CHEMCAD 5™

Version 5.0

Book of Examples

Part1: Steady-State Simulation

Table of Contents

What Is This Book About?

This book presents the applications of CHEMCAD 5 Process Simulation Software in various process industry areas, as different as oil refining and cosmetics manufacture. Exceptional ease of use of this program and the most popular hardware and software platform, the PC running all platforms of Microsoft Windows, have won CHEMCAD wide acceptance, from engineering companies, to process plants, to universities.

The book is a presentation of material for companies who are considering the purchase CHEMCAD 5.

We have created all pictures included in this book using CHEMCAD 5.

Fired Heater Summary

Equip. No.	1
Name	
Temperature Out F	400.0000
Heat Absorbed	48.4796
(MMBtu/hr)	
Fuel Usage(SCF)	71821.5875
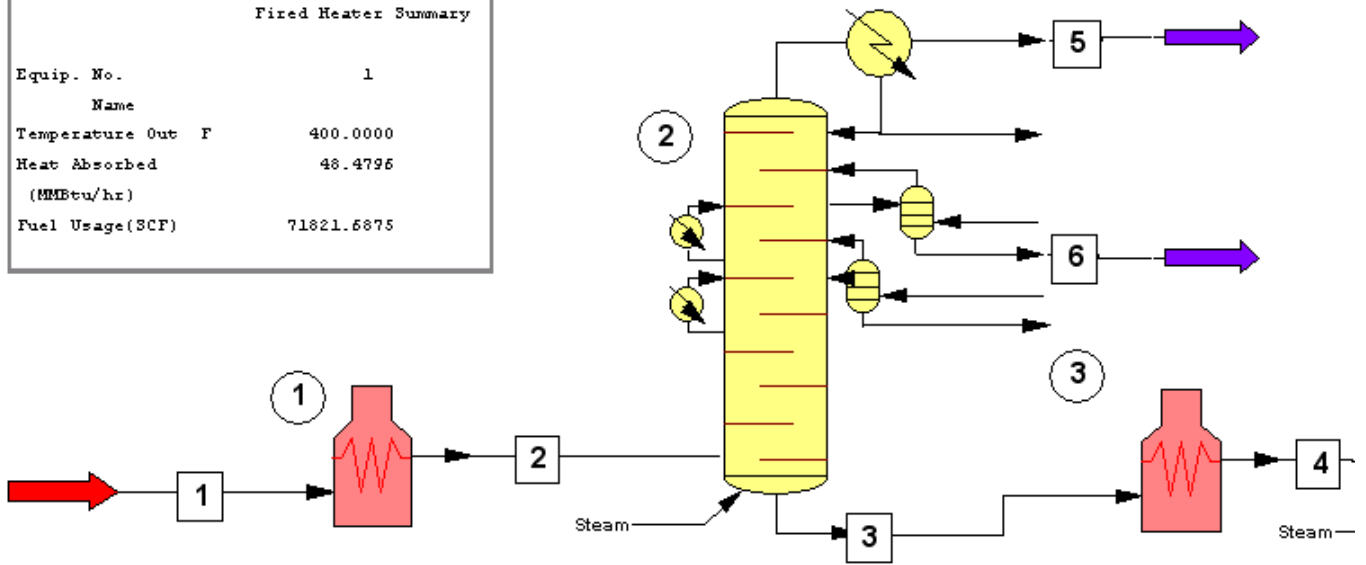
| Stream No.	1	5	6	7	8	9	10
Name							
- - Overall - -							
Molar flow lbmol/hr	1791.6	346.3	544.7	186.5	276.0	203.3	249.0
Mass flow lb/hr	310252.0	26875.7	61867.9	21922.5	47425.1	49269.9	103143.5
Temp F	150.0	100.0	278.2	100.0	394.1	515.7	614.5
Pres psia	58.0	48.0	54.1	20.0	23.9	24.4	25.0
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Degree API	34.9	84.8	49.4	47.7	33.1	25.3	15.3
Average mol wt	173.2	77.6	113.6	117.6	171.9	242.3	414.3
Actual dens lb/ft3	50.4	39.4	41.7	48.1	44.4	44.4	47.6
Actual vol ft3/hr	6154.2	681.7	1482.0	456.0	1067.4	1109.7	2166.0
Std liq ft3/hr	5848.9	658.6	1268.1	445.0	884.4	880.8	1716.1

Databoxes and graphics can be placed directly on flowsheet, forming the Main Process Flow Diagram. Individual Process Flow Diagrams can be also created and edited.

Atmospheric Distillation of Crude Oil
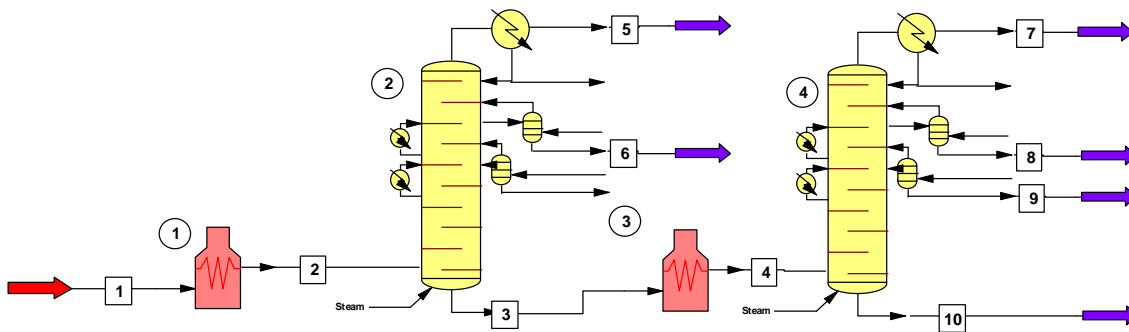
DESCRIPTION:

Crude oil is heated in a process furnace to 400 F. Then it enters the tower T-1001, near the tower bottom. The tower is equipped with 12 stages, a condenser, one side stripper for naphtha, one side heat exchanger, and one pumparound. The bottoms of the tower are heated to 600 F in the second furnace, and sent to the tower T-1002. The latter is equipped with 15 stages, a condenser, two side strippers (for kerosene and diesel oil), one side heat exchanger, and one pumparound.

The bottoms of both towers as well as all strippers are fed with live steam.
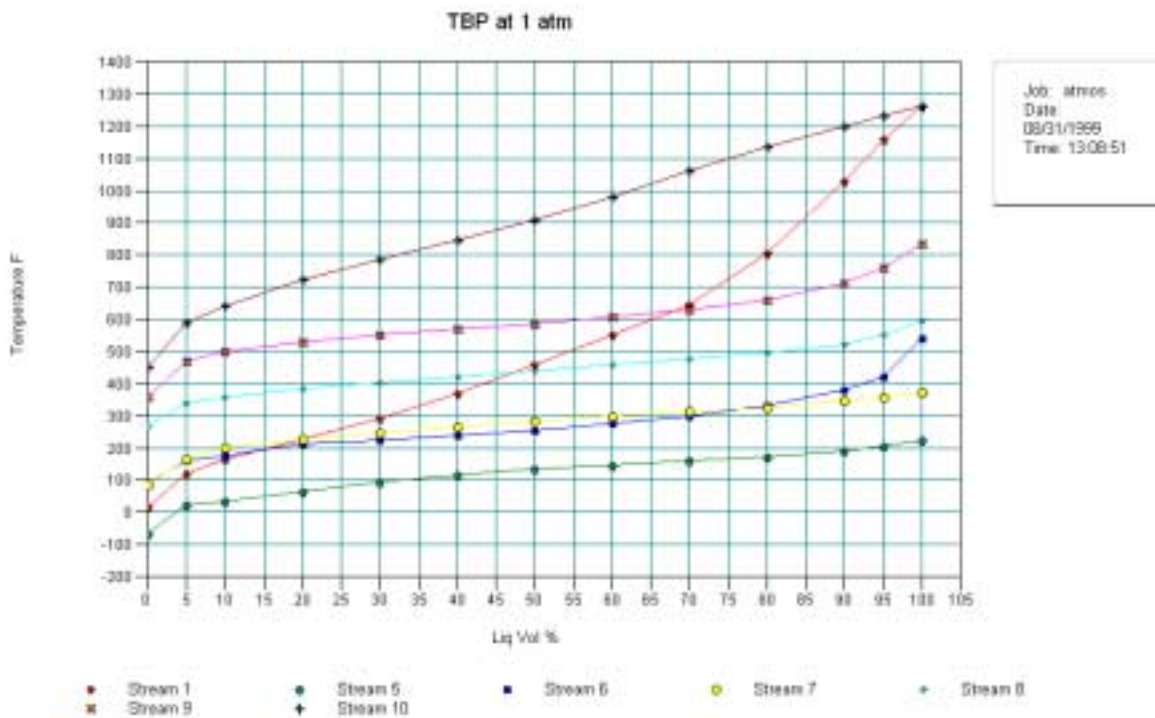
This example explains usage of the Tower Plus distillation model and a way of performing crude oil characterization.

