

...intuitive – reliable – powerful... Chemstations' Simulation Software

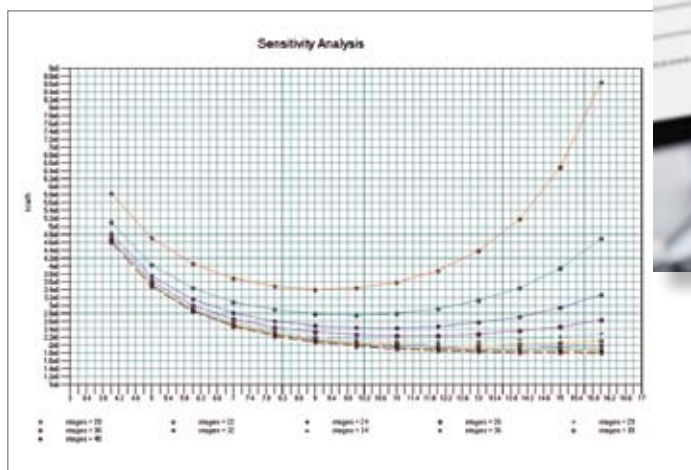
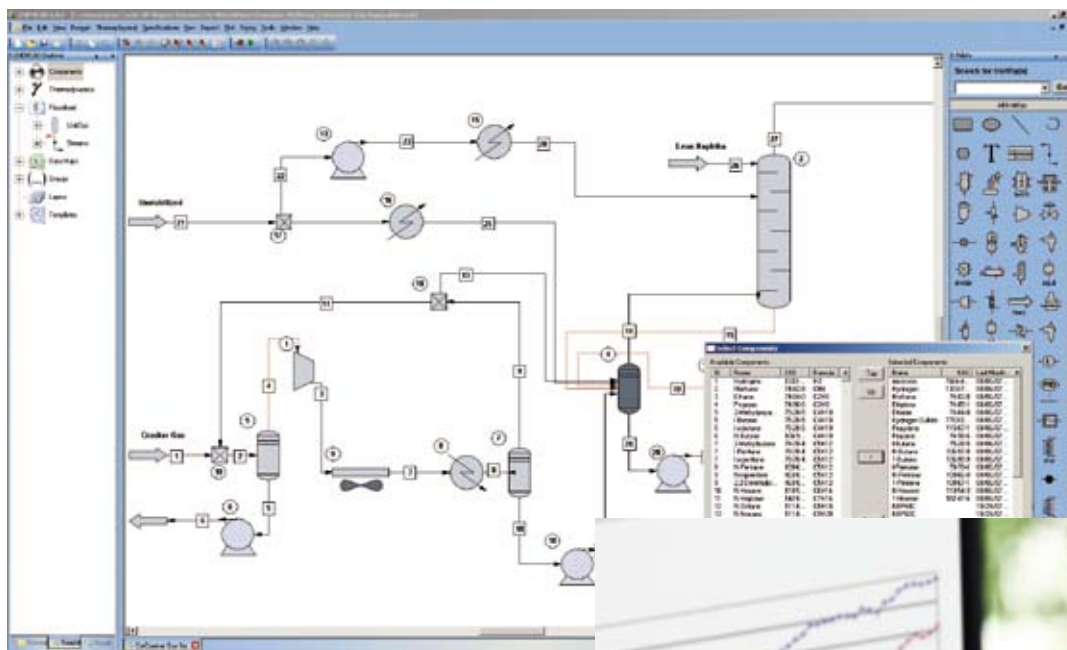
- ➔ CHEMCAD
- ➔ CC-BATCH
- ➔ CC-THERM
- ➔ CC-DYNAMICS
- ➔ CC-SAFETY NET
- ➔ CC-FLASH

Almost all processes in chemical, petro-chemical, pharmaceutical, mechanical and environmental process technologies can be simulated with CHEMCAD.

The entire CHEMCAD Suite, with its add-on modules, offers a powerful and efficient range of simulation programmes. Each programme can be acquired as a stand-alone version or as an add-on version to the main programme CHEMCAD. CC-SAFETY NET and CC-FLASH are already included in CHEMCAD.

Simulation with CHEMCAD is based on a large database including more than 2000 components for gases, liquids, solids and electrolytes. Extensive thermodynamic models are available to calculate phase equilibria and a graphical palette of common unit operations complete the user-friendly modern and intuitive interface of the CHEMCAD SUITE.

The user can quickly configure a graphical flowsheet of simple or complex processes and then enter data in a Windows® format to calculate the process, mass and energy balances,



which are reported in Excel or Word. Many unit operations can be calculated including capital cost estimation. CHEMCAD offers a wide range of graphical presentations with respect to physical properties, phase equilibria, heat curves, column profiles and sensitivity studies.

In our seminars you will be trained thoroughly in the use and application of CHEMCAD which will acquaint you very quickly with all the features of CHEMCAD.

The Experience

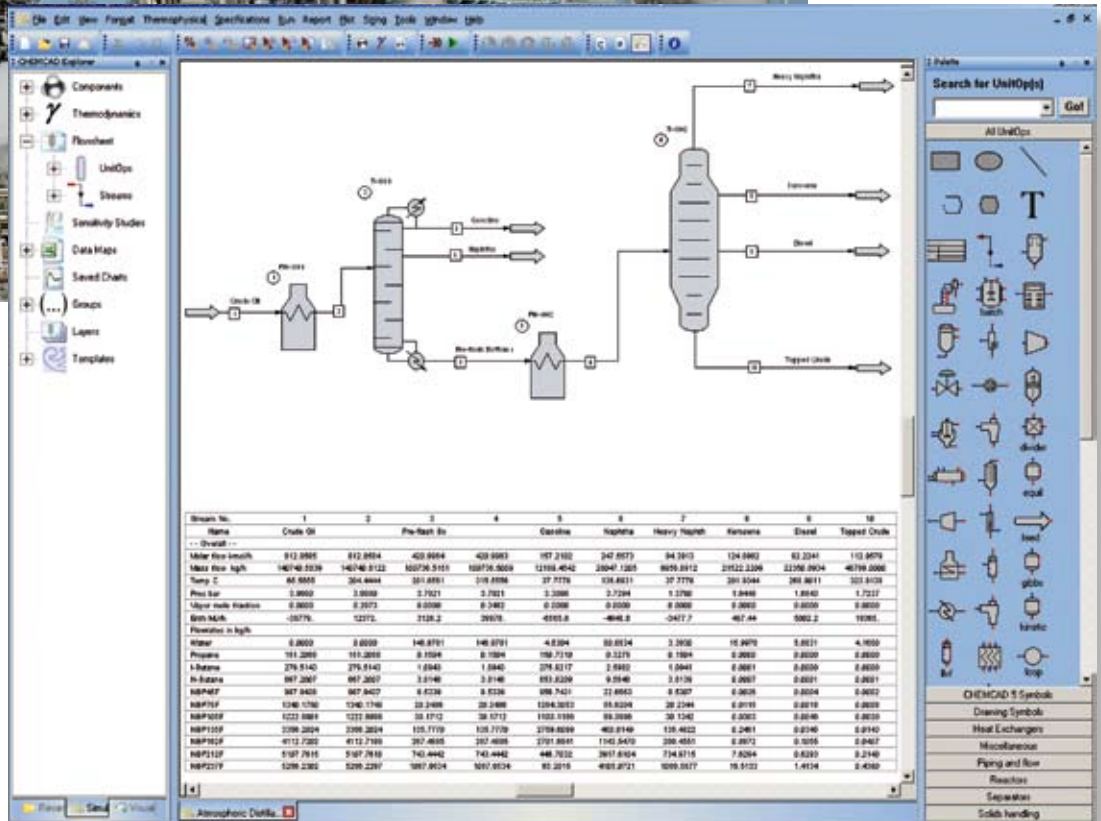
Throughout the world, many processes are being simulated successfully with CHEMCAD and giving excellent comparisons with reality. Based on this even established processes can be improved and optimised, thus avoiding expensive plant studies. From initial concept CHEMCAD is used in plant simulation in order to verify the realisation of an idea. When

using CHEMCAD a process goal is achieved within a very short timescale avoiding expensive laboratory or pilot plant trials. **Thus time and money are saved!**

CHEMCAD is an indispensable tool in order to explore emerging markets with new products.

