CHEMCAD Process Simulation Software under Windows 95/98/2000/NT demonstrated on an example of a continuous distillation as well as a batch distillation

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The new CHEMCAD has been released as version 5.0 and runs under Windows 95, 98, 2000 and NT, not only as a single installation but also as a network installation. CHEMCAD will run on all PCs and laptops working under Windows with the necessary Windows requirements.

CHEMCAD is a process simulation programme for quick calculation and simulation of chemical processes normally occurring in chemical, petro-chemical, pharmaceutical and environmental technology. Being an alternative to long-lasting manually done calculations CHEMCAD provides time saving calculations and simulations of small batch processes as well as large scale continuous chemical plants

A modern graphical package similar to AutoCad allows more than 40 different unit operations to be modelled, including the following:
Columns for reactive, azeotropic, extractive and batch distillation, extraction and scrubbing and gas washing.
Continuous reactors
Dynamic batch reactors
Compressors
Turbines
Pumps
Heat exchangers
Flash vessels (phase equilibrium)
Controllers
Crystallisers
Crushers
Cyclones
Sieves
And other unit operations.
These provide the ideal tools to develop and optimise chemical processes quickly and safely on the PC.

The data base included contains more than 1800 solids, liquids, gases and electrolytes, with more than 6000 binary data from the DECHEMA data bank. Other sources for vapour-liquid equilibrium, in combination with mixing rules and more than 20 thermodynamical models like Peng-Robinson, Soave-Redlich-Kwong, PSRK (Gmehling), NRTL, UNIQUAC, UNIFAC, mod. UNIFAC, Henry, etc., provide the ideal means to easily model processes with up to 200 chemical components and numerous unit operations.

The database can be quickly and easily extended to include customers' own components and own measured data. Incremental methods like Lyderson-Joback are available to estimate critical data, formation enthalpy and Cp values. Methods for the prediction of pseudo components from boiling analyses and regressions of measured data are also available. All data can be shown and plotted numerically and graphically.

The flowsheet to be simulated is not limited in size. The following figure 1 shows a flowsheet of a medium size plant designed to simulate a waste water plant where phenol and methanol are to be removed by extraction with methyl isobutyl ketone and vapour stripping. This procedure is based on a description in the literature which has been further developed by a study with CHEMCAD.

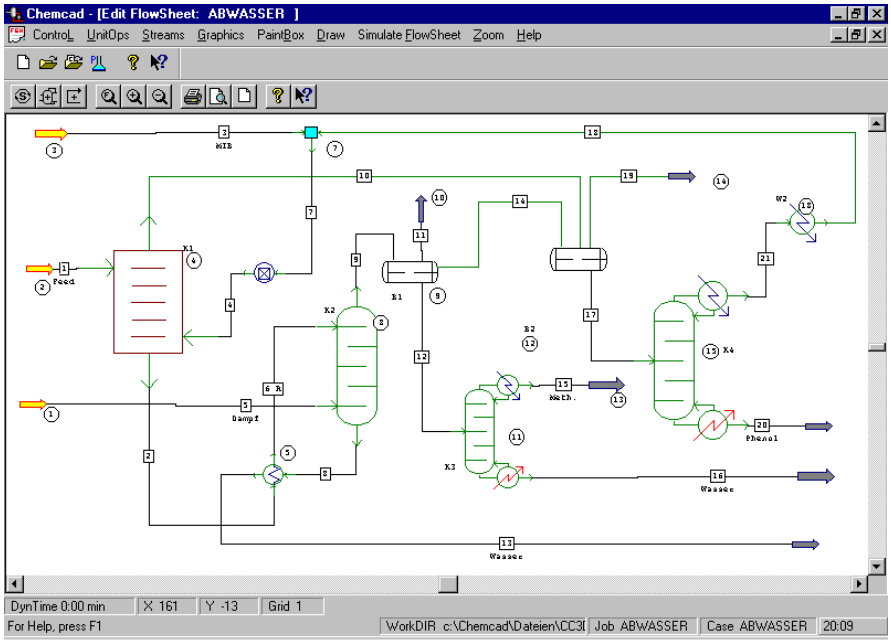

Figure 1
Waste Water Plant developed with CHEMCAD

Using CHEMCAD it was possible to draw conclusions about waste water processing and the costs involved.