TBP at 1 atm

Job: blending
Date:
08/31/1999
Time: 13:33:48

Temperature C

Liq Vol %

Stream 1   Stream 2   Stream 3

6
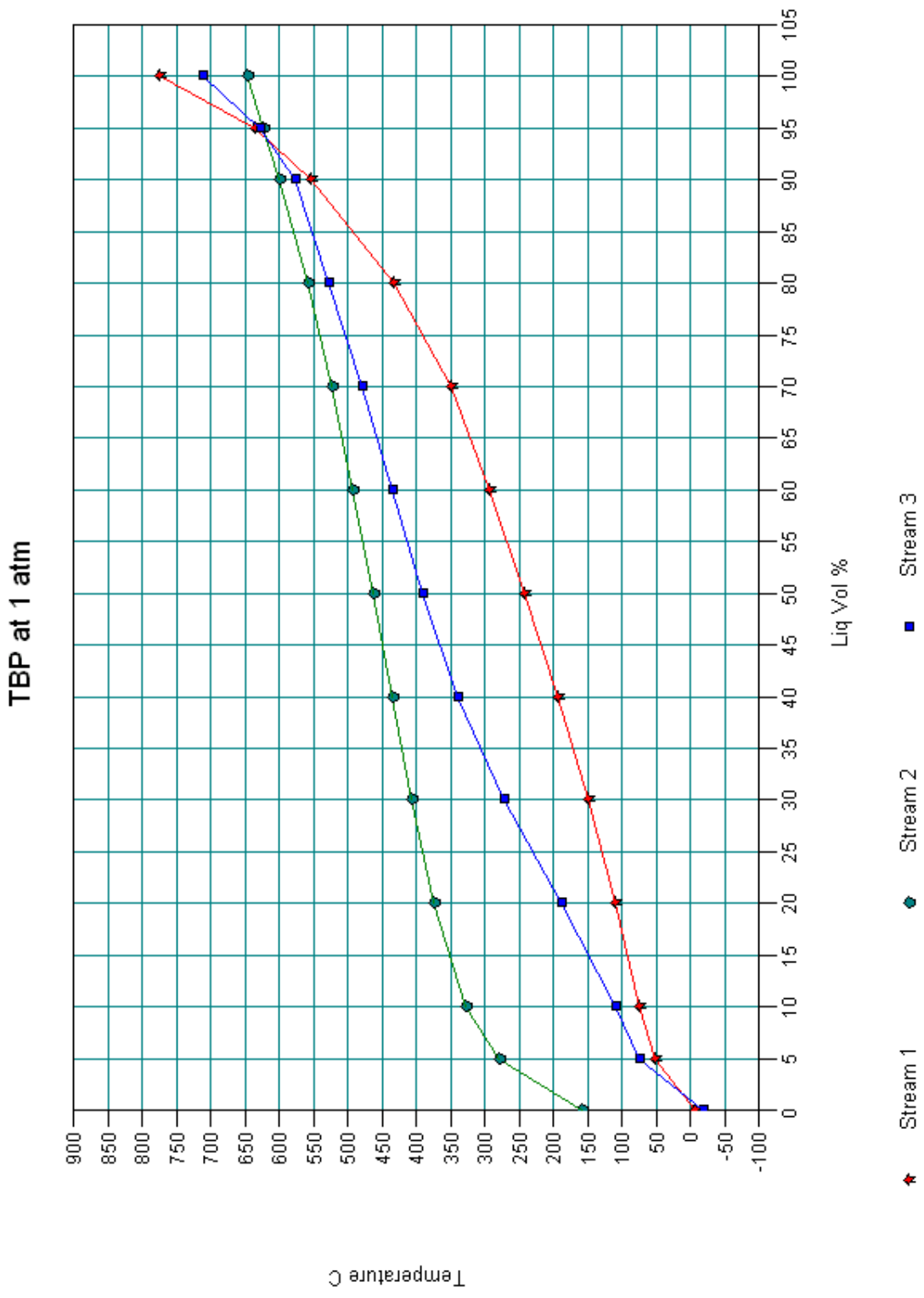
Blending of Crude Oil

DESCRIPTION:

CHEMCAD 5 has the ability to generate crude oil pseudo-components according to user provided distillation curves. CHEMCAD 5 supports the following blending options:
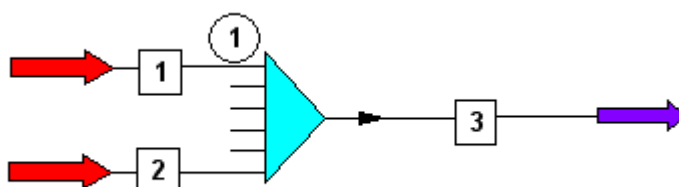
The "Blend" option can generate pseudo-components by averaging distillation curves of all streams under characterization.

The "No Blend" option allows characterizing crude oil streams individually, so pseudo-components generated from different streams can be distinguished in the product streams. This makes evaluation of distribution of various crude oils in the flowsheet easy.

CHEMCAD 5 does all reporting to user-selected editors or word processors, such as Microsoft Word, and graphics can be copied directly to the Windows Clipboard. This way, you can freely compose your reports using your favorite office software.

```
CHEMCAD 5.00
Page 1

Stream No.            3

TBP at 1 atm
Liq Vol %
     0              -18.4
     5               75.1
    10              110.2
    20              188.6
    30              272.6
    40              338.8
    50              390.1
    60              435.0
    70              480.0
    80              528.7
    90              576.6
    95              626.9
   100              711.5
```
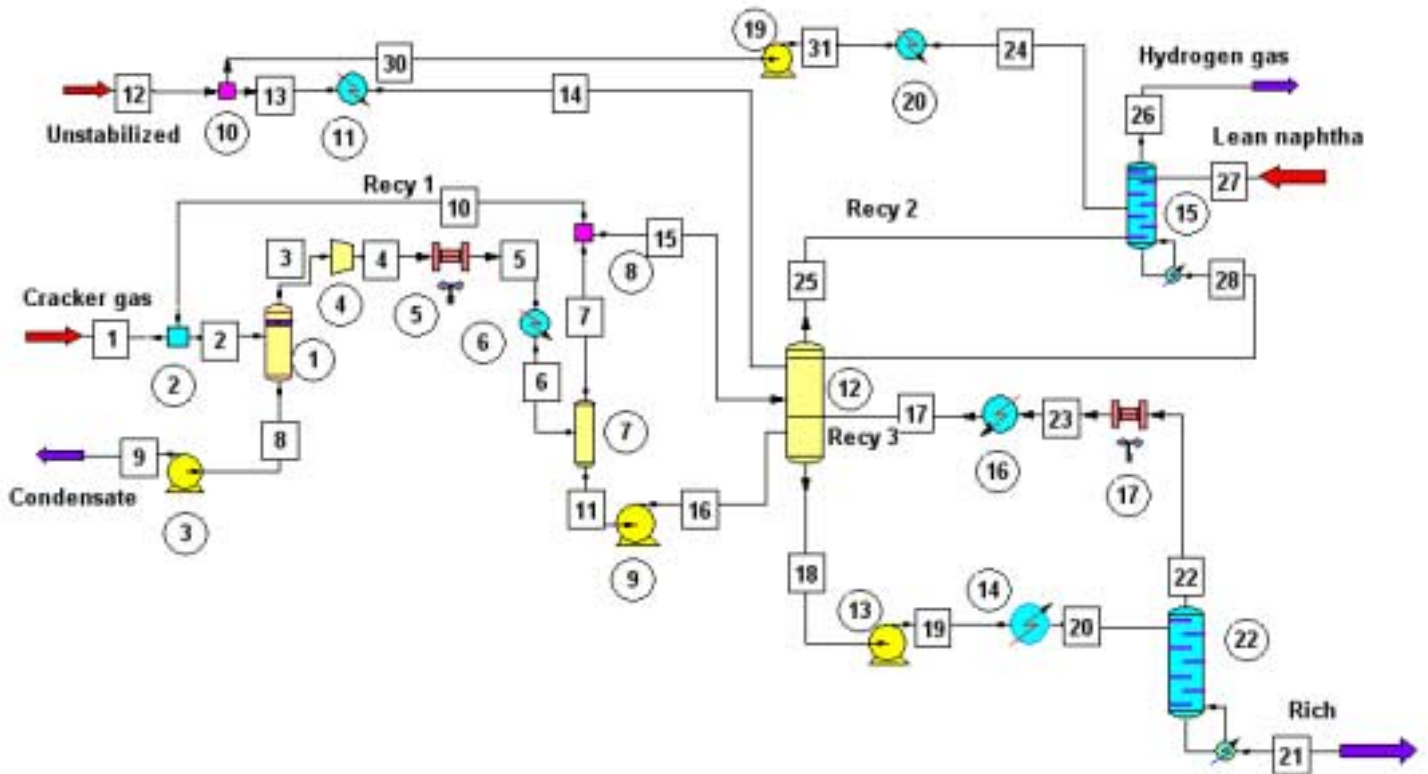
Cat-Cracker Gas Separation

DESCRIPTION:

This is a simulation of an existing process. Cracker gas is being mixed with recycled gas stream, flashed, compressed to 12 kG/cm2 G, cooled by air cooler and an aftercooler, and flashed again. Net gas and liquid from the compression stage are fed to a collector, which is a central point of the operation from the balance point. Off-gas of this collector is sent to the absorber, which is also fed with both stabilized (lean) and unstabilized naphtha. The top product of the absorber is hydrogen-enriched gas.

The bottoms are transferred to the central collector. The liquid product of the collector goes to the reboiled stripper (desorber), where the bottoms leave system as rich naphtha, and the top product returns to the collector. This flowsheet illustrates CHEMCAD's usefulness in modeling multi-recycled processes, applications of the Tower model for absorption, and desorption, as well as usage of special thermodynamic coefficients for ethylene-propylene systems.

De-Isobutanizer Sample
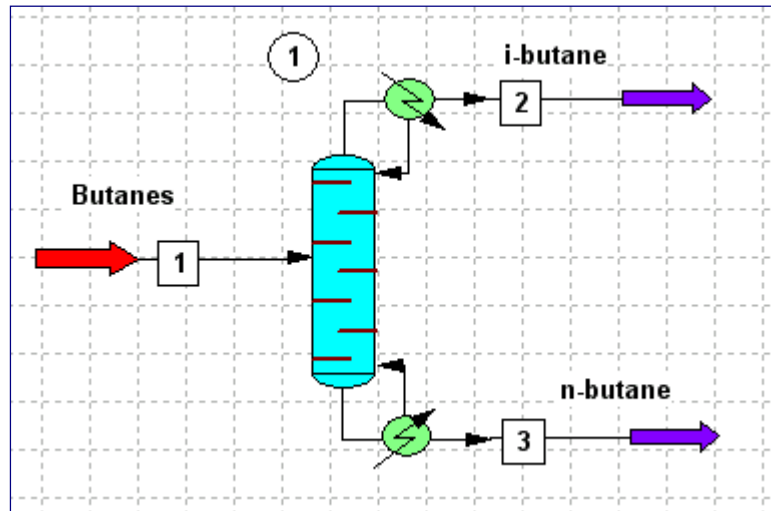
DESCRIPTION:

This example demonstrates how to make a preliminary design of an i-butane/n-butane splitter.