Questions concerning the physical properties, chemical equilibria or behaviour of mixtures – CHEMCAD provides reliable answers, results and solutions.

In your daily work take advantage of the numerous benefits offered by CHEMCAD, simulate your processes with CHEMCAD – we will be at your disposal with our support and advice any time free of charge.



CHEMCAD (steady state)

Typical Applications

- ➔ distillation (rectification)
- ➔ gas washing, absorption and desorption
- ➔ chemical reactions, kinetic and equilibria
- ➔ recycle processes, heat exchange, pressure drop
- ➔ handling of solids
- ➔ neutralisation of acids and alkalis

Advantages of CHEMCAD

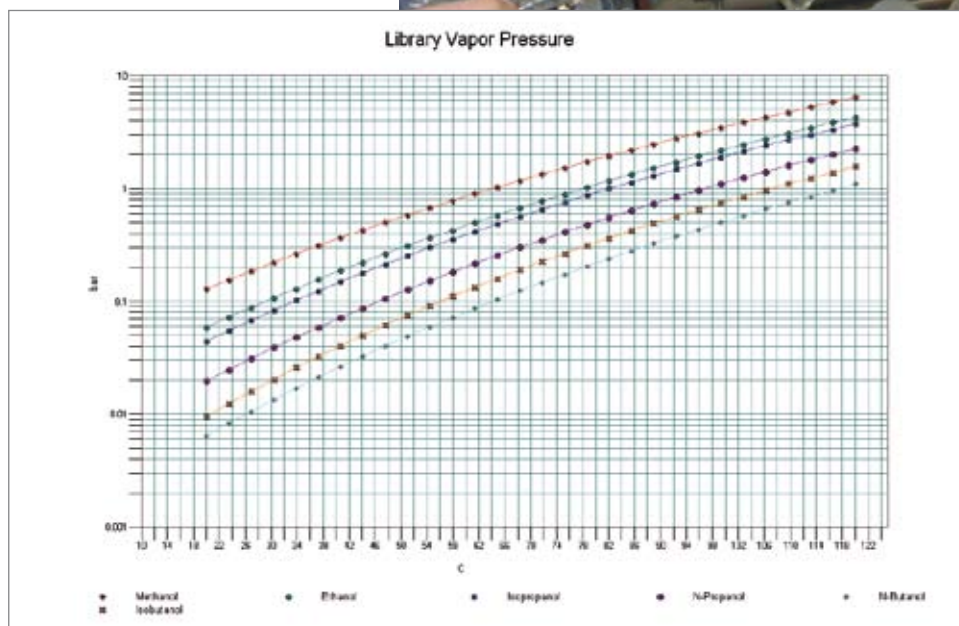
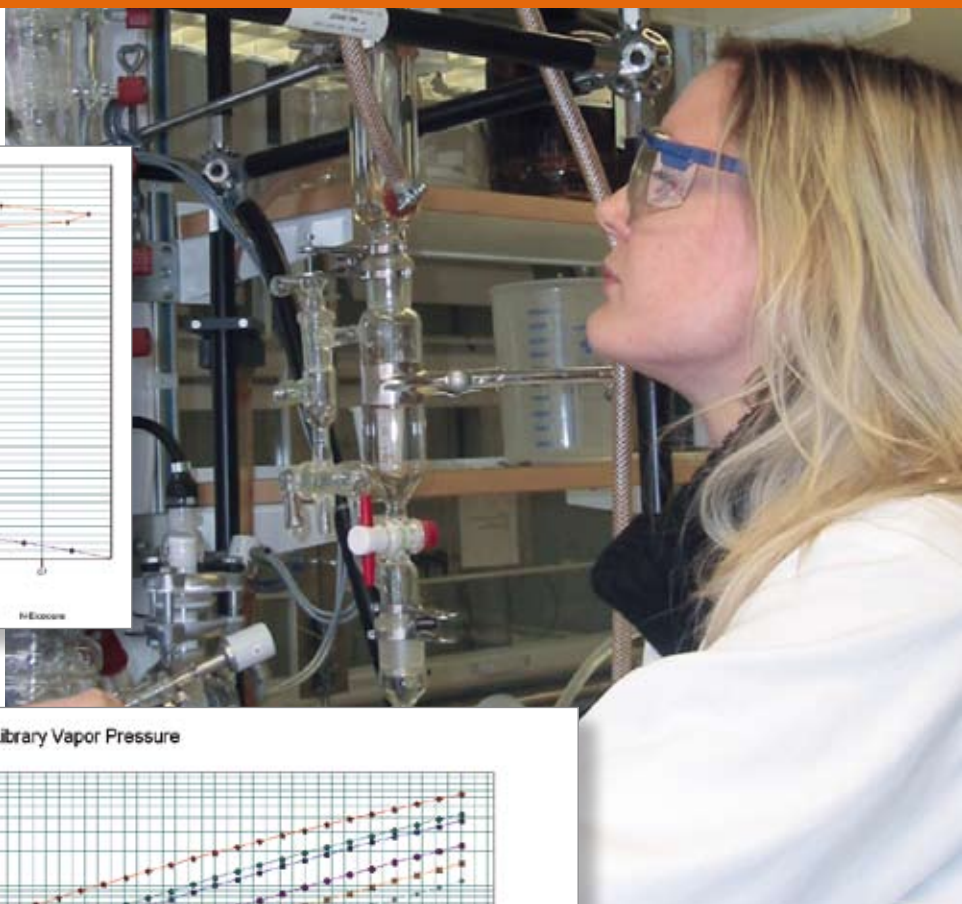
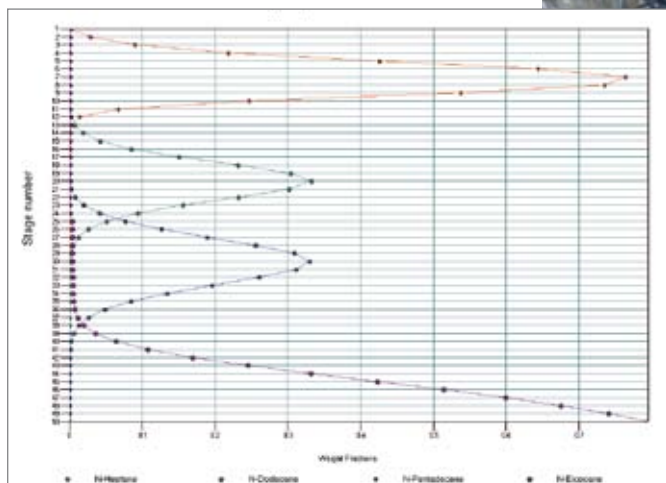
- ➔ CAD Flowsheet, easy to use
- ➔ unit operations for gaseous, liquid and solid processes
- ➔ data base with more than 2000 components (gases, liquids, solids and electrolytes)
- ➔ thermodynamic models for VLE, LLE and SLE

CHEMCAD represents the basic programme of the CHEMCAD Suite. CHEMCAD is the tool to simulate steady state processes. Once CHEMCAD is installed, you have the capability to acquire add-on programmes.

