CHEMSTATIONS

CHEMCAD SUITE - PROGRAM FEATURES
COMMON FEATURES

GENERAL FEATURES
Graphical user interface
Customized reports and PFD's
Interactive operation
Interfaces to spreadsheets (Microsoft Excel) and AutoCAD (.DXF)
User added unit operations, thermodynamics, components, and/or graphics symbols
In-line "C" language interpreter
Users may add their own .DLLs
Extensive online help
Extensive data checking
Flexible engineering units
OLE, COM, and Visual Basic integration

ENGINEERING DATA
Physical properties databank for pure components (DIPPR)
BIP database for activity coefficient equations
Electrolytes database
Vapor phase association database
Interface to corporate and/or third party databases

THERMODYNAMICS
Vapor phase association
Different K-Value models and/or enthalpy models for different units or trays
Different BIPs for different units or trays
Vapor-Liquid and Vapor-Liquid-Liquid equilibrium
Physical properties estimation of undefined components: group contribution methods available for pure and mixture properties estimation
Composite heat curve pinch analysis
Distillation curve assay analysis

K-VALUE METHODS
Equations of State
- Soave-Redlich-Kwong
- Grayson-Streed/Chao-Seader
- Peng-Robinson
- Benedict-Webb-Rubin-Starling
- API Soave-Redlich-Kwong
- Modified Soave-Redlich-Kwong (MSRK)
- Extended Soave-Redlich-Kwong (TSRK)
- Predictive Soave-Redlich-Kwong (PSRK)
- Elliott Suresh Donohoe (ESD)
- Statistical Associating Fluid Theory (SAFT)
- Peng-Robinson-Stryjek-Vara (PRSV)

Empirical
- ESSO (Maxwell-Bonnell)
- Vapor Pressure (Ideal Solution)
- Henry's Gas Law

Activity Coefficient Methods
- UNIQUAC (UNIQUAC with the new group and surface parameters)
- UNIFAC/UNIQUAC (UNIQUAC with the old group and surface parameters)
- UNIFAC VLE
- UNIFAC LLE
- UPLM (UNIFAC for Polymers)
- Wilson
- T. K. Wilson
- HRNM Modified Wilson
- Van Laar
- Non-Random Two Liquid (NRTL)
- Margules
- GMAC (Chien-Null)
- Scatchard-Hildebrand (Regular Solution)
- Wilson Salt

Special Systems
- Hydrocarbon-Water Solubility
- Amines (VLE and LLE)
- Sour Water
- Tri-Ethylene-Glycol/Water Dehydration
- Flory-Huggins Method for Polymers

User Supplied K-Values
- Polynomial K-values
- Tabular K-values
- Partial Pressures of Aqueous Mixtures
- User Subroutine
- User Specified Activity Coefficients

ENTHALPY METHODS
Equations of State
- Redlich-Kwong
- Soave-Redlich-Kwong
- Peng-Robinson
- API Soave-Redlich-Kwong
- Lee-Kesler
- Benedict-Webb-Rubin-Starling
- Peng-Robinson-Stryjek-Vara (PRSV)

Chemical Systems
- Latent Heat
- Electrolyte
- Heat of Mixing by Gamma

Special Systems
- Steam Table
- Mixed Model
- No Enthalpy (Mass balance only)

User Added Data
- Polynomial Enthalpy Model
- Tabular H's
- Heat of Solution Data
- User Subroutine

ELECTROLYTES
Pitzer and mNRTL methods for strong and weak electrolytes including temperature dependent interaction parameters
Binary and ternary interaction parameter database
Reaction equilibrium database including many common industrial systems; calculated from Gibbs free energy when data is absent
Expert system assistance for setting up electrolyte chemistry

REGRESSION
Pure component physical property regression
Multicomponent VLE/LLE regression from user data, UNIFAC, or infinite dilution data
Regression of electrolyte data

UTILITIES
EPA WAR Algorithm for environmental and health impact studies
Hydrate/Solid CO2 prediction
Total Organic Content/Chemical Oxygen Demand calculation
Plots – TPXY, Binodal, Residue Curve Map
Symbol Builder for custom graphic representations

Calculation of Relief Devices (DIERS)
- Design and rating of relief valves and/or rupture disks
- Bubbly, churn-turbulent, and homogeneous vessel models
- HEM, ERM, Henry-Fauske HNE, non-flashing liquid and single-phase vapor vent flow models
- API-520/52, API-2000, OSHA 1910.116, and NFPA-30 fire models, or specified heat rate.
- Inlet and outlet piping pressure drop calculations
- Comprehensive vessel and relief vent specification capabilities
- Atmospheric and pressure vessels