Given the feed's composition, flowrate and thermal state, and assuming pressure drops, a 50 theoretical stage tower equipped with a condenser and a reboiler was designed. Specified were a 99% recoveries of individual butanes to distillate and to bottoms. After several trials, an optimum feed stage location was found. The Eqsize/Trays option can do tray sizing, calculate pressure drops across trays, and estimate stage efficiencies by O'Connell and Chu correlations. Eqsize/Packing option can calculate pressure drop through a packed column, including a modern and accurate correlation of Mackowiak.

The CC-THERM module can do a rigorous design of the condenser and the reboiler, including pressure drops. The Tower model can be updated with these data and rerun, resulting in a rigorous design.

Tray Liquid Profile, Unit 1
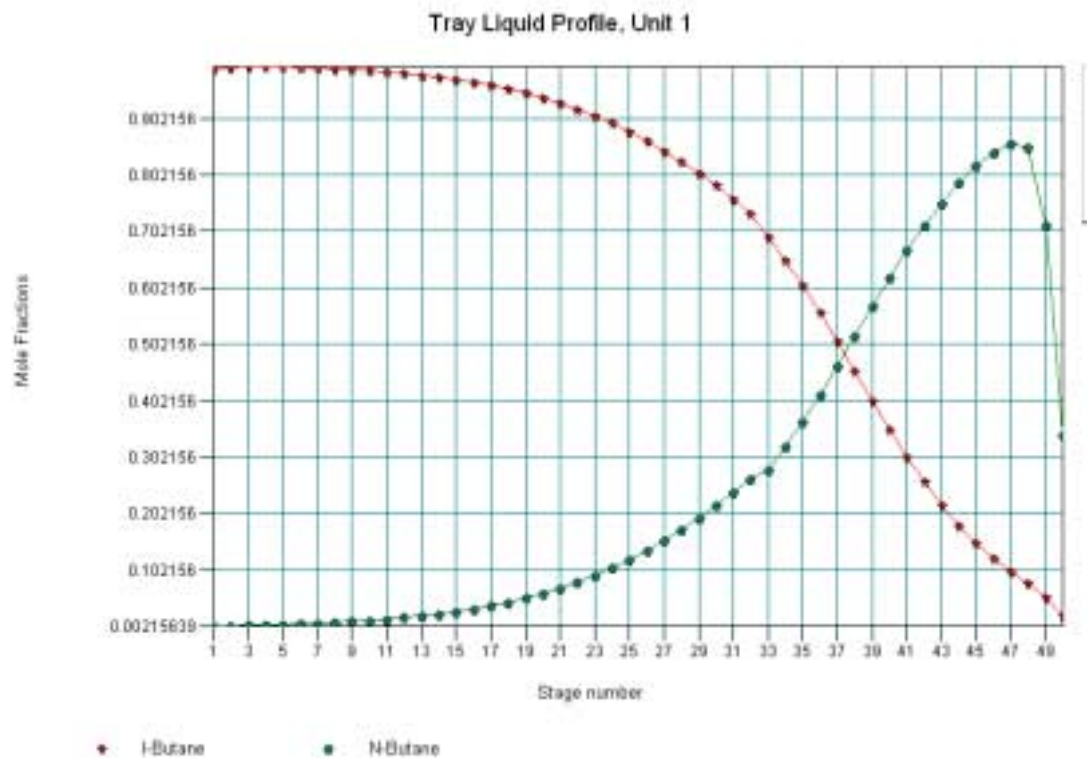
Hydrotreater Unit Simulation
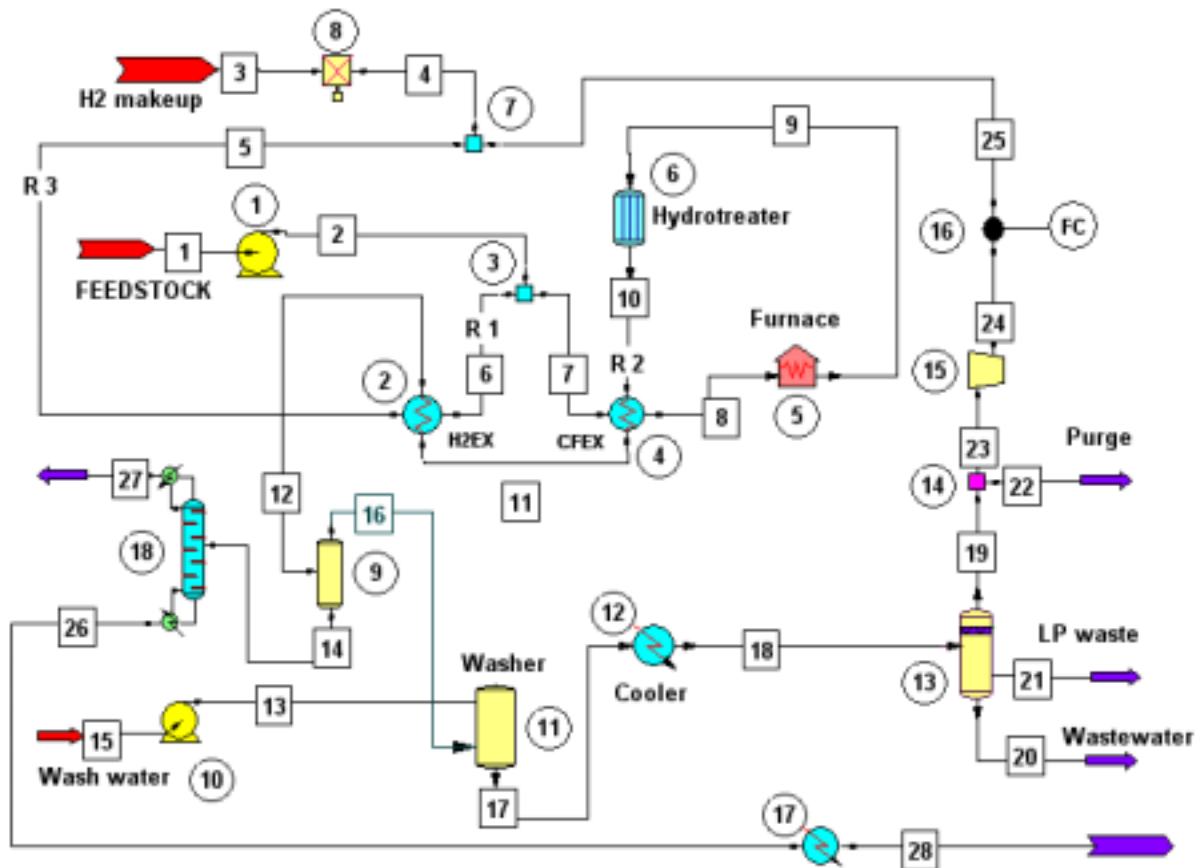
DESCRIPTION:

The example shows how to model refining technologies of undefined chemistry. The process is to remove sulfur and nitrogen impurities from C6+ petro cut by hydrogenation.

The feedstock is pumped from tankage and mixed with recycle hydrogen gas. Then it is preheated with hot reactor product gas in the CFEX heat exchanger. The reactor feed is then heated near to the reaction temperature in a process furnace, and introduced to the adiabatic hydrogenation reactor.

In the reactor, sulfur and nitrogen impurities are converted into hydrogen sulfide and ammonia respectively, and alkene bounds are being saturated. The heat of hot reaction gases is recovered in the CFEX exchanger.

Heat is further recovered in the H2EX heat exchanger, where the recycled hydrogen is preheated. The cooled mixture is sent to a drum separator, where gases are flashed off from the heavy liquid product. The gases are washed with process water, cooled, and sent to a flash drum, where light hydrocarbon product and wastewater are separated from the recycle gas. The recycle gas is purged to remove excess H_2S and NH_3 produced in the process, the gas is re-compressed and mixed with fresh H_2 make-up stream, and the recycle returns to the process.