The flowsheet is created in the user interface of CHEMCAD, the simulation is performed and the results are represented. A library of Unit Operations, which are required to build the flowsheet are provided on a palette.

What can be simulated with CHEMCAD?

Gaseous, liquid and solid processes, rectification, gas washing, absorption and desorption in columns, chemical reactions, heat exchange of fluids with condensation and vaporisation,



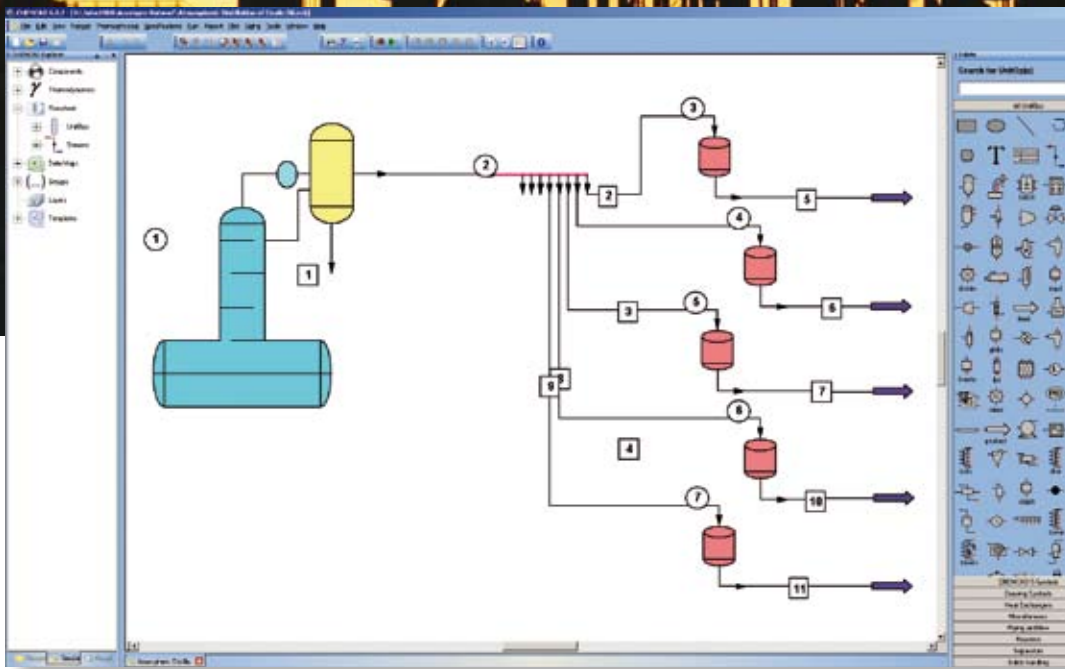
any phase equilibria with diagrams, transport of gases, liquids, mixed phases in pipes with pump, compressor, valves for pressure drop calculation, solid grinding and separation according to particle sizes and electrolyte reactions.

CHEMCAD is well-known for its easy and clearly structured user interface. CHEMCAD will lead you to a quick successful outcome. It will be a pleasure for us to have the opportunity to demonstrate CHEMCAD to you.

Frequently the unit operations have several symbols with the same algorithm. The data base consists of more than 2000 components, gases, liquids, solids and electrolytes with physical properties from e.g. DIPPR and phase data from e.g. Dechema Data Collection. The engineering units can be adjusted,

e.g. SI. Pipe flow calculations are recognised automatically by CHEMCAD. Convergency is achieved by special algorithms. Phase equilibria are calculated with models such as NRTL and UNIFAC. Equations of state models such as Soave-Redlich-Kwong are available. A thermodynamic wizard is available to assist in the selection of the best models based on the components and pressure and temperature parameters.

Many extension possibilities are available such as defining your own components based on the molecular structure, your own data for the calculation of physical properties and algorithms for Unit Operations and a powerful interface to Excel for calculation and reporting purposes.



Typical applications of CC-BATCH

- ➔ separation of a multi component mixture
- ➔ specification of a column up to 200 trays
- ➔ formation of fractions
- ➔ variable specification of fractions
- ➔ constant or variable reflux ratio operating mode
- ➔ further treatment of products in CHEMCAD
- ➔ 2-phase condensation

Advantages of CC-BATCH

- ➔ very fast simulation
- ➔ graphical presentation of the results
- ➔ easy to optimise processes

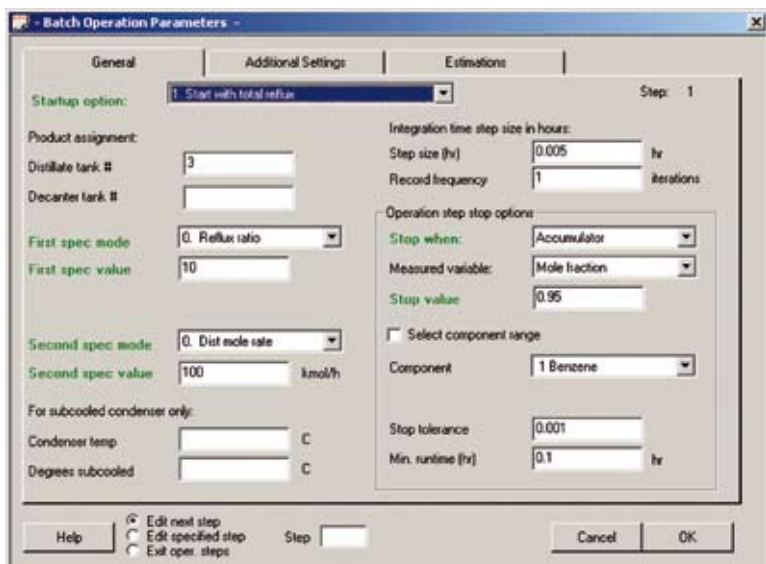
CC-BATCH

The programme CC-BATCH can be acquired as a stand-alone version or as an add-on version.

The batch distillation process is chosen in applications involving small volumes of complex multi component mixtures. The batch distillation process has some advantages as compared with a continuous rectification but experience is required to achieve an optimum solution. CC-Batch helps the user to reach this objective quickly.

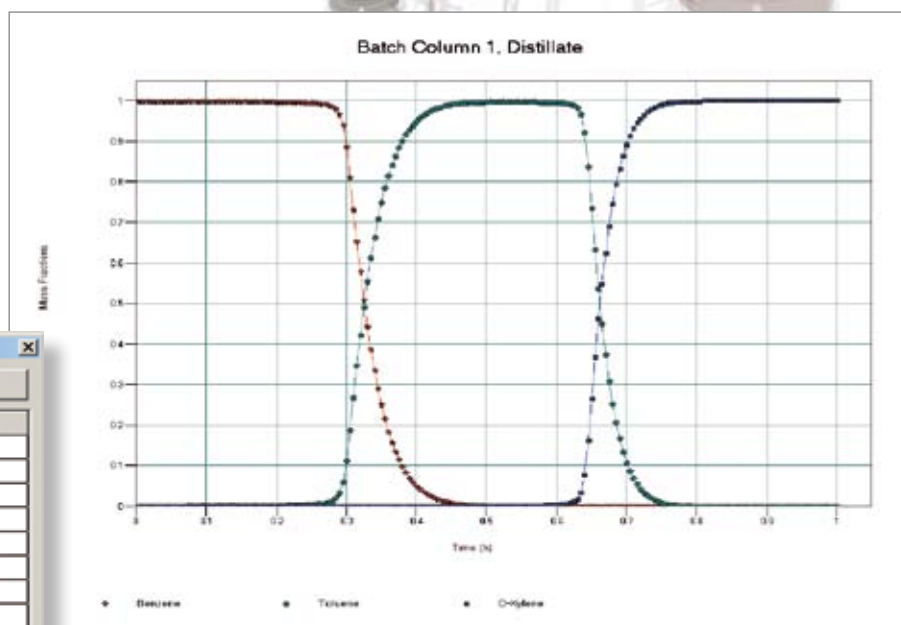
What can be simulated with CC-BATCH?