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CHEMCAD SUITE - PROGRAM FEATURES
CC-STEADY STATE

UNIT OPERATIONS
Calculator
Component separator
Compressor
Controller
Distillation Column (see detailed DISTILLATION section)
Divider
Excel Unit
Expander/Turbine
Fired heater
Flash
Heat exchanger
Liquid-liquid extractor
LNG Heat exchanger
Loop
Mixer
Node
Phase Generator
Pipe simulator
Pump
Reactor (see detailed REACTORS section)
Recorder
Stream reference
User Added Module
Valve
Vessel
Solids handling:
- Baghouse filter
- Centrifugal filter
- Crusher/Grinder
- Crystallizer
- Cyclone
- Dryer
- Electrostatic precipitator
- Hydrocyclone
- Screen
- Sedimentator
- Vacuum filter
- Venturi scrubber
- Washer

DISTILLATION
Shortcut and rigorous
Multiple column arrangements
Flexible specifications
Simultaneous Correction and Rigorous Inside Out algorithms
Up to 500 theoretical stages
Three phase distillation
Scrubbing and stripping
Mass transfer based distillation for packed and tray-ed columns
Automatically calculates the component diffusivities
Rigorous calculation of the mass transfer coefficient
User editable database of packing data from packing manufacturers
Calculation of ambient heat loss
Tray by tray tabular and plotted output

REACTIVE DISTILLATION
Reactions may be equilibrium or kinetic equation based
Reactions solved simultaneously with VLE
Flexible rate form, including user added
Purity and temperature specifications
Up to 300 reactions
Vapor and/or liquid reactions are permitted

REACTORS
Stoichiometric
Equilibrium
- Up to 300 simultaneous reactions

Water-gas shift data
Methanation data
Gibbs free energy minimization
Kinetic (PFR or CSTR)
Unlimited simultaneous reactions
Flexible rate form, including user added

FLOWSHEET CONVERGENCE
Sequential Modular convergence
Speed up methods (Wegstein, Dominant Eigenvalue)
Simultaneous Modular convergence for piping networks (when the Node unit operation is used)
Optimization algorithm – allows you to maximize or minimize a stream or unit operation variable (Objective Function) given certain independent variables and constraints.
Sensitivity and Parametric analysis with reporting
Unlimited size of flowsheet (unlimited number of streams and unit operations)

EQUIPMENT SIZING
Rigorous equipment sizing routines for:
- Trays (Sieve, Bubble cap, Valve)
- Packing (Random & Structured)
- Pipes
- Pressure Vessels
- Orifices
- Control Valves
- Three Phase Vessels
- Relief Devices (DIERS)

Spec (specification) sheets in Microsoft Excel with pre-built templates for:
- Baghouse filter
- Compressor
- Fired Heater
- Heat Exchanger (including TEMA sheet)
- Pump
- Distillation column
- Tank
- Valve

EQUIPMENT COST ESTIMATION
Calculates purchase and installed cost of major pieces of plant equipment

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CHEMCAD SUITE - PROGRAM FEATURES
CC-FLASH

GENERAL FEATURES

Shares core features with CHEMCAD:
Physical property database
Thermodynamics
Regression facilities
Flowsheet convergence
Limited unit operations available

UNIT OPERATIONS

Flash
Mixer
Divider
Equipment sizing routines are provided for orifices, pipes, valves, pressure vessels, and relief devices

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CHEMCAD SUITE - PROGRAM FEATURES
CC-DYNAMICS

GENERAL FEATURES
Full dynamic flowsheeting for operability, training, startup/shutdown
Graphical plotting of time dependent results
Online, real-time display of results during calculation
Calculation interrupt
Full integration into the CHEMCAD Suite and flowsheets

INTERACTIVE DYNAMIC SIMULATION
Additional mode of operation allowing user interactivity while the simulation is running
Open/close valves
Change setpoints
Introduce upsets
Mode for connectivity to operator training systems

CONTROL VALVES
Equal percentage or linear values
Valve coefficient (Cv)
Rangeability
Critical flow factor
Valve position function

CONTROLLER
PID (proportional – integral – derivative) action can be specified
Controller set points can be purity, temperature, pressure, level, flow, or any other flowsheet variable
Controller limits may be set:
With or without upper or lower limits
Relative to the set point
At a specified value
Cascade and split range controllers can be used
Sensor functions can be specified
RAMP Control
Time/Value table
Random Disturbance
Sine Wave