TEG Gas Dehydration–Regeneration
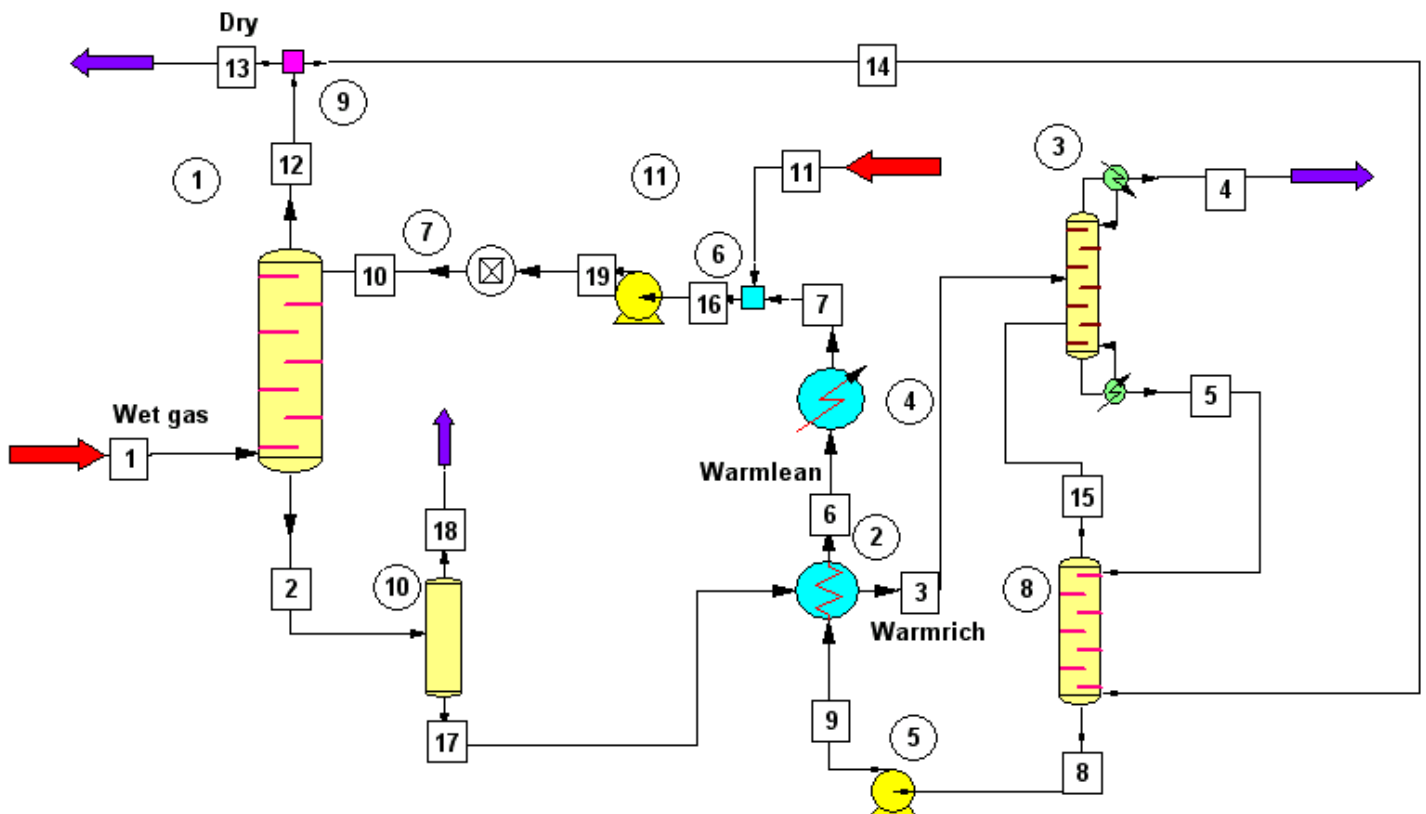
DESCRIPTION:

Currently, CHEMCAD includes 34 thermodynamic methods to determine phase equilibria, as well as electrolyte package and solids as built-in features. K-Value methods vary from very universal to specialized ones. Process natural gas dehydration with triethylglycol (TEG) has its own K-Value method in CHEMCAD 5.

The flowsheet describes a typical dehydration unit. Gas enters the unit at 85 deg F, saturated with water. It is dried in the dehydrator column at 500 psia by contact with lean TEG. The rich TEG is then flashed, heated and regenerated with a combination of indirect heat and a slipstream of the dried gas. The regeneration column has a reboiler, condenser and packed section below the reboiler. With this flowsheet, the water removal from a process or natural gas stream as a function of operating variables is calculated. The user may define circulating TEG flow, column pressures, flash pressure, stripping gas flow and heat exchanger performance.

Propane-Propylene Splitter
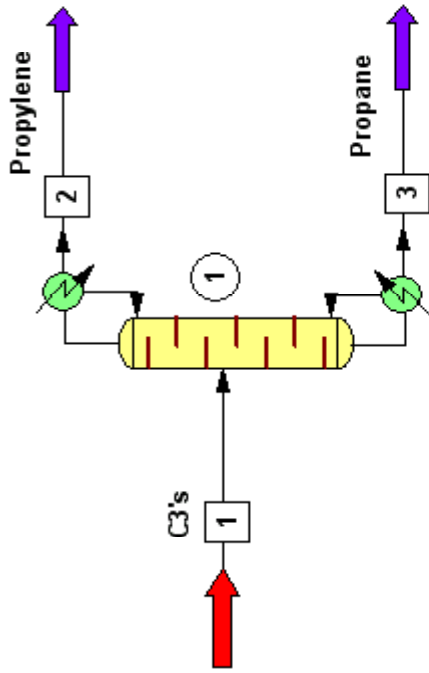
Stream No.	1	2	3
Name	C3's	Propylene	Propane
- - Overall - -			
Molar flow lbmol/hr	755.3	543.4	211.9
Mass flow lb/hr	32263.4	22869.3	9394.1
Temp F	107.0	97.0	123.1
Pres psia	240.0	220.0	250.0
Vapor mole fraction	0.0000	0.0000	0.0000
Enth MMBtu/hr	-9.0508	1.1518	-10.274
Actual vol ft3/hr	1098.7	759.0	334.2
Std liq ft3/hr	997.0	702.1	294.9
Std vap 60F scfh	286620.2	206225.8	80394.4
Flowrates in std vap scfh			
Ethane	113.8	113.8	0.0
Propylene	208713.3	205324.7	3388.5
Propane	75895.7	787.2	75108.5
N-Butane	1897.4	0.0	1897.4

Propane-Propylene Splitter

Tray Liquid Profile, Unit 1
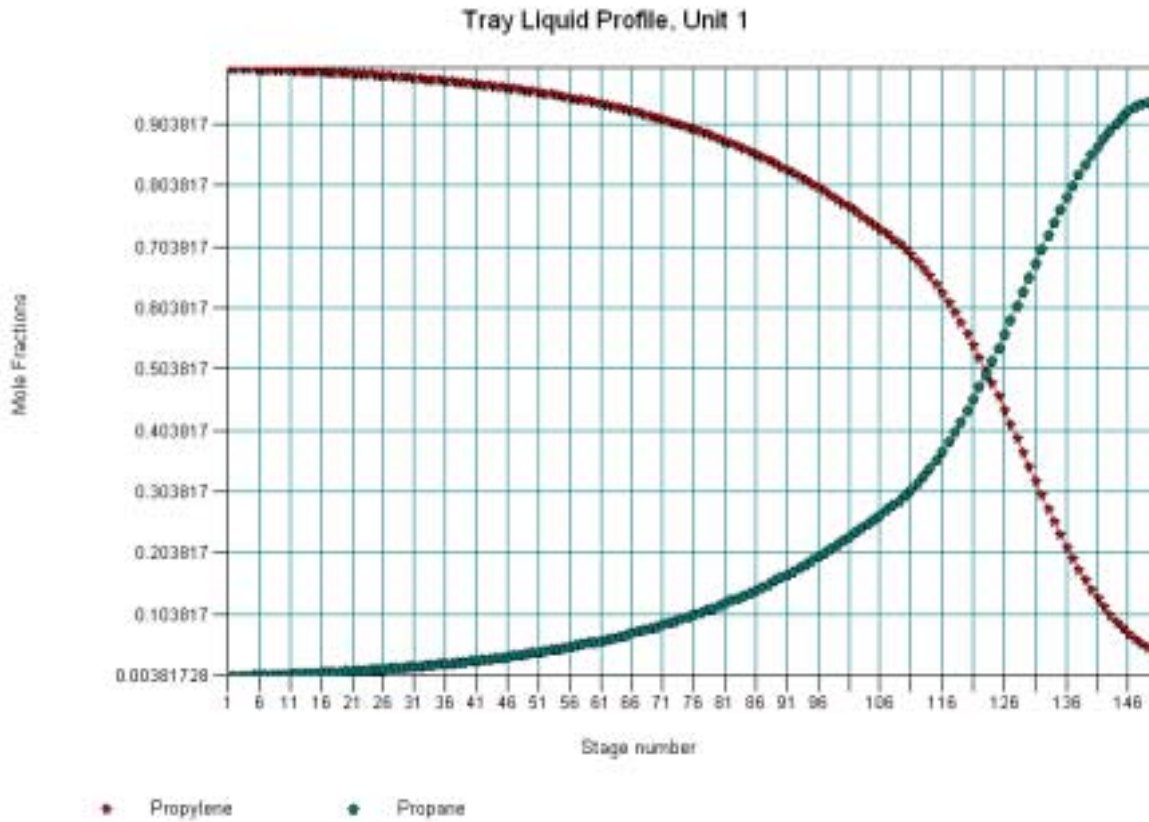
DESCRIPTION:

Propane and propylene are very difficult to separate one from another, as they are close-boiling components. Nonetheless, distillation at elevated pressure is a common technology, provided sufficient number of trays exists in the distillation column.

Calculations of a 148 actual-tray tower are presented in this example. The SCDS distillation model was used to accommodate big number of trays, and to account for actual trays.

Propane/propylene and ethane/ethylene vapor-liquid equilibria are affected by interactions between the components. Special Binary Interaction Parameters for the Peng-Robinson Equation-Of-State were used to reflect these non-idealities.

