen.

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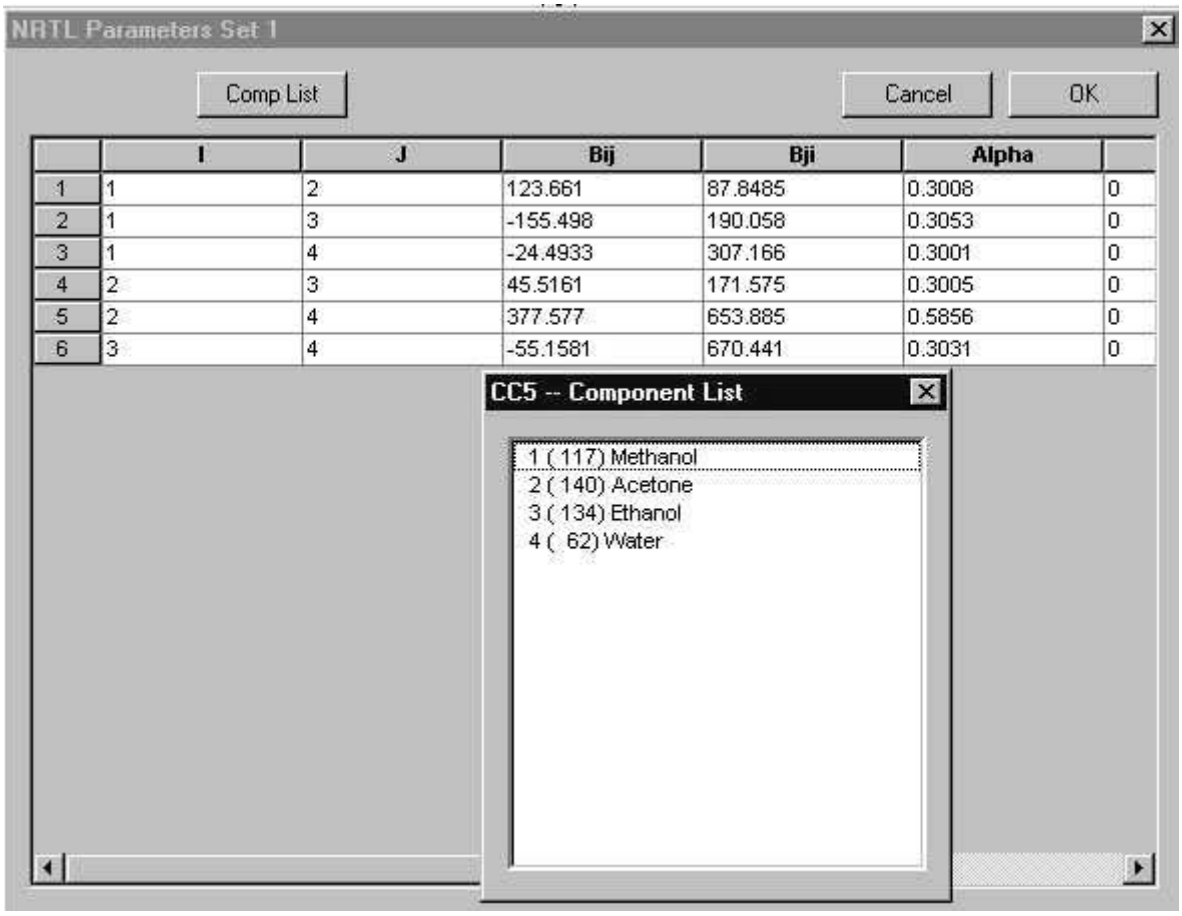

Figure 4
NRTL parameters for 4 components

Figure 4 shows the NRTL parameters of the 4 components. With this model, in combination with the binary parameters, the vapour-liquid behaviour in the column, on each of the 50 stages, as well as the vaporisation and condensation, is simulated. The integrated database contains more than 1800 gases, liquids, solids and electrolytes, the parameters for physical properties mainly coming from the DIPPR (USA) database and more than 6000 binary data from the DECHEMA data bank.