CC-BATCH allows a batch distillation, comprising a multi component mixture, to be simulated into fractions. Numerous specifications of fractions are possible enabling the user to simulate close to real conditions. The simulation can determine the optimum conditions for practical use in a short time.



Edit Streams

Stream No.	1	2	3
Stream Name	BTX		
Temp C	20	79.70264	122.4815
Pres bar	1	1	1
Vapor Fraction	0	0	0
Enthalpy MJ/h	505.1142	729.0761	266.7138
Total flow	3000	999.9995	2000.001
Total flow unit	kg/h	kg/h	kg/h
Comp unit	weight frac	kg/h	kg/h
Benzene	0.333333	999.9916	0.00852518
Toluene	0.333333	0.007941065	999.9921
O-Xylene	0.333333	8.280655e-011	1000



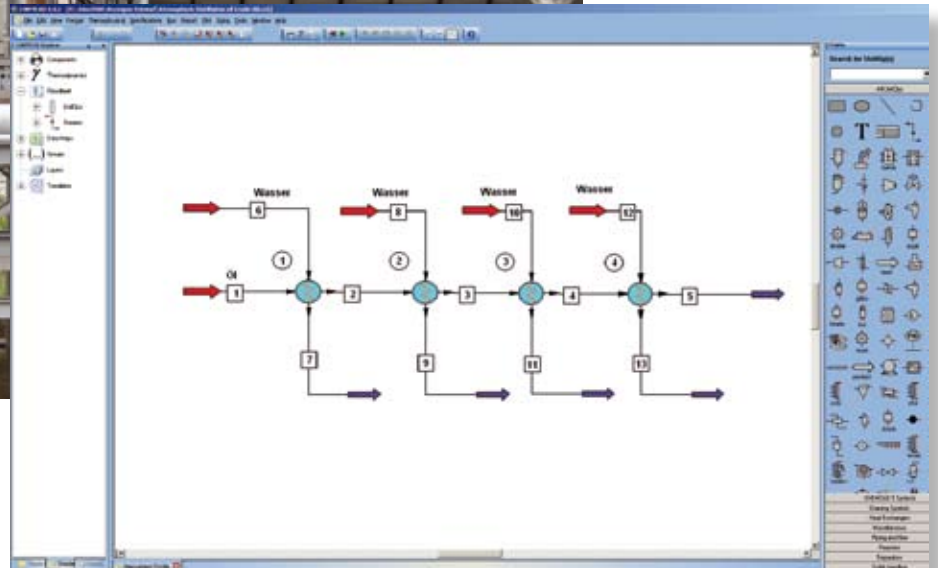
Conditions can be chosen for each fraction individually, e.g. with respect to time, composition in the distillate, in the product or in the still. During the course of the simulation the amount and concentration flow in the distillate, in the fractions and in the still, as well as the thermal requirements, can be reported graphically.

The calculation is so fast that several recalculations, using different parameters, can be done in order to achieve better results. Thus change over fractions can be minimised, mole fractions maximised and finally the thermal efficiency and timings of the batch distillation can be optimised. This leads to the fact that the optimum solution can be obtained very quickly. CC-BATCH provides many advantages as compared with alternative empirical methods.

It goes without saying that constant and variable reflux ratio operation can be simulated. In the latter case the reflux ratio starts with a low value and increases exponentially. Thus the optimum operating conditions in regards to thermal energy can easily be determined using CC-BATCH.

The fractions are collected in a vessel thus allowing further study in a steady state simulation.

CC-BATCH offers a great variety of features. Do not hesitate to test it.



CC-THERM

Typical applications of CC-THERM

- ➔ shell and tube, double pipe and plate heat exchangers
- ➔ air cooler
- ➔ calculation of the overall heat transfer coefficient (k or U) and the area

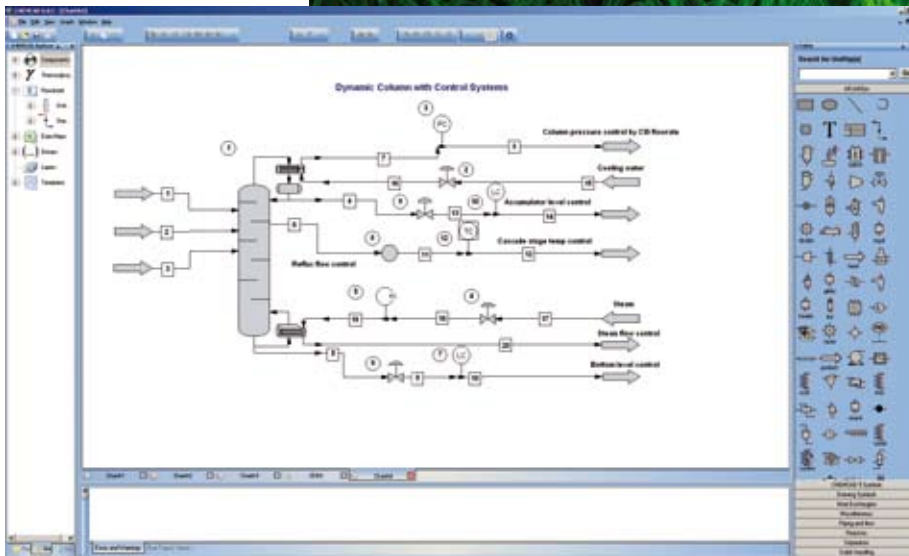
Advantages of CC-THERM

- ➔ vertical or horizontal condensation and evaporation (in case of shell and tube heat exchanger)
- ➔ choice of construction
- ➔ optimisation according to minimised area
- ➔ vibration analysis of pipes
- ➔ transfer of k or U -value and area to CHEMCAD
- ➔ heat curve compatible with other heat exchanger programmes
- ➔ TEMA sheet

CC-THERM is available as a stand-alone or as an add-on programme.

A heat exchanger in CHEMCAD is calculated thermally obtaining important parameters. CC-THERM is the tool to design this heat exchanger. As a result the heat transfer coefficient and the heat transfer area are calculated. Based on the heat exchanger construction data a comparison with the CHEMCAD calculation is obtained. It is possible to optimise the heat exchanger heat transfer area automatically by forcing design parameters such as tube length, tube passes, tube layout, shell diameter and baffle design and spacing.

The results can be combined with the CHEMCAD flow-sheet thus allowing an automatic calculation of the heat transfer coefficient with each CHEMCAD simulation.



CC-DYNAMICS

CC-DYNAMICS is available as a stand-alone or add-on programme.

When studying mass and energy balances the steady state simulation with CHEMCAD is the programme of choice. But, when studying time dependent processes the add-on programme CC-DYNAMICS is the perfect tool to simulate control processes and the behaviour in columns, equipment and reactors. The most important unit operations in CC-DYNAMICS are the dynamic vessel, batch reactor, dynamic column with hold up, PID controller, control valve and ramp controller.