More complex processes like coal tar distillation or mineral oil distillation can be simulated in their entirety with CHEMCAD. This is also applicable to other well-known processes in chemical process technology.

Using CHEMCAD for the simulation of a coal tar distillation column with approx. 40 components and 50 stages and a side stream, according to the UNIFAC method, the calculation needs less than 1 minute. Typical ingredients of coal tar are aromatics like benzene, toluene, o-xylene, naphthalene. With CHEMCAD their distillation can be modelled for continuous or discontinuous processes.

In a single continuous distillation column with a multicomponent mixture one component exits at the top and one at the bottom, other components have to exit via side streams. With CHEMCAD it is possible to model, using the concentration profile of the column, the efficiency with which several components can be produced from a single column. In the case of the batch distillation the recovery of several components is obtained in sequence depending on the time. This also can be simulated with CHEMCAD.

The following figure 2 shows a column profile of the a.m. mixture in a column of 40 theoretical stages (NTU).

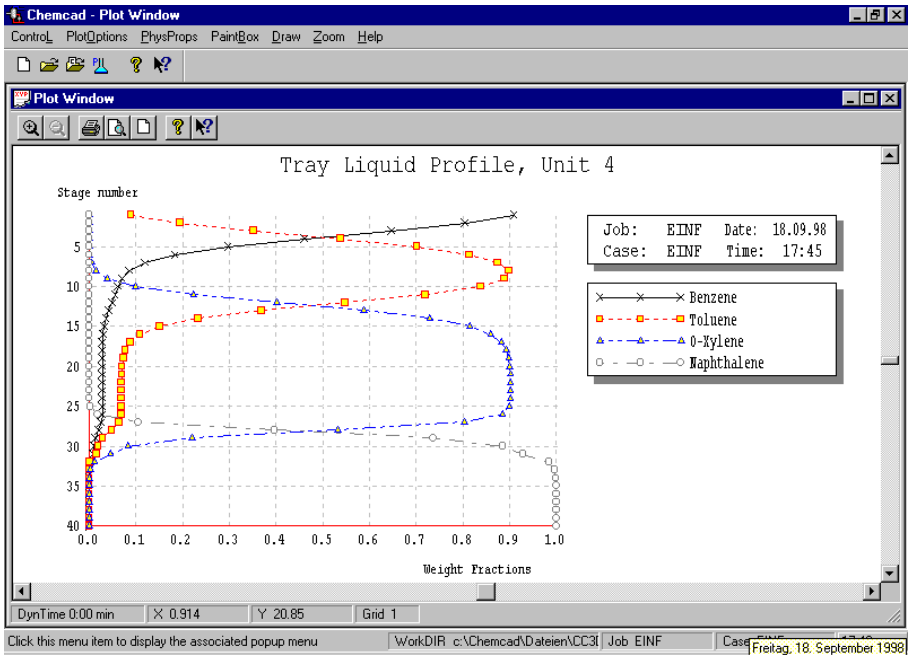

Figure 2
Column Profile for continuous distillation

The graphic shows that the maximum concentration of toluene and o-xylene (approx 90% each) are obtained at the 8th and the 29th stage (counted from the top) respectively. Benzene exits the top at a concentration of slightly more than 90 % and naphthalene exits the bottom with a concentration approaching 100%. To optimise these results a number of parameters were varied, the number of stages, their efficiency, the reflux ratio, the position of input and output stages, the outlet quantities and their phase – liquid or gaseous. The simulation allows these parameters to be varied, quickly and easily, as for convergence the latest column profile can be used. Activating the function "sensitivity analysis" is a great help. Parameter studies can thus be carried out automatically and the results can be shown graphically and evaluated. This leads to a considerable improvement in the purities of all components.