The condensation takes place using cooling water. The flow of water is controlled via pressure in order to maintain a condensation pressure of 1.013 bar. The actual pressure behaviour versus time is shown in the figure 5. It is interesting that initially the pressure shows a short and strong peak, but after approx. 10 minutes it stabilises.

The reality is that mass transfer and reduction of pressure in the column at start-up cannot be achieved instantly thus leading to pressure turbulence during start-up. This can be seen from actual operational data.

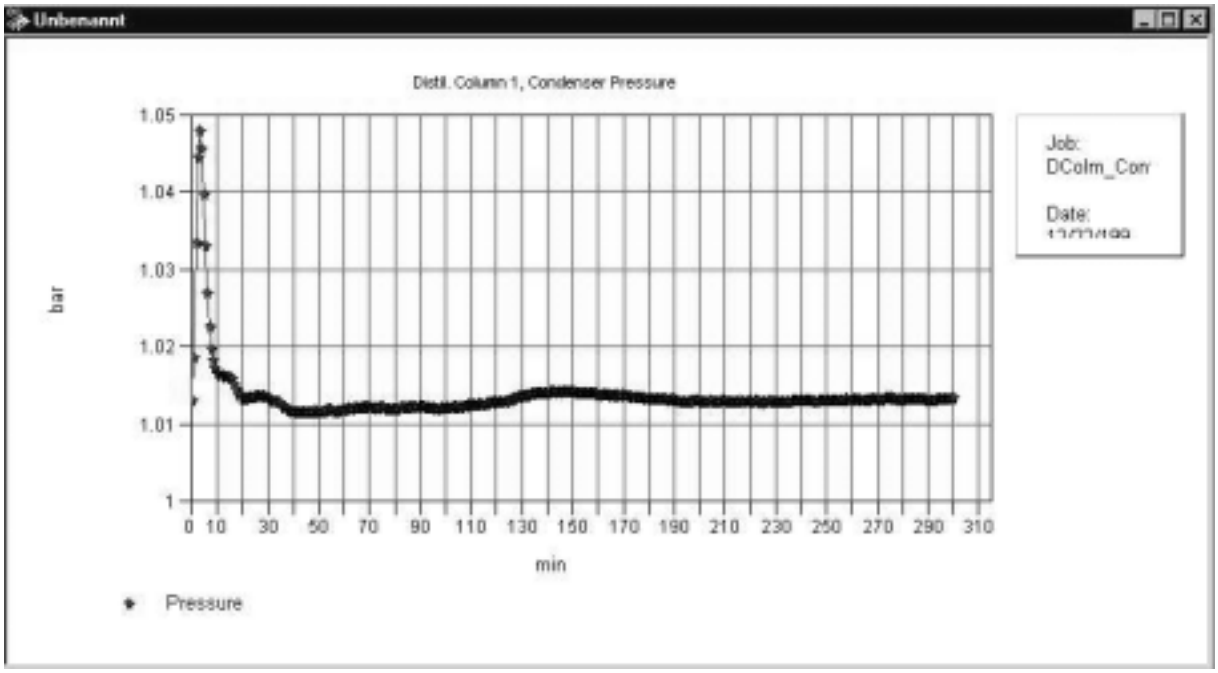

Figure 5
Loss of pressure during distillation

The flow of the distillate is dependent on the correlations for the control responses and is not constant, it starts at 35000 kg/h, increases to 80000 kg/h and gradually stabilises at 50000 kg/h as shown in figure 6. The reflux flow is controlled constantly whereas the flow of distillate is dependent on the Level control in the condensate collection vessel. This procedure is typical in practice to achieve the aim of maintaining steady state conditions.