DIERS ANALYSIS FACILITY
Practical, comprehensive, field tested DIERS (Design Institute for Emergency Relief Systems) analysis
This can be used to simulate emergency relief situations on a dynamic basis
The DIERS results are included in the heat and material balance of the dynamic vessel
OUTPUT
Time history reports and plots for:
All unit operation parameters including control valve position and controller output
All stream parameters

BATCH REACTOR (CC-REACS) FEATURES

CHEMICAL DESIGN
Unlimited number of species
Unlimited number of simultaneous reactions
Choice of Arrhenius, Langmuir-Hinshelwood, or user added rate equation forms
Regression of kinetic process data

REACTOR DESIGN
Multiple Coils and jackets
Service or process side heat exchangers and electric heaters
Heat transfer rate calculation; includes calculation of process and service side film coefficients
Vapor and liquid draws permitted
Batch, semi-batch or continuous operation
Vessel pressurization calculated

AUXILLIARY EQUIPMENT
Other unit operations may be used with the batch reactor to flexibly model the process, including: dynamic vessel, heat exchanger, mixer, divider, separator, valve, pump, etc.

CONTROL SYSTEM
User specified PID loops
Multiple ramp or step changes in setpoint
Control of reactor or jacket temperature differential
Level controllers
Pressure controllers
Cascade control
Heat-cool-chill system with safety interlocks
Split range controllers

KINETIC DATA REGRESSION
Can regress any combination of concentration, temperature volume and/or heat of reaction (Qr) data
Can fit multiple experiments in a single regression analysis
Can calculate the frequency factor, activation energy, component reaction order, Langmuir absorption parameters
Offers a variety of numerical methods to ensure that the regression is fast, accurate and can handle stiff systems
Accepts data from a wide range of calorimeters including the Mettler RC1 for which special features are provided
Graphical and tabular comparison of experimental and predicted results makes it easy for the user to evaluate the validity of the model

DIERS ANALYSIS FACILITY
Practical, comprehensive, field tested DIERS (Design Institute for Emergency Relief Systems) analysis facility for the reactor vessel
This can be used to simulate reactive emergency relief situations on a dynamic basis
The DIERS results are included in the heat and material balance of the reactor

OUTPUT
Graphical and tabular time history reports for:
Compositions
Pressure
Temperature
Heat of reaction
Utility flowrates
Liquid level
Reaction mass physical properties
Rates of formation
Yields
Conversions

DISTILLATION (CC-DCOLUMN) FEATURES

COLUMN FEATURES:
Can begin the simulation as a startup or from a steady-state condition
Holdups can be:
ignored
constant or variable
liquid and/or vapor
specified in mass, molar or volumetric units
specified for the condenser, reboiler, or any stages
specified on each stage
Pressure can be fixed or calculated
Simulation can be performed using rigorous mass transfer analysis or using the equilibrium stage approach
Packed columns can be calculated using rigorous mass transfer analysis or assuming equilibrium stages
Multiple liquid phases
Discrete event scheduler
Pressure drop calculations included
Reactive distillation allowed
Calculation of ambient heat loss

START-UP FEATURES:
Dry or Wet tray startups
Fixed or variable pressure
May specify startup duration time and reboiler duty
Open or closed loop control simulation

CONDENSER FEATURES:
Holdup can be:
Constant or variable
Specified in mass, mole or volume units
Set by a control valve
Reflux can be:
Specified in mass, mole or volume units
Set by a control valve
Distillate can be:
Specified in mass, mole, or volume units
Set by a control valve
Condenser U*A can be set. Cooling fluid flowrates can be fixed or controlled.
Condenser accumulator vessel specification options:
Orientation
Head type
Diameter and length
Initial liquid level

REBOILER FEATURES:
Holdup can be variable or constant
Bottoms liquid product rate can be:
Specified in mass, mole, or volume units
Set by a control valve
Reboiler U*A can be set. Heating fluid flowrates can be fixed or controlled.
Reboiler vessel options:
Orientation
Head type
Diameter and length
Initial liquid level

SIMULATION WITHOUT CONTROLLERS:
Condenser/Reboiler specification options:
Reflux/Reboil ratio or rate
Heat duty
Temperature
Flowrate
Component flowrate
Purity
Recovery
Component recovery
Component ratios
Side product specification options:
Liquid or vapor flows
Liquid or vapor draw ratios

OUTPUT
Complete stage information
Graphical and tabular time history for:
Condenser and reboiler
Any stage