Typical applications of CC-DYNAMICS

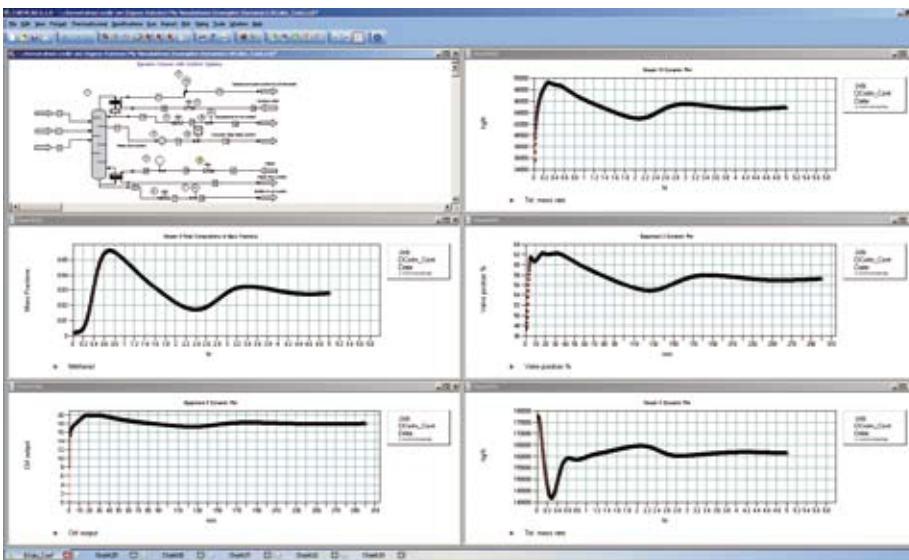
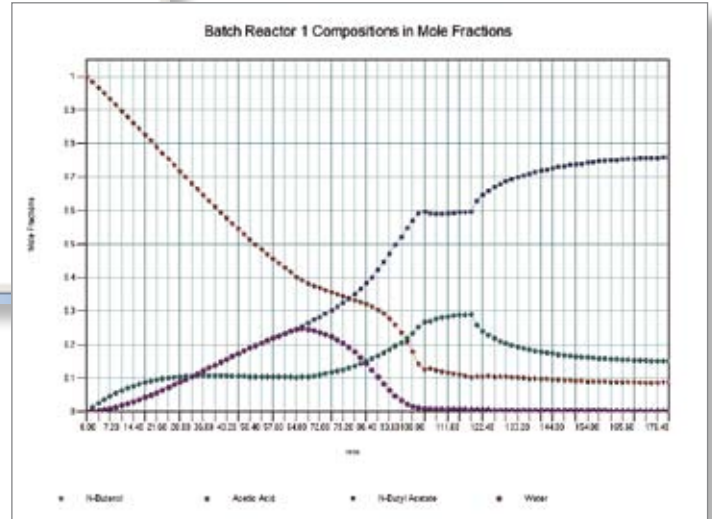
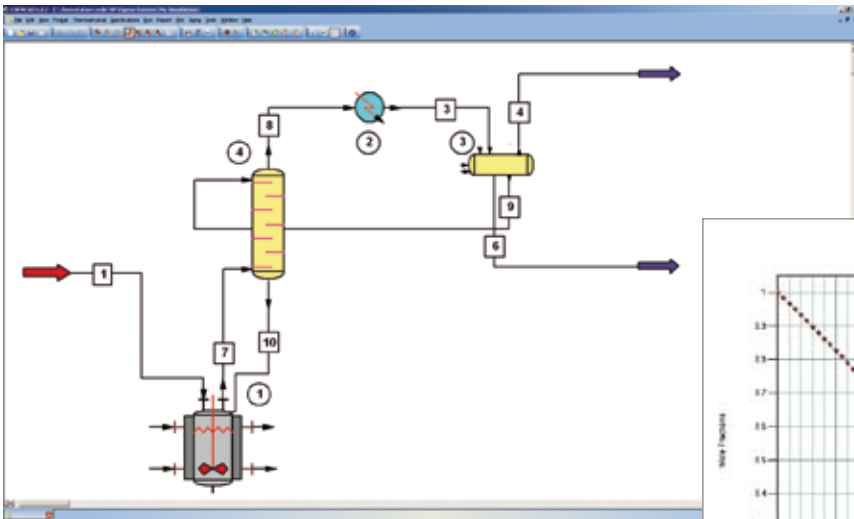
- ➔ dynamic simulation of processes
- ➔ dynamic column
- ➔ dynamic batch reactor
- ➔ PID controller
- ➔ control valve
- ➔ ramp controller
- ➔ dynamic vessel

Advantages of CC-DYNAMICS

- ➔ simulation of complex processes
- ➔ distillation, reactor
- ➔ semi batch reactor
- ➔ combination distillation with reactor
- ➔ control processes
- ➔ time controlled processes (batch processes)
- ➔ comprehensive graphical presentation of the simulation

What can we simulate with CC-DYNAMICS?

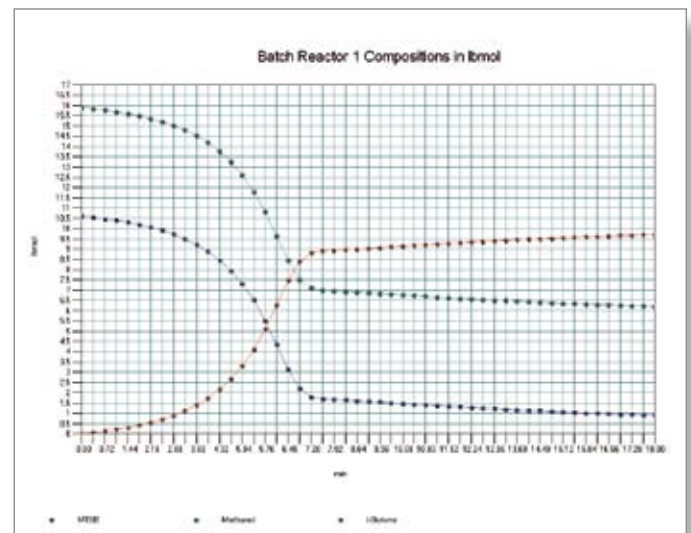
- reaction in a batch reactor with jacket heating and cooling
- level and pressure control in a vessel
- start up and shutdown simulation in distillation and absorption columns
- pressure drop in pipe networks including two phase flow
- emergency relief and flare systems
- filling and draining vessels, e.g. time controlled

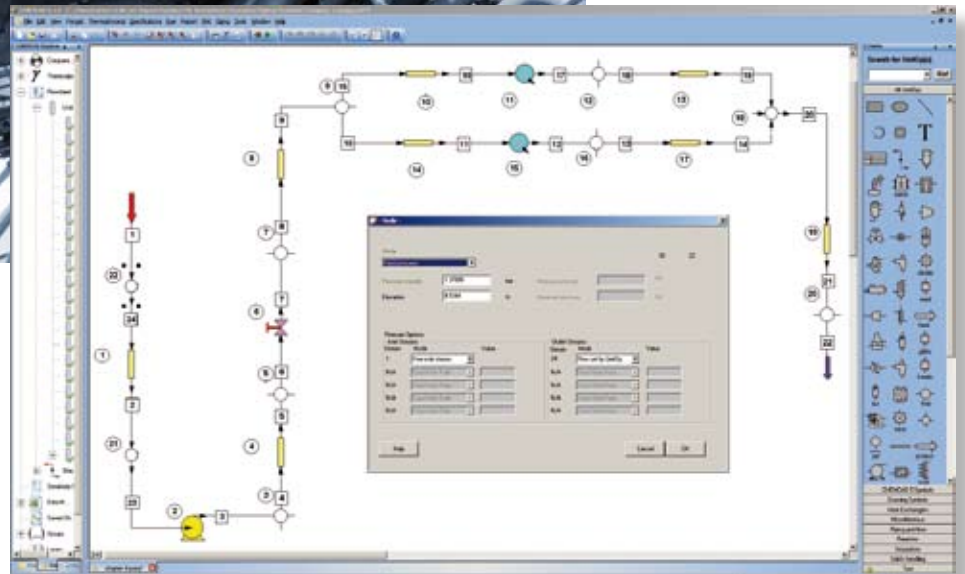


The Highlight

If a flowsheet contains steady state unit operations (e.g. flash, pump, valve, etc.) these can be included in the dynamic simulation. Data transfer between Excel and the simulation are achievable during the dynamic run allowing process parameters to be changed using customer algorithms.