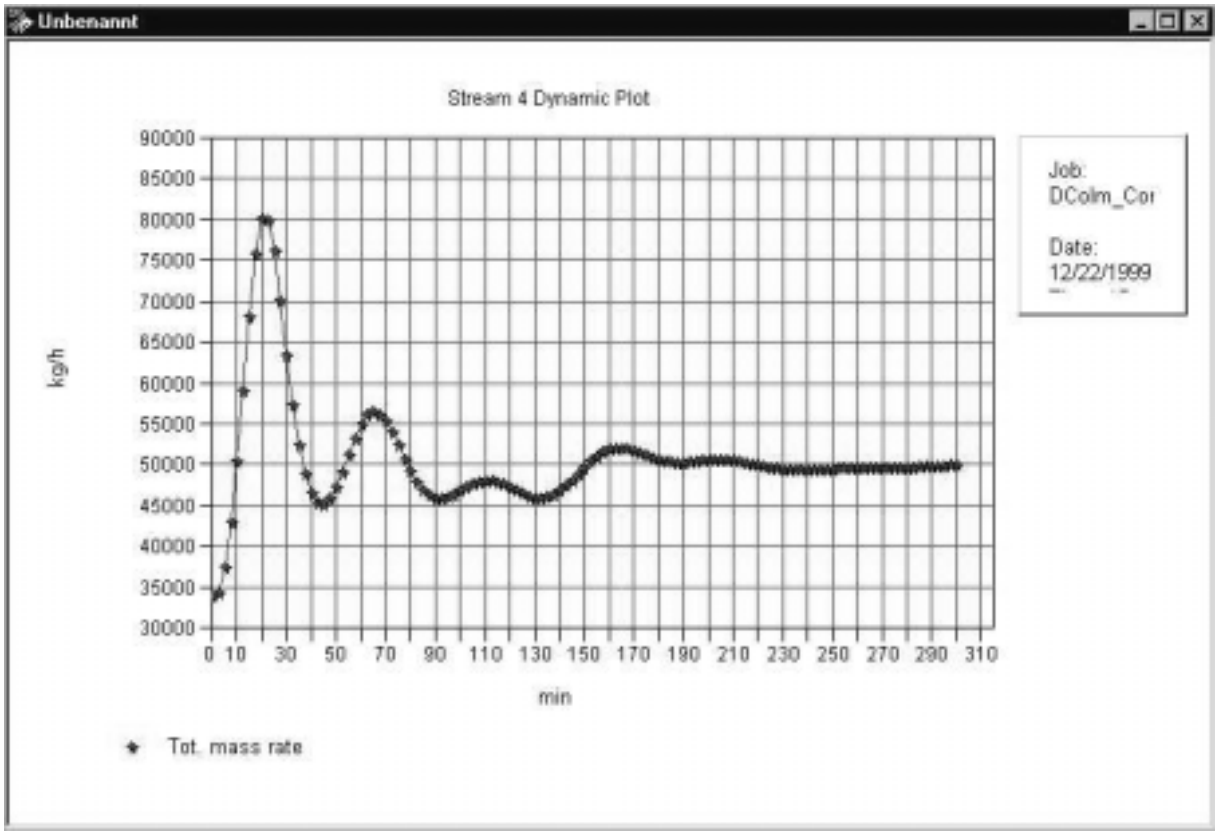

Figure 6
Amount of distillate during distillation

Likewise, the distillate composition, as shown in figure 7, is not constant initially. The concentration of acetone is high at the beginning and stabilises at a lower value after approx. 20 minutes. This is due to the high initial reflux ratio compared to steady state conditions after the reflux ratio has stabilised.