Tray Vapor Profile, Unit 1
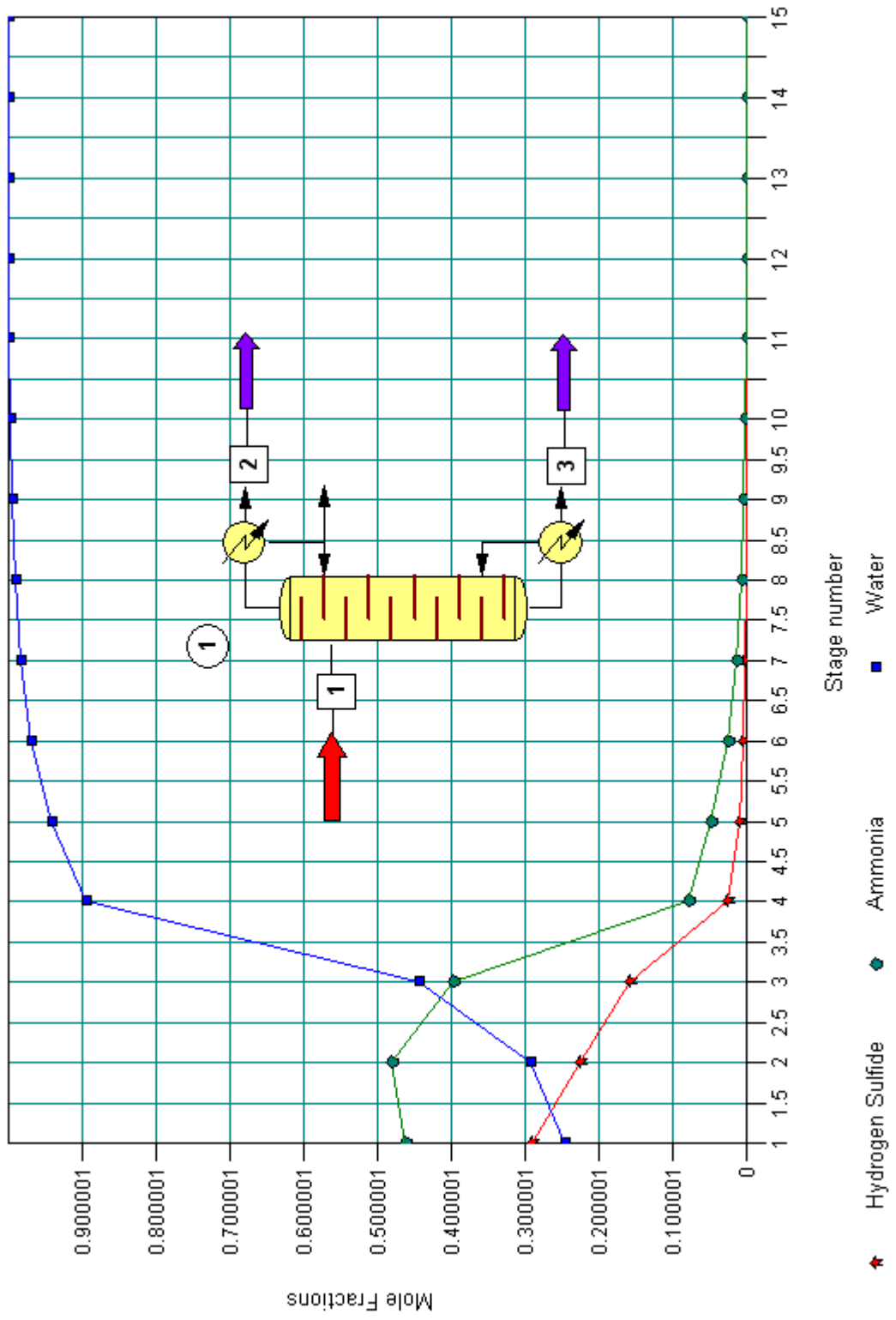
Sour Water Stripper
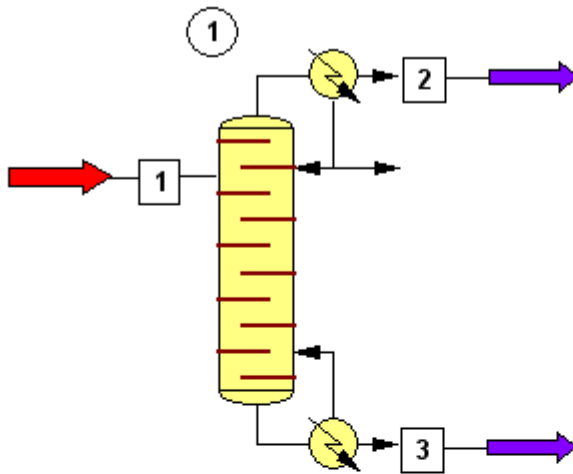
Stream No.	1	2	3
Name			
– – Overall – –			
Mass flow lb/hr	69503.7	343.2	69160.5
Temp F	140.0	148.1	218.7
Pres psia	56.9	14.4	16.8
Vapor mass fraction	0.0000	1.000	0.0000
Component mole fractions			
Hydrogen Sulfide	0.00	0.29	0.00
Ammonia	0.00	0.46	0.00
Water	1.00	0.25	1.00

DESCRIPTION:

In this example, the Tower Plus (TPLS) model has been used to simulate stripping wastewater from Hydrogen Sulfide and Ammonia down to the level of 5 ppm. This is another application of the TPLS model, which is normally used to simulate atmospheric and vacuum distillation of crude oil.

The tower is equipped with a reboiler, and a pumparound is used to generate internal reflux.

A special thermodynamic model, SOUR, has been used to calculate equilibria in the system.

The picture below is the Process Flow Diagram including a Stream Databoxes. CHEMCAD 5 allows to place Stream and Equipment Databoxes on a PFD, and you are free to select properties and the units of measure that would appear there.

D1160 at 10mmHg

Temperature C

Liq Vol %

Stream 1   Stream 2   Stream 3   Stream 4   Stream 5

18
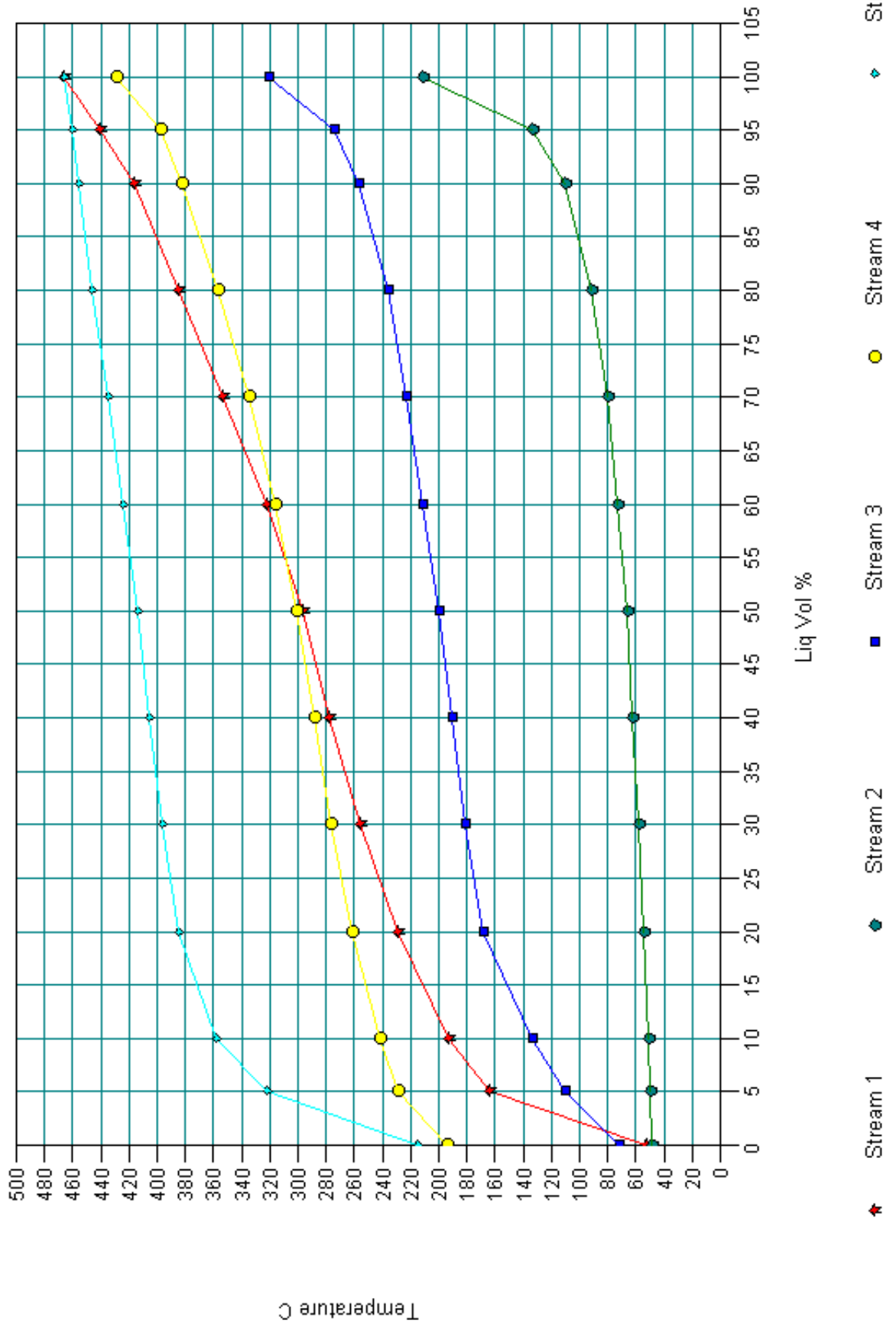
Vacuum Tower with TBP Assay

DESCRIPTION:

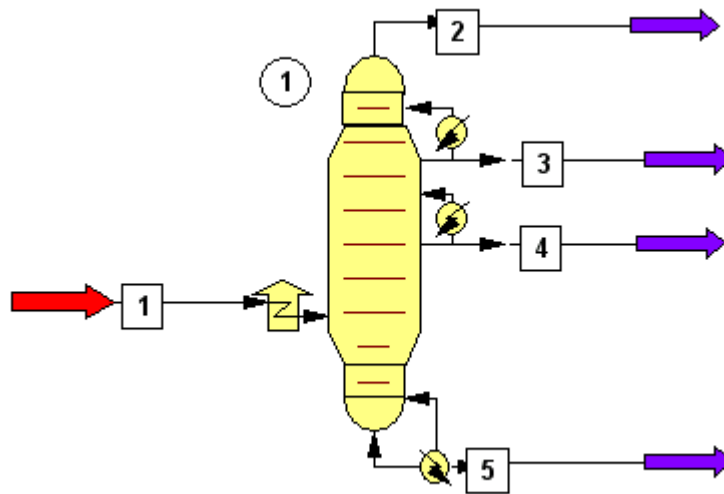Atmospheric residue is distilled under vacuum into fuel oil, two grades of vacuum gas oil, and vacuum residue. The preheated feed stream enters the bottom part of the tower, which is additionally heated. Two pumparounds provide internal reflux.

The process has been modeled with a Tower Plus (TPLS) distillation module.

