

CHEMCAD 5.0

THE NEW AND QUICK GENERATION OF PROCESS SIMULATION

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One does not necessarily expect a process simulation programme that can be handled easily or that will calculate very quickly. The reason for using such a programme is to simulate a complex chemical process, which normally would need weeks or even months.

The process engineer therefore, will be surprised to learn how easily the new CHEMCAD 5.0, working under Windows, is able to handle a variety of processes for the chemical, petrochemical, pharmaceutical and environmental technologies.

It is surprisingly easy for the beginner to create a flow sheet, to choose the required chemical components for his process and to find the correct thermodynamic model. The data input is quick and easy for initial components and unit operations. All the necessary steps are now available to simulate a process. After the simulation is run, a complete mass and energy balance of the process can be obtained.

First the beginner draws a flowsheet. A palette provides the necessary process units. This palette is shown in Figure 1, right hand side. More than 50 symbols help the process engineer to create a complete flowsheet. Almost all the commonly used process units are available. The size of the flowsheet is unlimited.

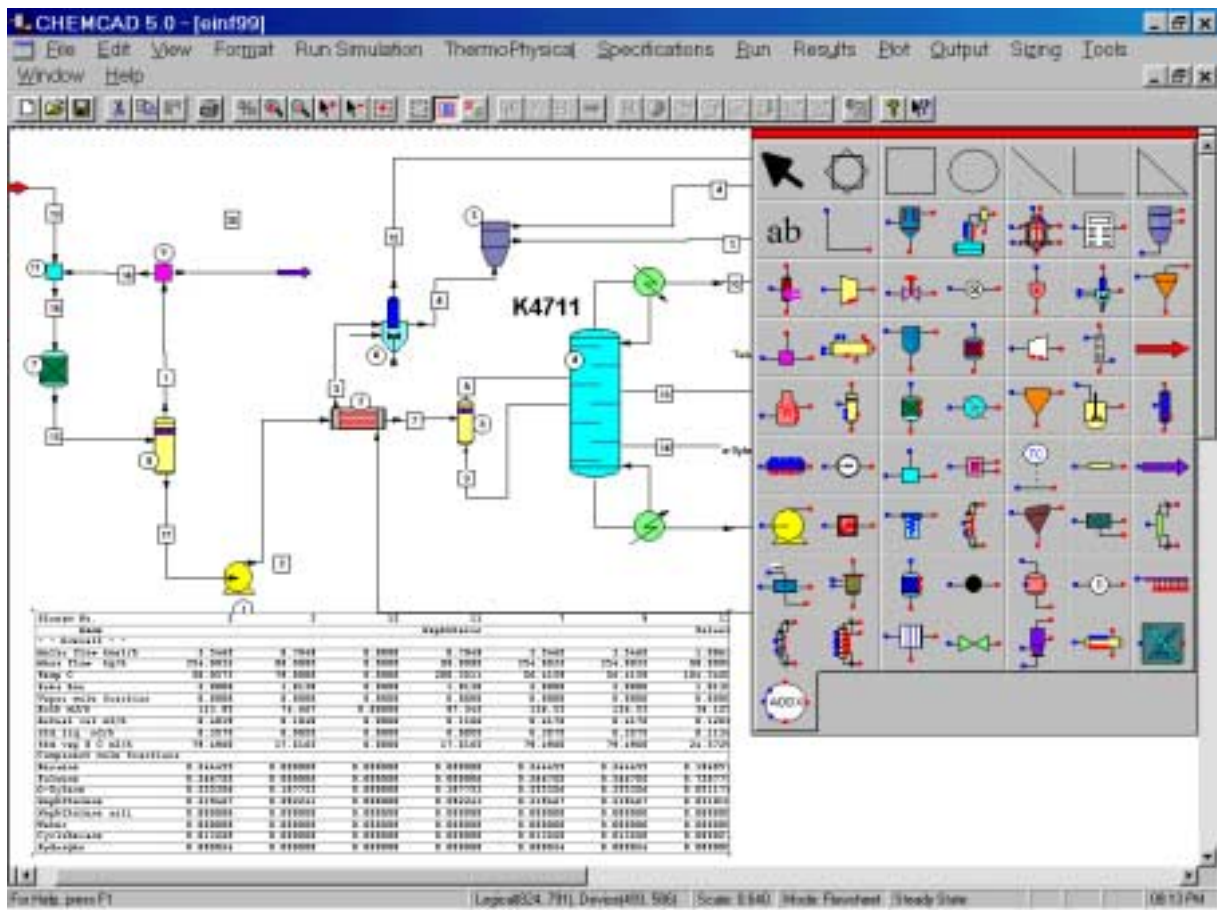


FIGURE 1
Flowsheet of a dehydration with distillation and crystallisation.