Batch distillation can also be simulated with CHEMCAD and, therefore, represents an alternative to continuous distillation. The following figure 3 shows the progress with respect to the time of a batch distillation with the same multi-component mixture.

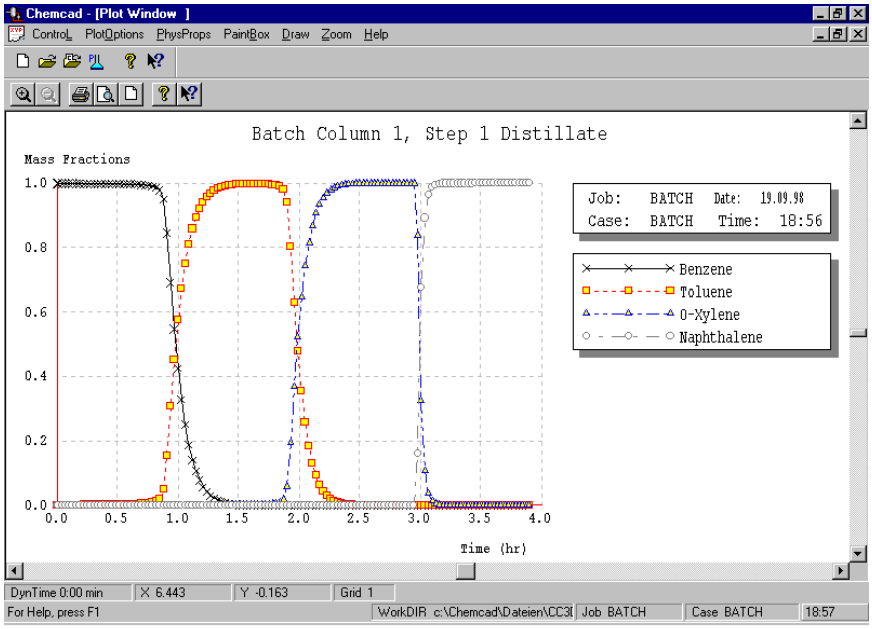

Figure 3
Time profile of a Batch Distillation

In order to achieve the maximum purity of each component, CHEMCAD allows the time periods at the batch column to be fixed thus obtaining the correct main and side fractions. The criteria to interrupt the time periods can be determined by time or depending on the result. So the first fraction can be terminated when the benzene concentration is below 99.5 % for example. An intermediate fraction can be terminated as soon as the toluene concentration reaches 99.9 %., etc.

Thus it is possible to produce numerous fractions which can be fed to separate tanks. With CHEMCAD it is possible to create a flowsheet of the batch distillation as well as the continuous simulation. Moreover the intermediate fractions can be fed to a new batch distillation and then redistilled.

If 2 liquid phases are formed in the mixture which has to be distilled the corresponding vapour-liquid-liquid-phase equilibrium is calculated. This is especially important in case of condensation and probable separation of the distillate. Thus, heavy and light phase of the condensate can be separated. Thus dry (water-free) ethanol can be separated from an ethanol-water mixture by adding n-pentane or benzene.

The calculation method for distillation in CHEMCAD is done to a high standard in accordance with the matrix method. A quick convergence and short simulation time is therefore guaranteed. In most cases the user need not be concerned with the details of the internal calculation, this is done automatically by CHEMCAD.

In addition to the actual simulation, CHEMCAD allows sizing calculations of columns, heat exchangers, vessels, pumps, etc. and includes a cost prediction. More utilities include TOC analysis, formation of hydrates on oxygen, simulation of blowdown vessels, Relief valve sizing according to DIERS theory, etc.

CHEMCAD can be extended with customer’s own unit operations produced as DLL data, Excel data sheet or module in Visual Basic.

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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