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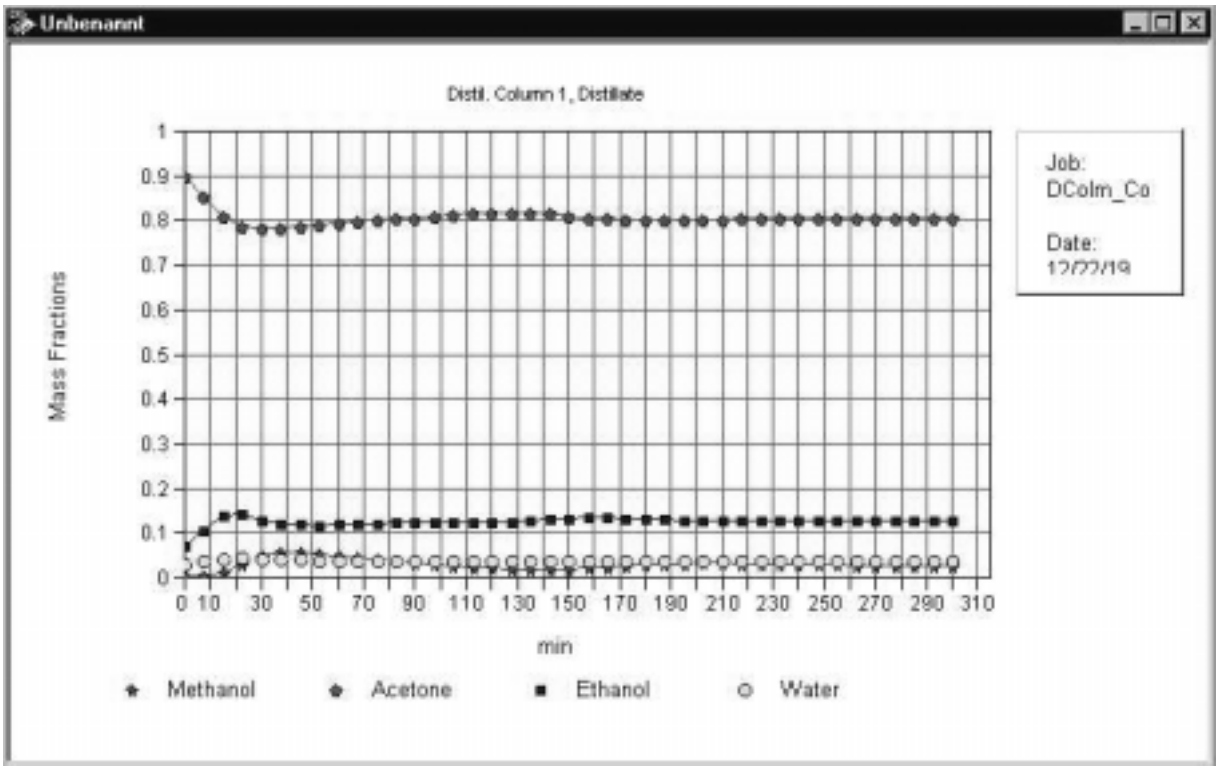

Figure 7
Composition of the distillate

The changing value of the reflux ratio can be shown, although it is a mathematical parameter. Figure 8 shows the reflux ratio during distillation. Considerable deviations can be seen, especially during the first 3 minutes. Initially the reflux ratio has a value of 2.5, which then drops dramatically down to 1, before finally stabilising at a value of 1.7.