The process in Figure 1 shows a chemical reaction, phase separation, distillation and crystallisation with heat exchanger and dryer. In this example cyclo hexane is dehydrated and led in a circuit. The products benzene, toluene, o-xylene and naphthalene are preheated and distilled in a column. The naphthalene is cooled down, crystallised and dried. The reactor unit operation calculations are carried out in accordance with the principle of minimising the free Gibbs' reaction energy and thus calculate the composition of equilibrium without reaction equation.

After the simulation, the results can be shown numerically in WordPad, Word, Excel or graphically. A strong feature is the inclusion of numerical data output as PFD directly into the flowsheet as shown in Figure 1.

With almost 50 unit operations (column, reactors, heat exchanger, compressor, valve, pump, cyclone, etc.), 20 thermodynamic models (NRTL, Unifac, SRK, etc.), almost 1900 chemical components and 6000 binary data from DIPPR and DECHEMA Data Collection and a graphical windows platform the process engineer is able to take advantage of the extremely efficient tool CHEMCAD 5.0 when it comes to design and optimisation of new and existing plants.

With CHEMCAD 5.0 almost all processes for the chemical, thermal and mechanical process engineering industry can be designed, simulated and optimised within a very short time.

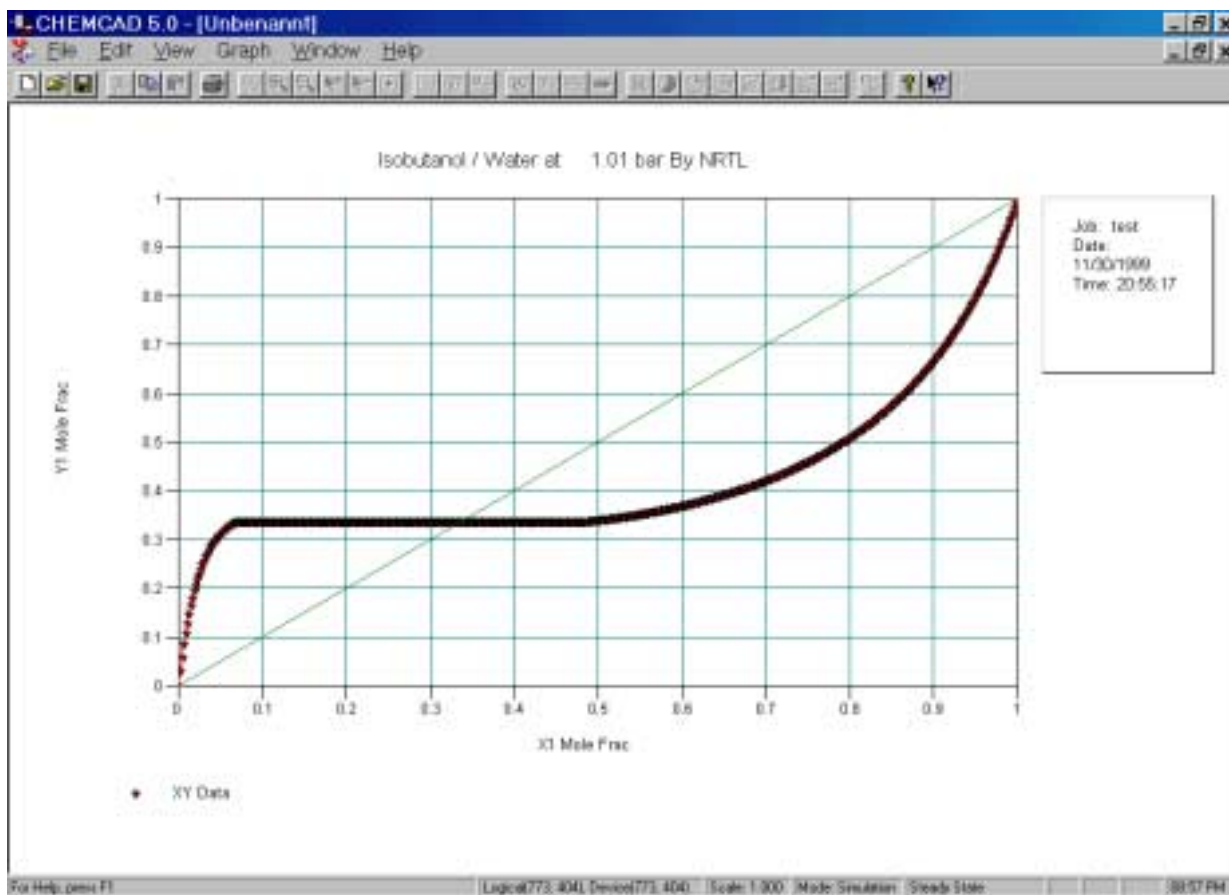


Figure 2
Vapour-liquid equilibrium n-butane-water according to NRTL.

The graphical presentation of physical properties and phase equilibrium is a further important tool in CHEMCAD 5.0, it can, for example, be used to predict the separation possibilities of a multi component mixture.

Figure 2 shows the phase equilibrium of the binary mixture n-butane-water at 1.013 bar according to the NRTL model. The heterogeneous azeotrope, (i.e. the mixture gap) of the 2 components is recognisable. It is also possible to show graphically ternary liquid-liquid equilibrium thus giving a good basis for the consideration of separation in a decanter in an extraction process.

The graphical presentation of physical properties such as viscosity or vapour pressure is possible for single components and mixtures of components. Figure 3 shows the vapour pressure for a group of some aromatics in a double logarithmic form.