The example shows how flexible as to specifications the TPLS module is. (For instance, you may replace a condenser with a pumparound, or the reboiler with side heat exchanger, if you need it.) It also demonstrates characterization of the oil feed by TBP assay. (The figure below shows feed and product characterization curves after automatic TBP-D1160 inter-conversion). A thermodynamic K-Value model most suitable for vacuum distillation of heavy material was selected.
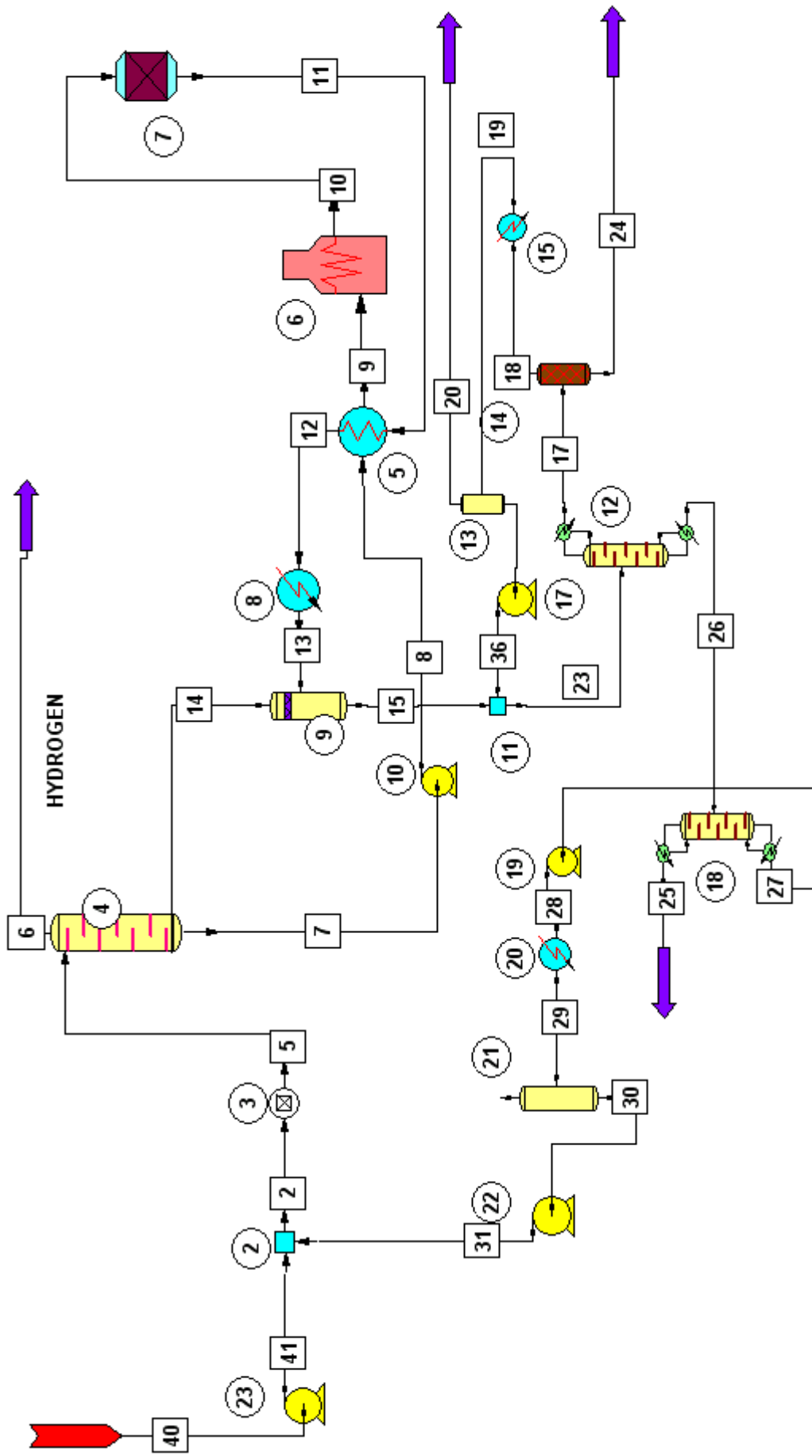
Methyl-Ethyl Ketone Manufacture, 15,000 metric tons per year

HYDROGEN

MEK Process. Dehydrogenation of sec-Butanol

DESCRIPTION:

The flowsheet shows a technology to make 15,000 MTPY of methyl ethyl ketone (MEK) by sec-butanol (SBA) dehydrogenation. It is a design study.

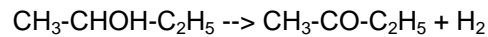Fresh SBA is pumped onto the top of a scrubber (1), where residual MEK is removed from a byproduct hydrogen stream. Then SBA is vaporized and superheated before it enters the reactor system (6), where sec-butanol is dehydrogenated in a vapor phase reaction over a solid catalyst:

$$CH_3\text{-}CHOH\text{-}C_2H_5 \text{ --> } CH_3\text{-}CO\text{-}C_2H_5 + H_2$$

The reaction is highly endothermic and it is typically carried out in several reactors connected in parallel or in series.

According to literature (Kirk-Othmer), conversion of 90 % can be achieved fairly easily.

The reactor effluent is condensed, and hydrogen is flashed off. Crude MEK enters the distillation column (7), where MEK-H2O azeotrope goes to the top. The product is dehydrated on a rock salt bed, and the MEK-rich phase is condensed and recycled to the azeo column. Dried mixture of unconverted SBA and MEK is then distilled into 99.5 wt. % MEK product and SBA, the latter being recycled to the process feed stream.

Example in the Training Book explains handling multiple recycles, a reactor model, non-ideal VL equilibria, controllers, and modeling special operations, like rocksalt bed unit.
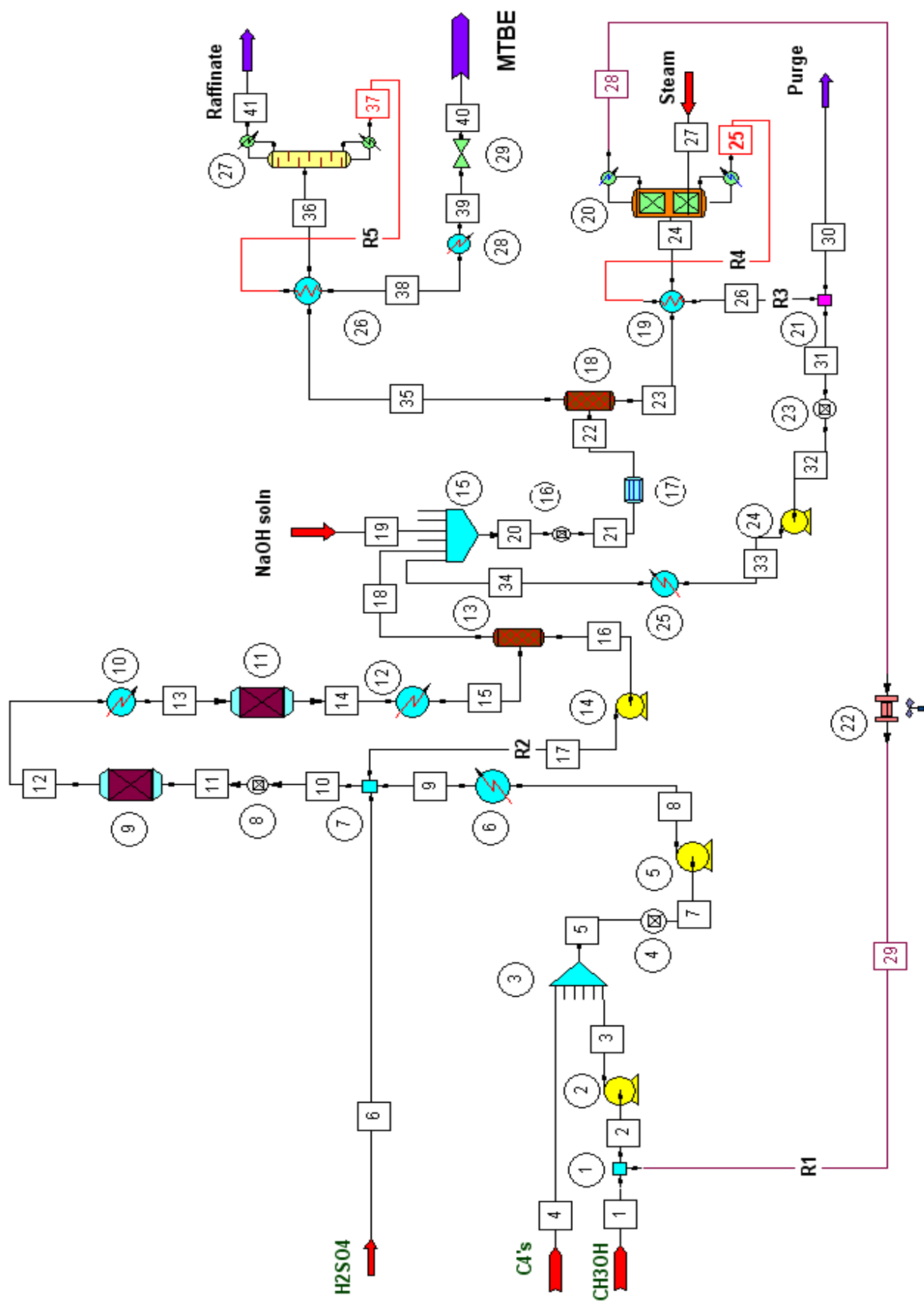
MTBE Process with H_2SO_4 Catalyst

DESCRIPTION:

MTBE is made commercially by catalytic reaction between methanol and i-butylene. A widely used catalyst is an acidic ion exchange resin. This flowsheet shows the alternate route, where sulfuric acid is used as catalyst. The flowsheet was made according to published data. (Al-Jarallah, A.M., and Lee, A.K.K., "Economics of new MTBE design", Hydrocarbon Processing July 1988.)

The process is to make approximately 100,000 metric tons per year of the MTBE product.

A mixture of fresh and recycled methanol is mixed with a C4 stream and a mixture of fresh and recycled sulfuric acid, and reacted at elevated temperature and pressure in two sets of multistage, intercooled reactors in liquid phase. Most of H_2SO_4 is then separated in the settler and recycled to reaction. Sour organic phase is then neutralized with alkali and washed with water. Methanol is recovered from the aqueous phase by stripping with live steam and recycled to the process. The wash water recycle is purged to avoid Na_2SO_4 build-up. Washed organic phase is distilled to separate the MTBE product from spent butanes.