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CHEMCAD SUITE - PROGRAM FEATURES
CC-THERM

GENERAL FEATURES

Design mode
Rating mode
Fouling Rating mode
Simulation mode
Full integration into the CHEMCAD Suite

OUTPUT

Tabular and graphical reporting features including TEMA and/or API datasheets
A detailed tabulated analysis report
A detailed report of overall exchanger values
A zone-by-zone report of the heat curve, fluid properties, heat transfer and pressure drop calculations
The stream information inlet/outlet with H, T, P, and component flow rates
Optimization data

SHELL AND TUBE

Calculation of all TEMA types
Tubeside process types:
- Sensible flow (vapor or liquid)
- Forced evaporation
- Falling film evaporation
- Vertical thermosyphon
- Horizontal condensation
- Vertical condensation
- Reflux condensation

Shellside process types:
- Sensible flow (vapor or liquid)
- Forced evaporation
- Horizontal thermosyphon
- Horizontal condensation
- Vertical condensation

Exchangers may have evaporation on one side with condensation on the other with any combination of subcooling and superheating
Full stream analysis performed on the shellside
Zone-by-zone analysis is performed (2-31 zones, user defined)
Conditions and properties automatically generated at all zones and can be user modified
Complete materials library for tubes, pipes, shells, bonnet, and tubesheets
Dry- or wet- wall condensing
Thermosyphon mode
5 stream exchangers (evaporators with separate outlet streams for vapor and liquid) calculated

SHELLSIDE

Shells in series or parallel
Shell as pipe or plate
Sealing strips permitted
Diameter or max. diameter may be specified

TUBESIDE

Tubes may be bare or fin
Turbulators may be used on inside of the tube
Tube OD, gauge, pattern, and pitch may be specified
Tubesheet thickness calculated to determine effective area
U-bend radius and/or efficiency may be specified
Tube length or max. tube length may be specified

BAFFLES

Baffles may be single segmental, double segmental, triple segmental, full circle, no-tubes-in-window, or rod
Specify or have the program optimize the baffle spacing, cut, and direction
Optional impingement baffles

CLEARANCES

Select from available clearance standards or user defined clearances

MISCELLANEOUS

Safety factors may be specified
Entrainment ratios
Kettle diameter
Shellside or tubeside coefficient may be fixed
Tube axial stress
Vibration analysis
Zone-by-zone analysis of heat transfer and pressure drop calculations

TECHNIQUES

Sensible Heat – A full stream analysis is performed on the shell side, and several optional methods on the tube side. Defaults are pre-selected.
Condensers – The program handles horizontal, vertical, or reflux condensers. Several methods are available, however, defaults are pre-selected.
Reboilers and Evaporators – A variety of methods are available for diverse fluids and applications
Stream Analysis – Baffle by baffle calculation on the shellside explicitly accounts for the effects of clearances and shellside configurations on heat transfer and pressure drop. This analysis can be extended to include finned tubes, turbulators, sealing strips, impingement plates, sparger pipes, and many other construction variables.
Detailed Zone Analysis For Two Phase Flow – Rigorous accounting for changes across the exchanger by dividing it into zones. At each zone, the conditions, properties, flow regime, and applicable heat transfer mechanism are calculated. The program then applies the appropriate formula to calculate the pressure drop and film coefficients.

AIR COOLED

TECHNICAL FEATURES

Handles the following applications:
- Sensible cooling
- Horizontal condensing
- Vertical condensing
- Reflux condensation

The program has its own fintube databank. This databank contains all necessary information describing fintube geometry and characteristics from the manufacturers' catalog. The user may specify his/her own fintube data if so desired.
Dry wall and wet wall condensing can be accommodated.
Conservative and non-conservative condensing methods are available.
Fan data from the following manufacturers are provided in the program:
- Checo
- Moore
- Environment Element Corporation
- Aerovent
- Hudson

TECHNIQUES

Tubeside Heat Transfer – The tube side heat transfer coefficient is calculated differently for condensation and sensible flow.
Condensation – The program calculates Horizontal, Vertical and Reflux condensers. Default methods are pre-selected.
Sensible Flow – Several methods are available for calculation, with pre-selected defaults.
Airside Heat Transfer – The program uses the ESDU method for staggered tube arrays and the method of Schmidt for in-line arrays.
Zone Analysis – The unit is analyzed using zones specified by the user. The program automatically sets up zones and properties of each zone, but permits the user to edit or override any or all values calculated by the program.