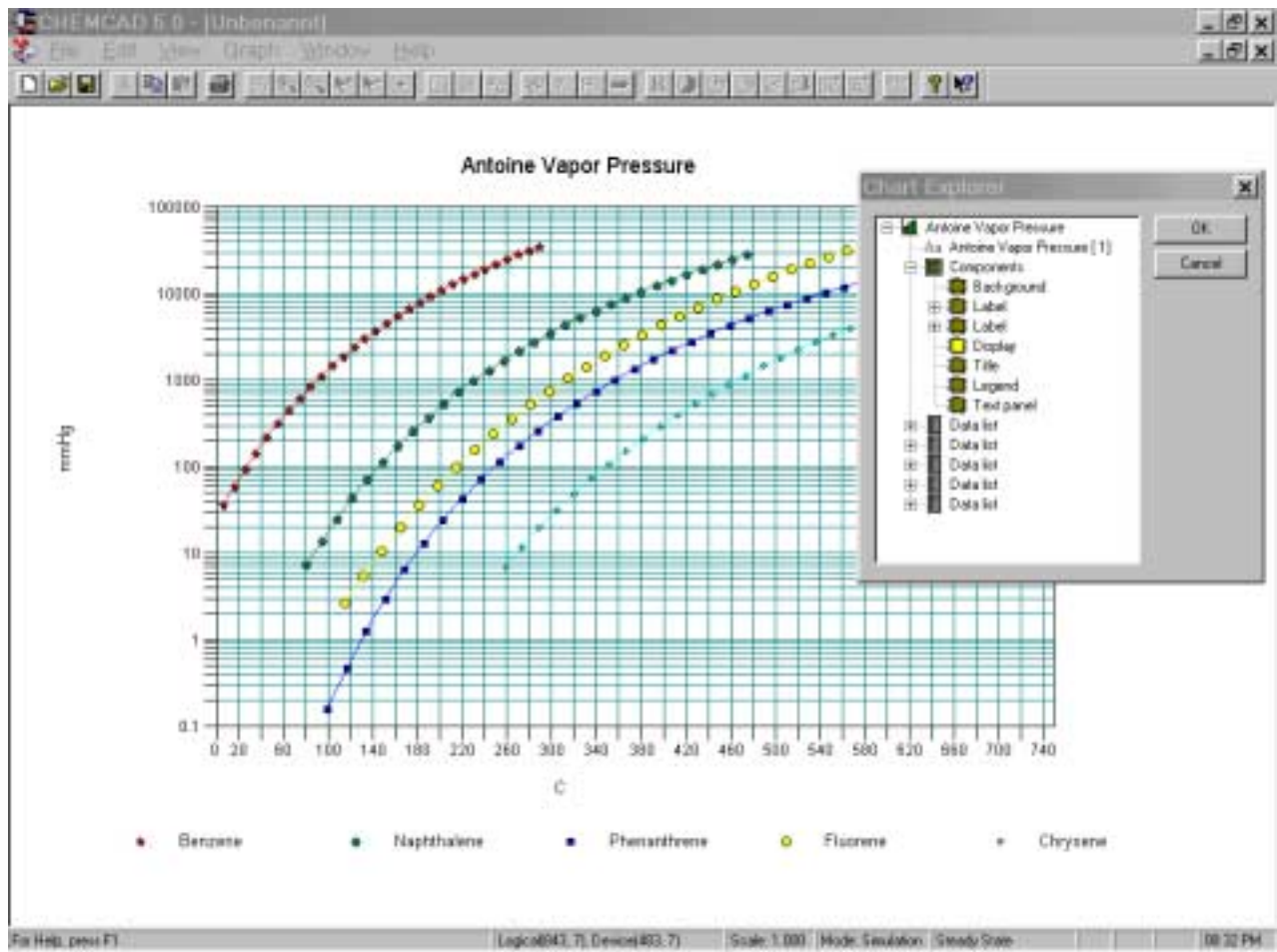


Figure 3
Vapour pressures of some aromatics according to Antoine

The help window shows the various possibilities for graphical treatment. The database can be extended with any customer's own data and physical properties. Initially CHEMCAD calculates using increments of a molecule according to the modified Lydersen method (as described in the VDI Heat Atlas, some basic data are indispensable for the simulation). Due to proven correlations CHEMCAD completes the physical properties calculation thus quickly providing the physical properties basis, which is necessary for the process simulation. A very efficient regression calculation is also provided, which allows measured data to be used for user specific components.

Using the sensitivity study as well as optimisation, CHEMCAD provides a highly efficient method to study a process. Thus the minimisation of energy, maximisation of yield, product optimisation etc. can be achieved.