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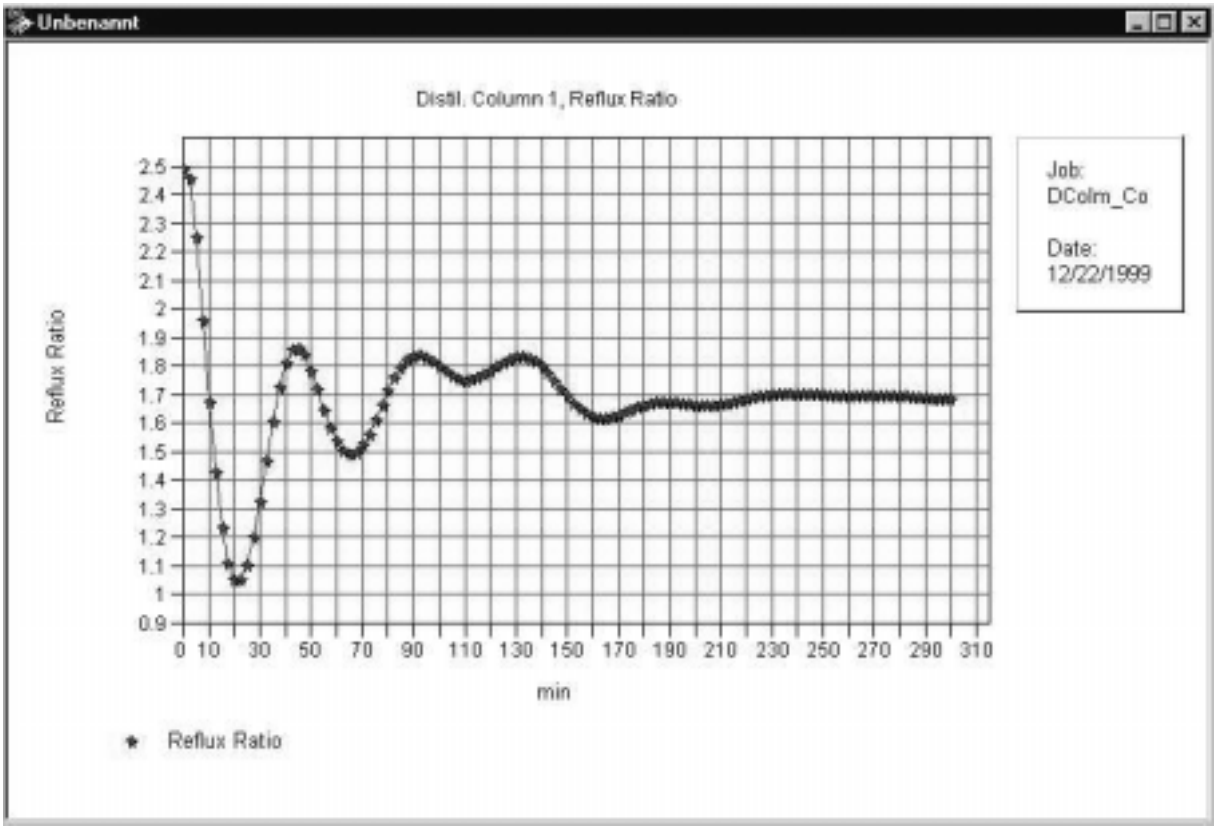

Figure 8
Reflux ratio

If further investigations concerning the composition of the distillate allied with the question of why the reflux ratio is so high at the beginning are required, then this procedure is quite simple, as the programme (CC-Dynamic Column) not only provides a great amount of graphical presentations but also allows adjustment of parameters for PID controllers and control valves.

After each adjustment of the parameters the dynamical simulation can be run again and the results can be viewed. Thus the engineer requiring preliminary sizing data for a distillation column can now carry out a realistic PC simulation and optimisation of the control and the can view the results. Thus it is possible to obtain answers concerning start-up, intermediate and steady state behaviour.

The simulation is done in such a way that all unit operations, i.e. column, controller, valve, etc. are elements in a differential equation, though each individual unit operation is calculated at steady state. The corresponding Euler-Cauchy algorithm takes these elements as single functions and then they are

considered in numerical order and solved within a defined range. Special iteration methods are used to ensure an accurate simulation.

The column itself can be chosen with a number of theoretical stages, with stage efficiency parameters and also as mass transfer columns with packing or trays. There are many options for the column such as separation of two liquid phases, extractive distillation, azeotropic distillation, reactive distillation, electrolyte distillation, etc. these being selected by the user according to his requirements.

In order to compare several graphical presentations it is possible to show them altogether on the screen. Figure 9 shows the graphs discussed above along with a plot of reboiler duty versus time. This new data confirms that the reflux ratio starts with a high value at the beginning of the distillation. The reboiler duty is 80500 MJ/h initially then increases rapidly 10 approx 110000 MJ/hr before gradually stabilising at 100500 MJ/h. This initial oscillation, however, takes approx. 160 minutes and thus influences the reflux ratio and subsequently the separation efficiency of the column.