PLATE AND FRAME

TECHNICAL FEATURES

Sensible to sensible heat transfer, which constitutes about 90% of all plate and frame applications.
Rating mode – The inlet and outlet streams are taken from the flow sheet and the user supplies the complete details of the exchanger geometry and dimensions and fouling factors. The program determines whether the exchanger is too large or too small for the given application.
Fouling rating mode – The inlet and outlet streams are taken from the flow sheet and the user supplies the complete details of the exchanger geometry and dimensions. The program calculates the fouling factors required to obtain the specified performance from the exchanger.
Film coefficients may be calculated by the program or specified by the user.
Chevron and intermating plates can be handled. The dimensions, geometry, and properties of the plates may be user specified if so desired.
Multiple cold side and hot side passes can be calculated. The LMTD correction factor is applied in such cases. Multiple pass performance factors are also applied.
A plate materials database is provided with the program.
The overall heat transfer coefficient is calculated as the inverse of the sum of all the heat transfer resistances from one bulk fluid to the other. The film heat transfer coefficient, h, is dependent on the fluid velocity, fluid properties, and plate geometry. Heat transfer correlations for specific plate designs are obtained experimentally and the data are frequently proprietary to the manufacturers.
Pressure drops are calculated for both sides of the best exchanger.

DOUBLE PIPE

Calculation of U-tube or straight tube double pipe exchangers (sensible to sensible only)
Allows multitube arrangements

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CHEMCAD SUITE - PROGRAM FEATURES
CC-BATCH

GENERAL FEATURES
Graphical plotting of time dependent results
Online, real-time display of results during calculation
Calculation interrupt
Full integration into the CHEMCAD Suite and flowsheets

COLUMN FEATURES
Any number of operating steps
Up to 500 theoretical stages
Reservoir feeds
Side product accumulators
Stage heaters and coolers
Calculation of ambient heat loss
Stage and condenser hold-ups (stage holdup profiles)
Simultaneous Correction and Rigorous Inside Out algorithms
Rigorous column sizing for trayed and packed columns available at the end of each operating step

OPERATING STEP OPTIONS
Startup from total reflux or from fixed liquid on all stages
Specifications may include a variety of options for the distillate, boil-up, reflux, condenser, and heat duties.
Dump accumulators at any time
Add material at any time
Stop criterion may be based on the accumulator, distillate, residual charge, or time
User-defined pressure profile (linear or non-linear)
Alternate stop criteria permitted

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CHEMCAD SUITE - PROGRAM FEATURES
CC-SAFETY NET
(all CC-SAFETY NET features are in CC-STEADY STATE)

UNIT OPERATIONS
Node – point in the piping network where pressure change occurs for some specified reason. Other unit operations go to and from nodes.
Pipe – models the pressure drop through a pipe segment or set of segments.
Pump – to move incompressible flow. Performance curve can be entered.
Compressor/Expander – to move compressible flow. Performance curve can be entered.
Flash – for phase separation under specified conditions.
Valve – simple valve for specifying outlet pressures, pressure drops, etc.
Control valve – comprehensive valve module for calculating pressure drops and/or flow through the valve based upon valve size and characteristics, flow conditions, and material properties.
Heat Exchanger – add or remove heat from a stream.

ADDITIONAL EQUIPMENT FACILITIES
Fittings and elbows – a library of fittings and elbows is provided with PIPE. Flow resistance may also be entered as L/D.
Commercial pipe schedules are built into the program.
Equipment sizing routines are provided for orifices, pipes, valves, and pressure vessels.
Equipment spec sheets are provided and can be customized.
Purchase and installed costs of major equipment can be estimated.
Equipment symbols can be added or customized by the user.
Vapor venting depressurizing facility provided.

FLUID FLOW METHODS
Darcy-Weisbach Equation – for single phase flow either compressible or incompressible.
Baker Method – for two phase flow. Determines if the flow is dispersed, bubble, slug, stratified, plug, annular or wave flow and applies appropriate equation.
Beggs and Brill Method – for two phase flow. Identifies the flow as segregated, intermittent, distributed, or transition flow to select correct equation parameters.
Isothermal flow equation – for long distance transmition lines.
Hazen-Williams equation – for water sprinkler fire protection systems.
Fritzsche equation – pressure drop formula for steam systems.
Critical flow – Critical flow of compressible fluids is always detected and reported. At the user's option, it will limit flow.

DIERS (DESIGN INSTITUTE FOR EMERGENCY RELIEF SYSTEMS)
Fully integrated into the program calculations

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