The dynamic simulation of processes with CC-DYNAMICS is fast and realistic. CC-DYNAMICS enables the user to simulate close to reality. Important details concerning the process and its control are obtained but also product and physical properties.





CC-SAFETY NET

CC-SAFETY NET is part of CHEMCAD but it can also be acquired as a stand-alone programme

Typical applications of CC-SAFETY NET

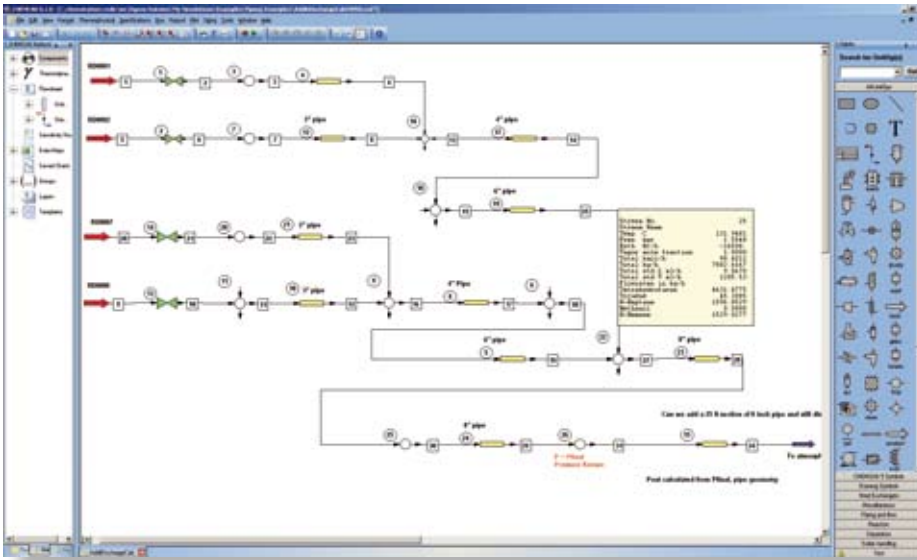
- ➔ pipes networks with pumps and compressors
- ➔ emergency relief and flare networks
- ➔ influence of control valves

Advantages of CC-SAFETY NET

- ➔ pressure drop in complex pipe networks
- ➔ relief device calculations according to DIERS
- ➔ mass and energy balances with component physical properties

What can be simulated with CC-SAFETY NET?

Complex pipe networks with pump, compressor, turbine, valve, and relief devices based on a CHEMCAD flowsheet. The simulation of safety and relief valves is carried out in accordance with DIERS technology. As a result the mass balance of all streams, their stream direction, physical properties and physical condition are obtained, with two phase streams and their regime being recognised automatically. Several fluid flow models can be chosen for pressure drop calculations. Performance data can be entered for pumps, compressors and turbines allowing the typical performance in plants to be simulated, e.g. pressure drop and mass flow in an isometric pipe system.



The 'Node' dialog box displays the following data for Node 7:

- Mode: **Variable pressure**
- Pressure at node: **2.00267** bar
- Elevation: **10.3632** m
- Minimum pressure: **1.37895** bar
- Maximum pressure: **5.51561** bar

Below the main data, there are sections for 'Inlet Streams' and 'Outlet Streams', each with a table for 'Stream', 'Mode', and 'Value'. The 'Inlet Streams' table has one entry for stream 7 with a mode of 'Flow set by UnitOp'. The 'Outlet Streams' table has one entry for stream 8 with a mode of 'Flow set by UnitOp'. Buttons for 'Help', 'Cancel', and 'OK' are at the bottom.

The 'Pipe Sizing and Rating (PIPE)' dialog box has several tabs: Specifications, Properties, Calculated Results, Valves, Fittings, and Heat Transfer. The 'Specifications' tab is active, showing the following settings:

- Method: **2 Single Phase flow**
- Sizing option: **5 Given size, Pin and Pout, calc flowrate**
- Number of segments: []
- Pipe diameter: **0.1016** m
- Pipe Schedule: **40**
- Pipe Length: **10.668** m
- Elevation: **2.4384** m
- Friction factor model: **0 Churchill**
- Optional pipe case studies:
 - Pipe diameter case #2: [] m
 - Pipe diameter case #3: [] m
- Enter one of the following:
 - Roughness factor: **4.572e-005** m
 - Pipe Material: **None**
- Include holdup in dynamic simulation
- Include gas expansion factor

Buttons for 'Help', 'Cancel', and 'OK' are at the bottom.

As CC-SAFETY NET uses the data base and the thermodynamic models for phase equilibria in CHEMCAD, it is not necessary to enter physical properties and physical conditions. Changing the flowsheet or the data can be easily done allowing the study of various scenarios.

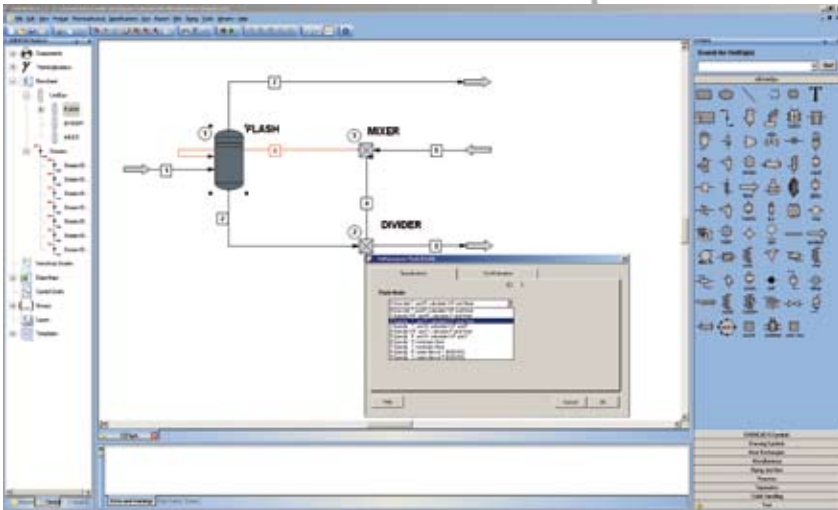
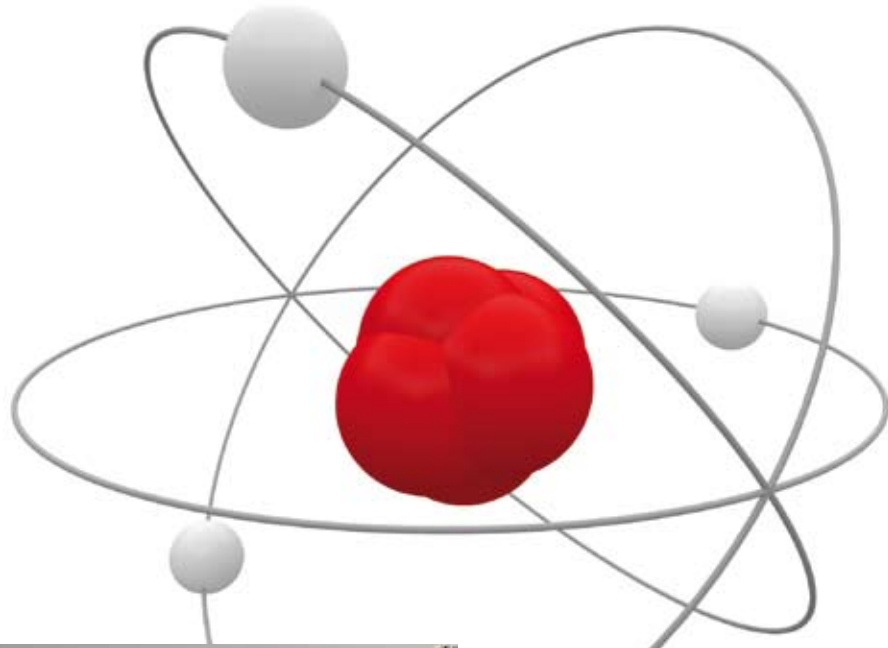
CC-SAFETY NET represents the ideal programme to investigate complex piping systems and their stream behaviour under various conditions, e.g. closing of a valve, pressure change at the entry or exit.