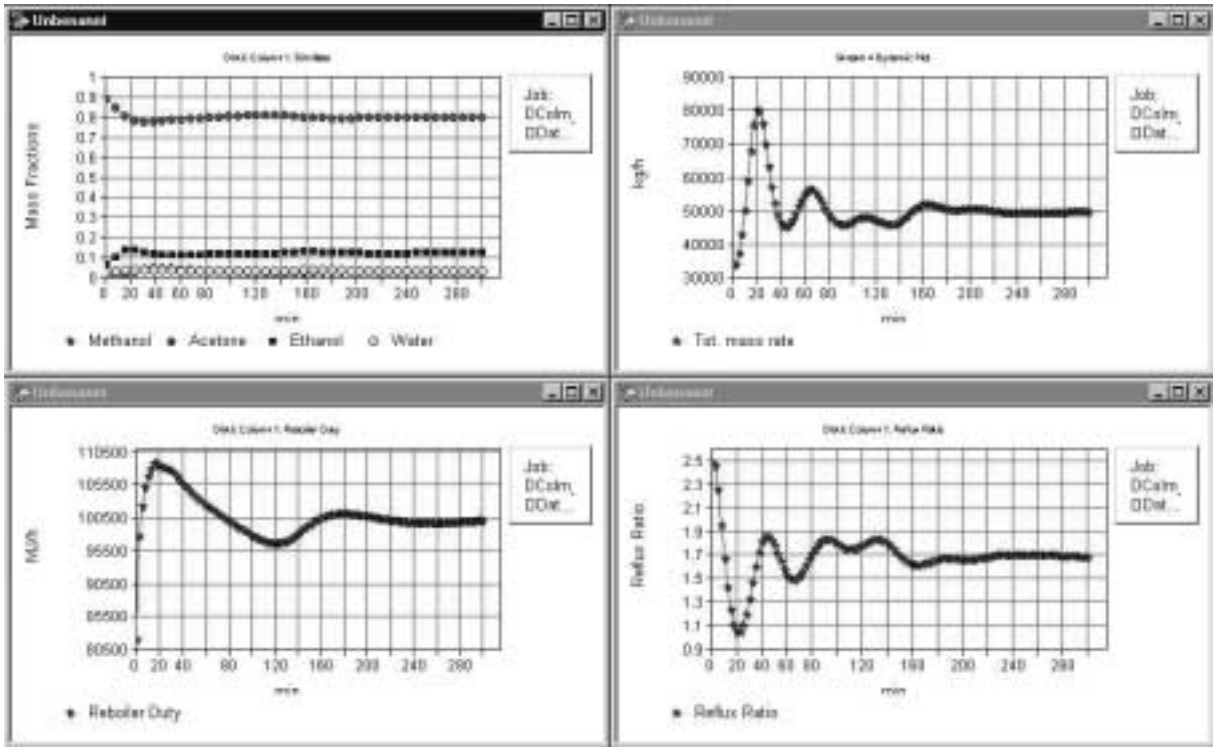

Figure 9
Multiple graphical presentation of several plots

In addition CC-Dynamic Column allows the printouts of numerous data such as column profile, composition of all streams, physical properties, design data and cost calculation of the column. These are printed as text files or Excel tables. With the CHEMCAD program, sensitivity studies and targets can be automated. Phase equilibrium data can be shown in TPXY diagrams in order to estimate the separation possibilities of binary components. It is also possible to obtain the phase equilibriums from physical property data.

Examples as well as a tutorial are available for demonstration and trials. The software is available free of charge for the period of 4 weeks.

CHEMCAD is an ideal PC Windows programme for the development and optimisation of chemical processes. CHEMCAD has been successfully marketed for 12 years and is distributed in Western Europe by Chemstations Deutschland GmbH in Wesel who also render support and seminars. In England, the UK agent is P&I Design Ltd, Thornaby, Cleveland. CHEMCAD was programmed and developed in the United States of America.

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