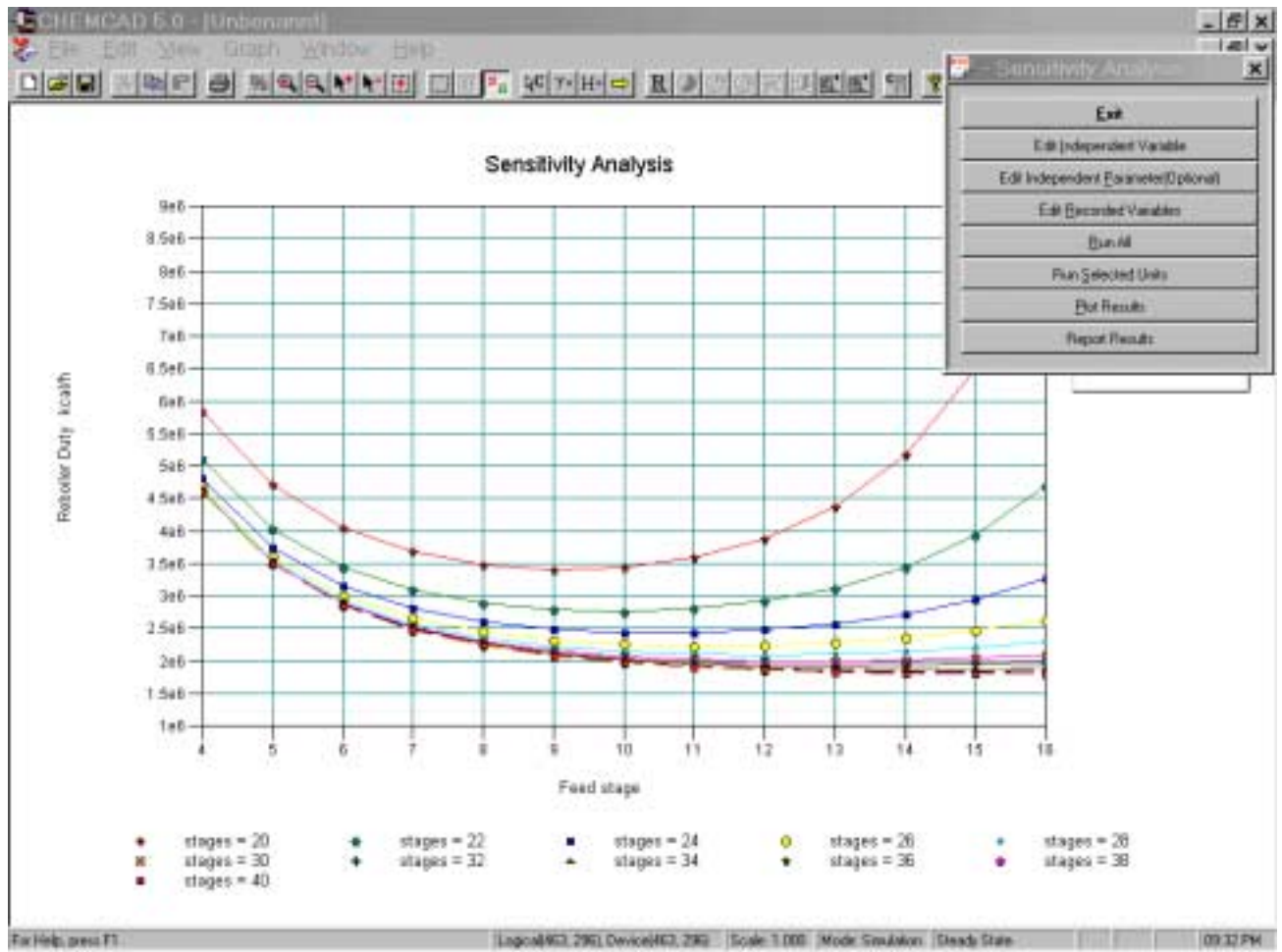


Figure 4
Sensitivity study for number of stages and position of the feed stage

Figure 4 shows the results of a study to minimise the efficiency of the reboiler in a distillation column depending upon the number of stages (x axis) and the position of the feed stage (parameter). The CHEMCAD 5.0 optimisation will calculate the minimum reboiler efficiency automatically with the help of proven numerical search algorithms within given limits.

Design calculations are available for columns, vessels, heat exchangers, valves, relief valves (DIERS), pipes and control valves. A cost prediction is available for most of the unit operations based on studies in the Chemical Engineering magazine, USA. Adjustment to match users' own experience is possible, as well as modifications to the calculation itself. With this, the user can carry out initial estimates for the construction and operation of the plant.

The menus, as well as the symbols for the unit operations, can be adjusted to specific user requirements. Programming of users own unit operations is also possible. The reports obtained in Excel are available as data interfaces. Graphics

can also be transferred to Excel. Thus the CHEMCAD 5.0 results can easily be used in other programmes.

The main application range of CHEMCAD 5.0 is in the design and optimisation of new and existing plants, i.e. continuous distillation, batch distillation, continuous reactors, batch reactors, heat exchangers, phase equilibrium, gas plants, gas washers, electrolyte processes, combustion, dynamical processes with controllers, solids component crushing and solids separation etc. It is also possible to calculate columns as a bottom column or as a mass transfer column.

Combined with controllers it is possible to simulate columns dynamically to allow the investigation of start-up and normal behaviour.

The main advantages of CHEMCAD 5.0 are

- easy handling
- easy to learn, supported by frequently offered seminars teaching the main topics (thermodynamics of mixed phases, physical properties and usage of main unit operations)
- extraordinary compatibility with results obtained in practice
- extremely high speed of calculation
- support 8 hours a day
- information rendered by own homepage <http://www.chemstation-eu.com>. Here numerous documents updated daily with application examples are provided ensuring the necessary confidence in usage and handling of CHEMCAD especially after a long break.

CHEMCAD 5.0 will run on all Windows platforms (95, 98, 2000, NT). CHEMCAD 5.0 has been programmed under C++ and due to the extensive Windows familiarity of the programmers, CHEMCAD will run quickly and with great stability.

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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