The Training Book explain the importance of Convergence Parameters in converging big, multi-recycled flowsheets. Calculations of *WAR Environmental Report* have been demonstrated. This feature allows the user to assess the environmental impact of waste streams.
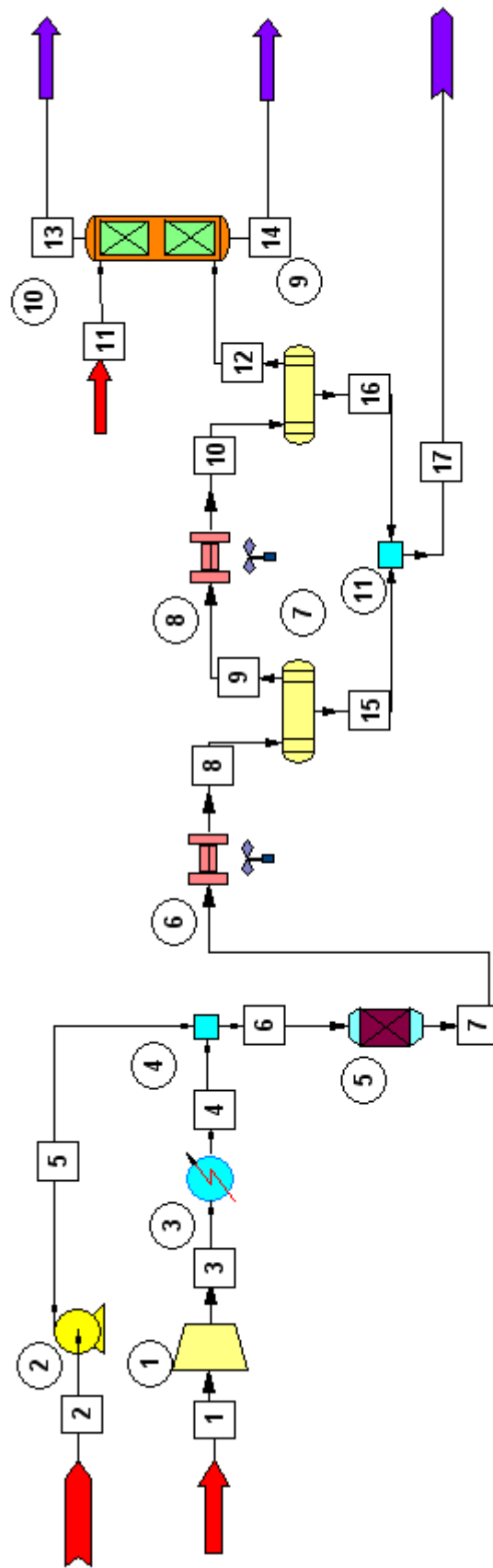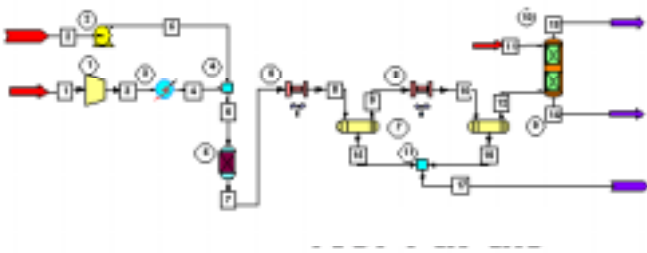
The Phthalic Anhydride Process

DESCRIPTION:

One of the routes to make Phthalic Anhydride (PA) is to oxygenate o-Xylene with air in a catalytic process.

Extensive laboratory/computational work has been carried out to develop actual kinetic model for the reactor. Then the data were input to CHEMCAD's Kinetic Reactor model as the Extended Kinetic Equation. Heat transfer was also included into the model.

As we were not permitted by the technology owner to publish data, the Training Book example involves simpler model for a similar process.

Reactive absorption has been employed to model a scrubber converting anhydrides into respective carboxylic acids.

```
                    Scds Rigorous Distillation Summary

Equip. No.                        10
        Name
No. of stages                      2
1st feed stage                     1
2nd feed stage                     2
Top pressure  bar              1.0132
Reactive distillation ?            Y
Reflux mole  kmol/hr         1560.7957
Reflux mass  kg/hr           30083.8094


Reaction Stoichiometrics and Parameters for unit no. 10

 No. of liquid reactions = 2
 No. of vapor reactions  = 0
 Mole unit: 2   Act. E unit : 3  Vol. unit : 2
 Time unit: 2   Press. unit : 0  Temp unit : 0

 Tray reaction volumes

      Stg       Liq rxn vol       Vapor rxn vol
       1       2.0800e+001        0.0000e+000
       2       2.0800e+001        0.0000e+000

Reaction   1   Type =   0    Phase =   0
A =  1.0000e+001  E =  0.0000e+000  Para3 =  0.0000e+000

Comp   Stoich.    Exp.factor   Adsorb Fac.   Adsorb E    Adsorb Exp.
  2   -1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000
 10   -1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000
 11    1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000

Reaction   2   Type =   0    Phase =   0
A =  1.0000e+001  E =  0.0000e+000  Para3 =  0.0000e+000

Comp   Stoich.    Exp.factor   Adsorb Fac.   Adsorb E    Adsorb Exp.
  3   -1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000
 10   -1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000
 12    1.00e+000  0.0000e+000  0.0000e+000  0.0000e+000  0.0000e+000
```

```
                  Compressor Summary

Equip. No.                        1
        Name
Type of Compressor:               2
Pressure out  bar             1.6000
Efficiency                    0.7500
Actual power  kW             603.0629
Cp/Cv                         1.3989
Ideal Cp/Cv                   1.3975
Calc Pout  bar                1.6000
Theoretical power  kW        442.3389
```
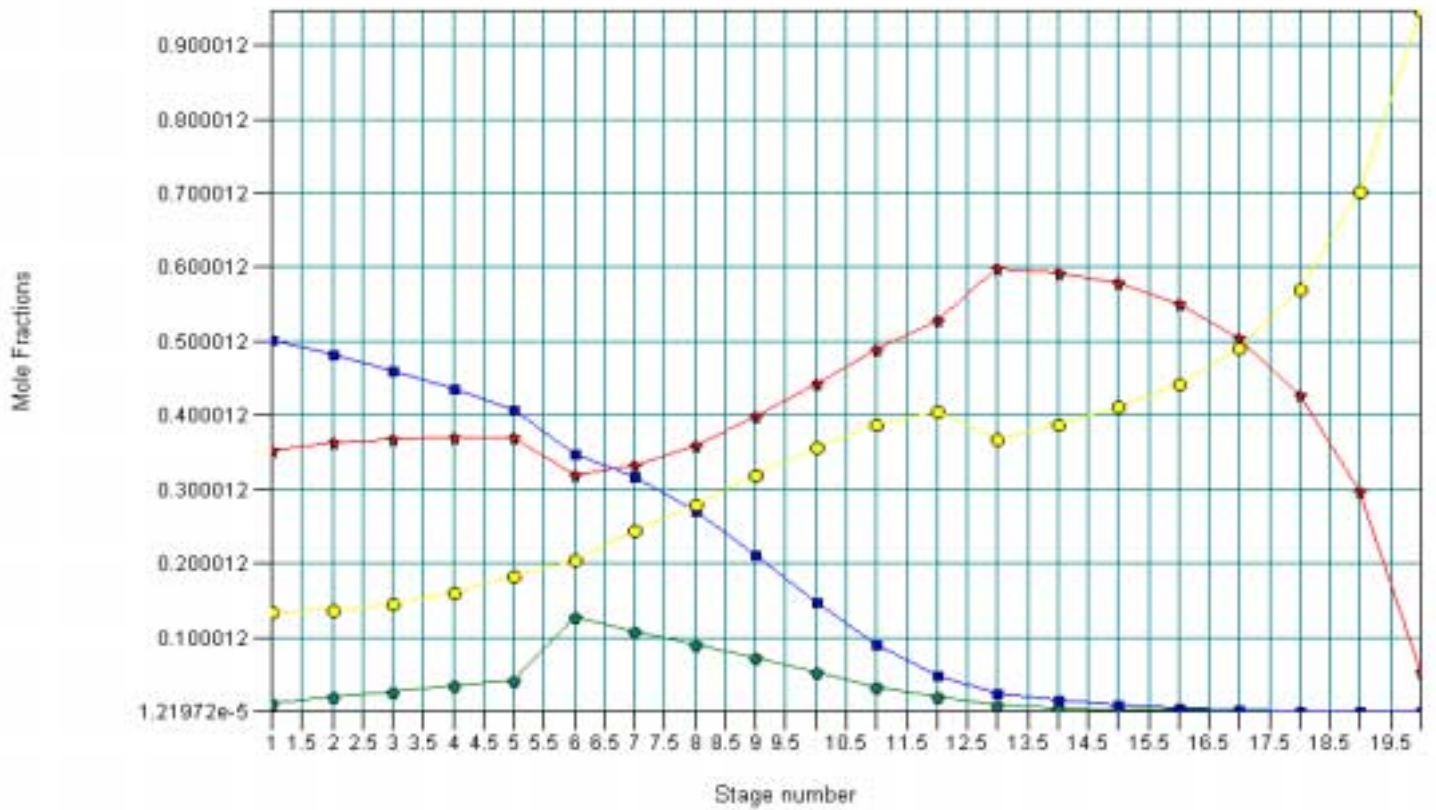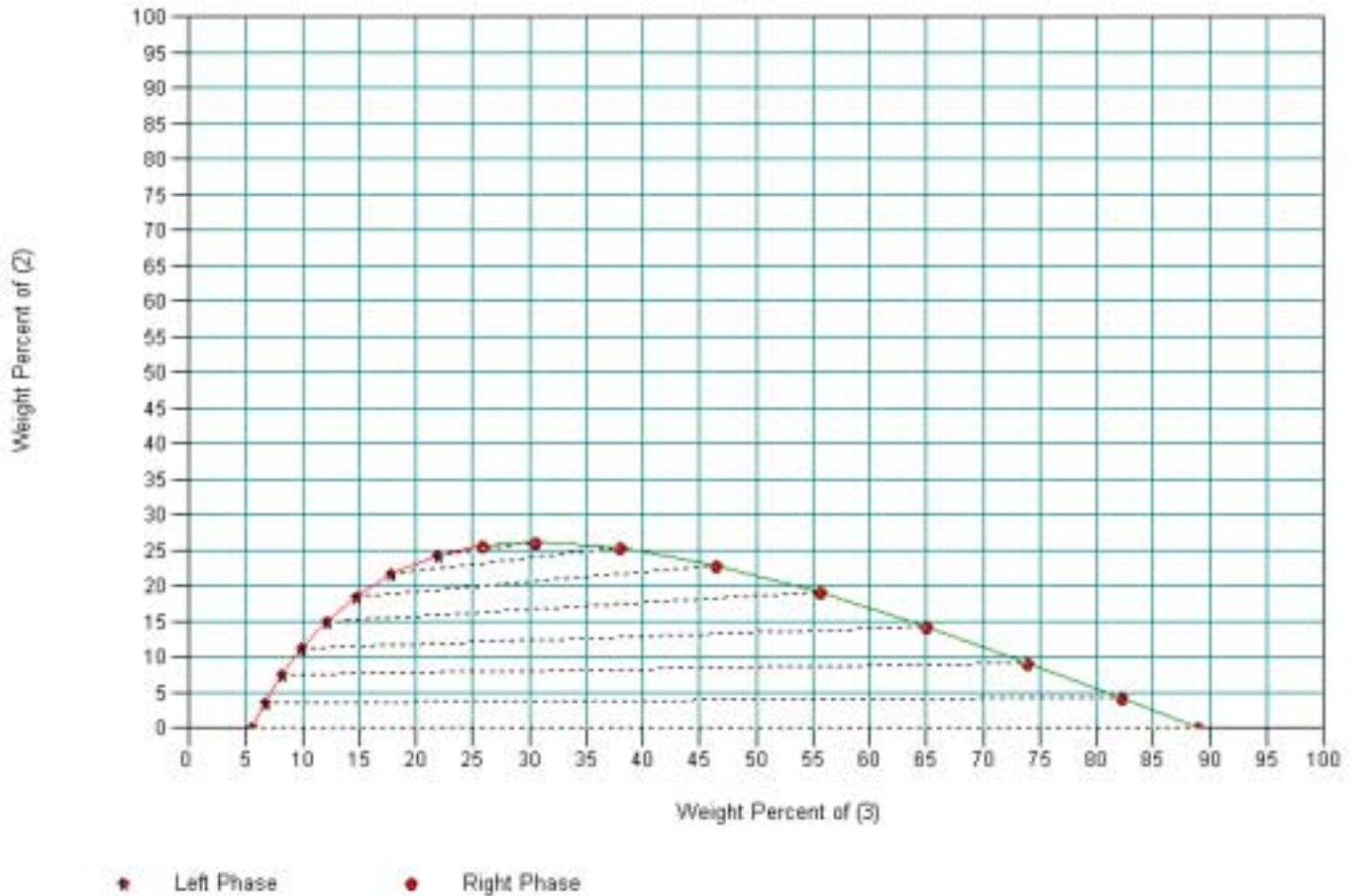
Tray Liquid Profile, Unit 1