All the features of CC-SAFETY NET are available in CHEMCAD.

The Highlight

CHEMCAD uses Nodes to simulate pipe networks as well as a special algorithm: simultaneous modular. Here the flowsheet is treated as a matrix. This enables a quick calculation and a good convergence of complex processes.

User data can be entered for valves and pipe fittings.



Typical applications of CC-FLASH

- ➔ mixing of streams
- ➔ stream dividing
- ➔ phase equilibria

Advantages of CC-Flash

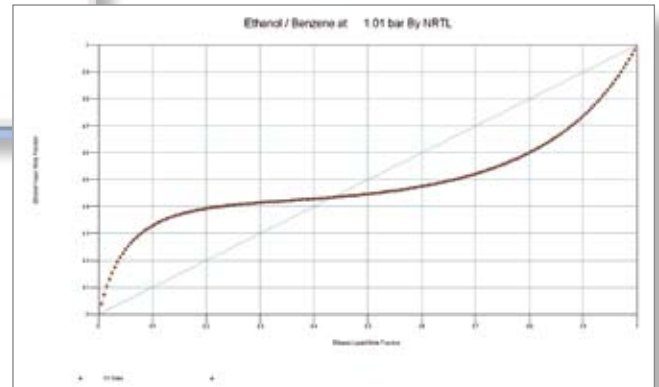
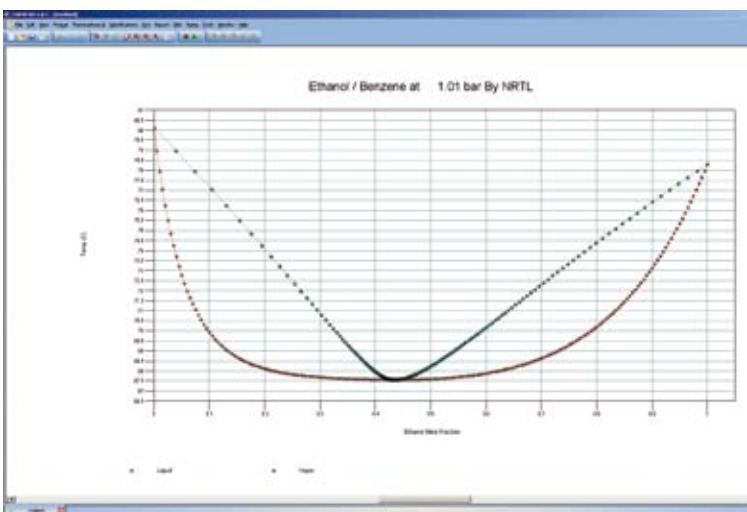
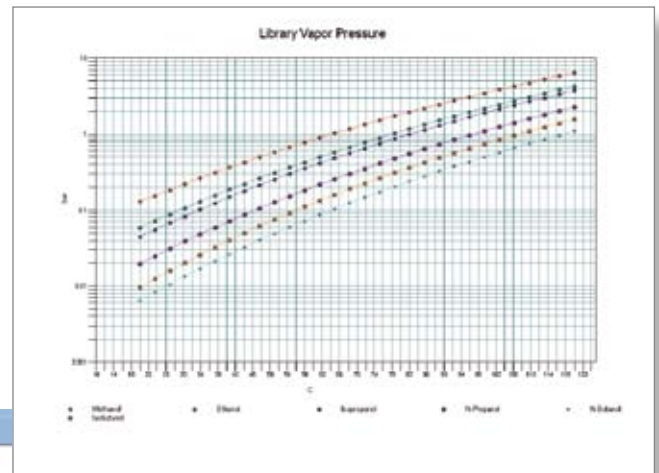
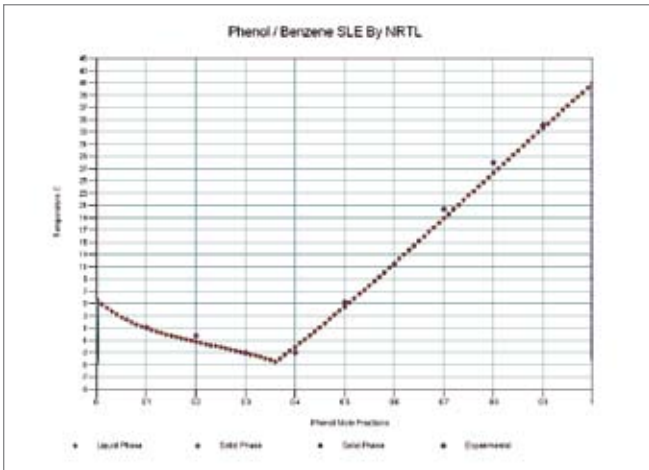
- ➔ physical properties
- ➔ mixed physical properties up to 200 components
- ➔ vapour-liquid-equilibrium (VLE)
- ➔ liquid-liquid-equilibrium (LLE)
- ➔ solid-liquid-equilibrium (SLE)
- ➔ electrolyte equilibrium
- ➔ data base with more than 2000 components (gases, liquids, solids, electrolytes)
- ➔ models: NRTL, Unifac, SRK, Henry, MEA, DEA, MDEA, Amine etc.

CC-FLASH

CC-FLASH is part of CHEMCAD but also can be acquired as a stand-alone version.

What can be simulated with CC-FLASH?

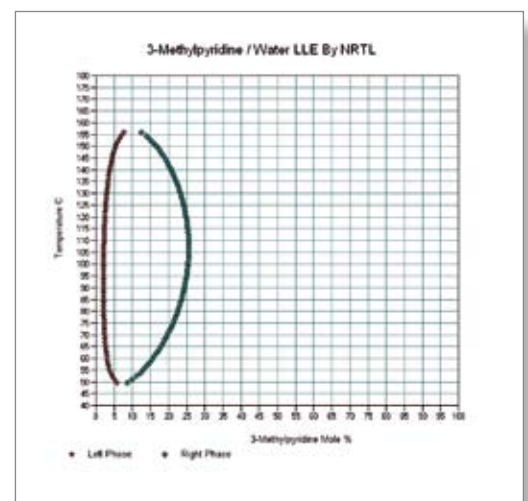
Phase equilibria including VLE (vapour-liquid-equilibrium), LLE (liquid-liquid-equilibrium), SLE (solid-liquid-equilibrium) of multi component mixtures, dew and bubble points, two phase condition, mixture condition, liquid interfaces graphical presentation of binary and ternary phase equilibria, residue curves, and physical properties of multi component mixtures. User components can be added to the data base.



It is possible to create a simple flowsheet using unit operations contained in CC-FLASH, e.g. a pressure drop reduction with several sequential flashes or a mass balance in a distribution system. All properties of CC-FLASH are part of CHEMCAD.

Unit operations contained in CC-FLASH are: flash, mixer, divider.

A useful feature of CC-FLASH is the presentation of physical properties and phase equilibria allowing the user to obtain important data out of the large data base very quickly for his daily work. The search for components in the data base can be done using name, formulae, CAS number and CHEMCAD ID number.





Process software to match your simulation needs!

You have the possibility to build your personalised CHEMCAD Suite:

- ➔ Chose the programmes which meet your requirements
- ➔ Chose the time you need

Programmes of the CHEMCAD SUITE

- ➔ CHEMCAD STEADY STATE
- ➔ CC-BATCH
- ➔ CC-THERM
- ➔ CC-DYNAMICS
- ➔ CC-SAFETY NET
- ➔ CC-FLASH

Your need – our recommendation

- ➔ You have a project with a life of 2 to 3 months
 - Leasing per month is recommended
- ➔ The time needed for the project is not known in advance; CHEMCAD is not used every day; once in a while you will want to verify and check older calculations
 - Leasing on an hours basis is recommended
- ➔ Frequently CHEMCAD is used by you and your colleagues to simulate and optimise projects
 - We recommend leasing a license with unlimited use of hours

It goes without saying that Maintenance-Update-Support is included in the leasing time.



Service

It is our main concern to provide the best possible service to our customers. This service includes

Maintenance – Update – Support (MUS)

Maintenance

Our software is subject to a steady ongoing development and improvement. We forward your wishes, needs and requirements to our programmers.

Update

Active customers with a valid MUS agreement can download from our website helpful information, job examples, programme releases. Officially released updates will be forwarded by us.

Support

Our support covers English and German speaking hotline, either by phone or email. Our CHEMCAD experts, with years of experience, will be at your disposal. Support is subject to an active MUS agreement.

Seminar

You will be trained thoroughly in the use and application during our frequently carried out seminars for beginners and advanced. After a 2 day seminar for beginners you will be able to run CHEMCAD and take benefit from its application in your projects.

On request we will train you in your company according to your special needs. Ask for an offer.

www.chemstations.de

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Technical Information

Hardware and Software requirements

The minimum requirements are:

Processor: 500 MHz or higher
System: Windows 2000, XP or Vista
Graphic cards with 128 MB or higher
Hard disk memory: 750 MB
For some features Microsoft Office® is required

CHEMCAD modules, features and unit operations

Here you will find a summary of features and properties of the CHEMCAD Suite to allow you to find the modules that satisfy your requirements.

FEATURES	CHEMCAD STEADY STATE	CC-BATCH	CC-THERM	CC-DYNAMICS	CC-SAFETY NET	CC-FLASH
VB/COM/OPC/DATAMAP	Yes			Yes		
Sensitivity/Optimization	Yes			Yes	Yes	
Sizing (Line/Valve/Orifice/Vessel)	Yes			Yes	Yes	
Run Steady State	Yes	Yes	Yes		Yes	Yes
Run Dynamics				Yes	Yes	
Run Recycles	Yes			Yes	Yes	
Costing	Yes			Yes	Yes	
Reconciliation	Yes			Yes		
Sizing Columns	Yes	Yes		Yes		
Sizing Heat Exchangers			Yes			
Economics	Yes			Yes		
Reports (incl. Excel)	Yes	Yes	Yes	Yes	Yes	Yes
DIERS	Yes			Yes	Yes	
CO ₂ solid	Yes			Yes	Yes	Yes
Hydrates	Yes			Yes	Yes	Yes
Depress	Yes			Yes	Yes	Yes
TOC/COD	Yes			Yes	Yes	Yes
Pure Regression	Yes	Yes	Yes	Yes	Yes	Yes
BIP Regression	Yes	Yes	Yes	Yes	Yes	Yes
Electrolyte Regression	Yes	Yes	Yes	Yes	Yes	Yes
Rate Regression	Yes			Yes		
Units Calculator	Yes	Yes	Yes	Yes	Yes	Yes
Execute Parser	Yes			Yes		
Environmental Report	Yes	Yes	Yes	Yes	Yes	Yes
Simple Calculator	Yes	Yes	Yes	Yes	Yes	Yes
Spec Sheet	Yes	Yes	Yes	Yes	Yes	

UNIT OPERATIONS	CHEMCAD STEADY STATE	CC-BATCH	CC-THERM	CC-DYNAMICS	CC-SAFETY NET	CC-FLASH
Baghouse Filter	Yes			Yes		
Batch Column		Yes				
Batch Reactor				Yes		
Calculator	Yes			Yes		
Centrifugal Filter	Yes			Yes		
Component Separator	Yes			Yes		
Compressor	Yes			Yes	Yes	
Control Valve	Yes			Yes	Yes	
Controller	Yes			Yes	Yes	
Crusher/Grinder	Yes			Yes		
Crystallizer	Yes			Yes		
Cyclone	Yes			Yes		
Divider	Yes			Yes	Yes	Yes
Dynamic Vessel				Yes	Yes	
Electrostatic Precipitator	Yes			Yes		
Equilibrium Reactor	Yes			Yes		
Excel Unit	Yes			Yes		
Expander	Yes			Yes	Yes	
Fire Heater	Yes			Yes		
Flash	Yes			Yes	Yes	Yes
Gibbs Reactor	Yes			Yes		
Heat Exchanger	Yes		Yes	Yes	Yes	
Hydrocyclone	Yes			Yes		
Kinetic Reactor	Yes			Yes		
LL Extractor	Yes			Yes		
LLV Flash*	Yes			Yes		
LNGH Exchanger	Yes			Yes		
Loop	Yes			Yes		
Mixer	Yes			Yes	Yes	Yes
Node	Yes			Yes	Yes	
Phase Generator	Yes			Yes		
PID Controller	Yes			Yes	Yes	
Pipe Simulator	Yes			Yes	Yes	
Polymer Reactor						
Pump	Yes			Yes	Yes	
Ramp Controller	Yes			Yes	Yes	
Recorder*	Yes					
Run Subflowsheet META Unit	Yes			Yes		
SCDS Distillation Column	Yes			Yes		
Screen	Yes			Yes		
Sedimentator	Yes			Yes		
Shortcut Column	Yes			Yes		
Solid Dryer	Yes			Yes		
Solid Washer	Yes			Yes		
Stoichiometric Reactor	Yes			Yes		
Stream Reference	Yes			Yes		
Tank		Yes				
Time Delay				Yes	Yes	
Time Switch		Yes		Yes		
Tower Distillation Column	Yes			Yes		
Tower Plus Distillation Column	Yes			Yes		
User Added Module	Yes			Yes		
Vacuum Filter	Yes			Yes		
Valve	Yes			Yes	Yes	
Venturi Scrubber	Yes			Yes		
Vessel*	Yes			Yes		

*These UnitOps will be phased out eventually.



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