Water/Ethanol/Ethyl Acetate at   30.00 C By NRTL

★ Left Phase   ● Right Phase

Ethyl Acetate by Reactive Distillation
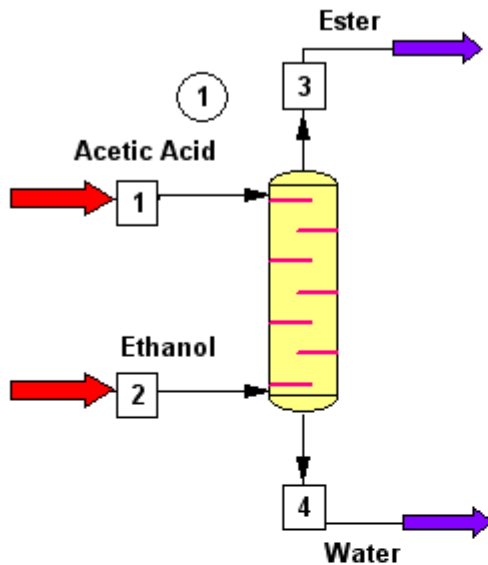
Stream No.	1	2	3	4
Name	Acetic Acid	Ethanol	Ester	Water
- - Overall - -				
Molar flow kmol/hr	25.0	50.0	48.7	26.3
Mass flow kg/hr	1501.3	2106.6	3094.5	513.5
Temp C	70.0	70.0	71.5	90.3
Pres bar	1.2	1.2	1.0	1.0
Component mole fractions				
Ethanol	0.00	0.86	0.35	0.05
Acetic Acid	1.00	0.00	0.01	0.00
Ethyl Acetate	0.00	0.00	0.50	0.00
Water	0.00	0.14	0.14	0.95

DESCRIPTION:

For reversible reactions, the equilibrium state can be shifted in desired direction by, i.a., adding one of reactants in excess or removing products from the reaction mass. This principle is the background of reactive distillation technique. Products are separated and removed from the distillation column due to difference in their relative volatilities, and due to counter-current reactants' flow, reactants are in excess to each other at several column stages.

This example shows how easily CHEMCAD 5 can cope with reactive distillation and extremely non-ideal systems. Not only is a reversible reaction there; Acetic Acid, Ethanol, Water, and Ethyl Acetate form a thermodynamically complex system with two-liquid phases and vapor phase association. For a chemical engineer, though, the only task is to correctly select thermodynamic models, enter reaction(s) equilibrium or kinetic coefficients, and specify the column as he would do with more 'typical' distillation; CHEMCAD 5 will do the rest.

CO2 separation by Benfield process
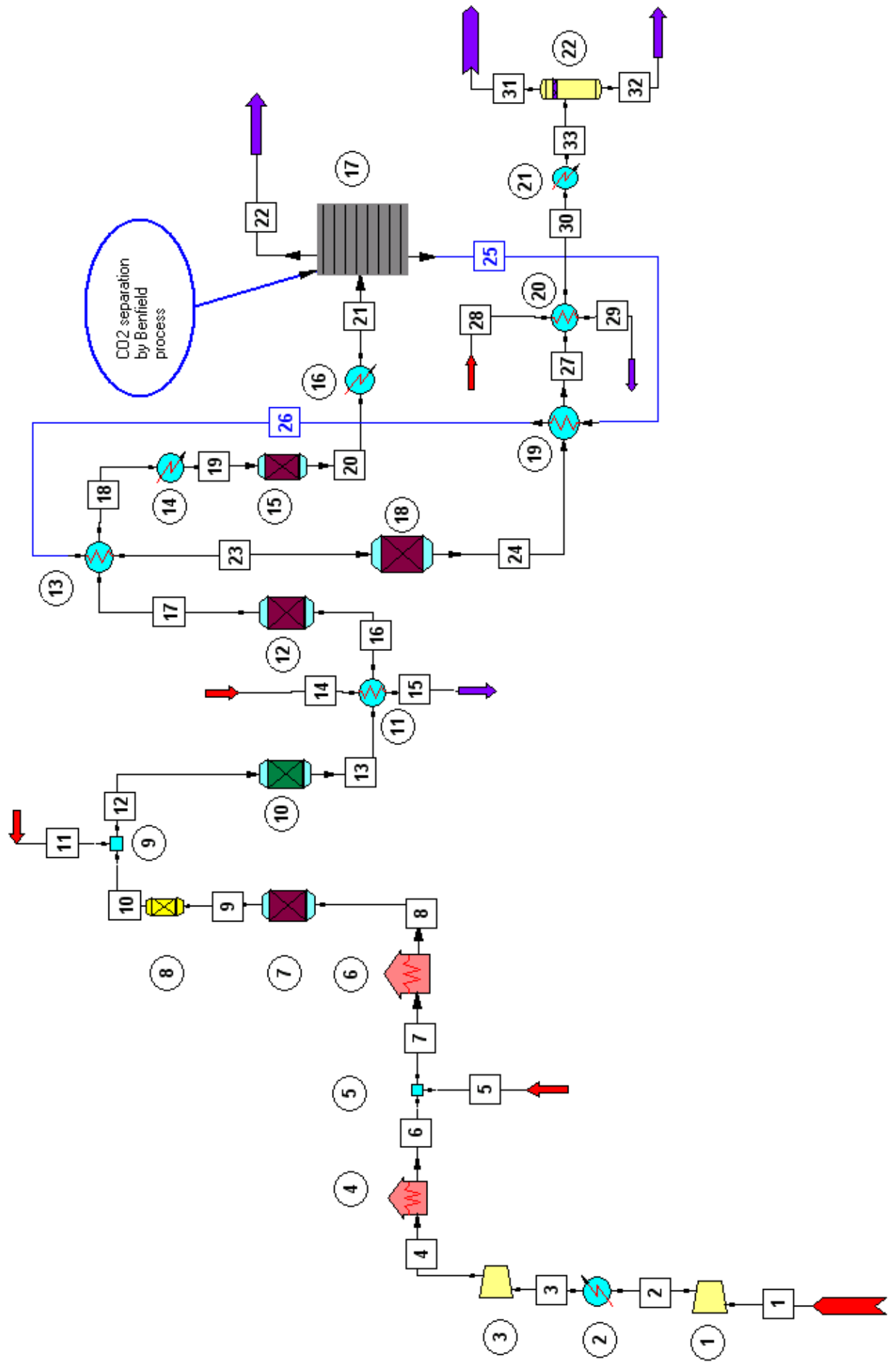
Ammonia Syngas Plant

Exchanger 19 Heat Curve

Stream 24   Stream 25
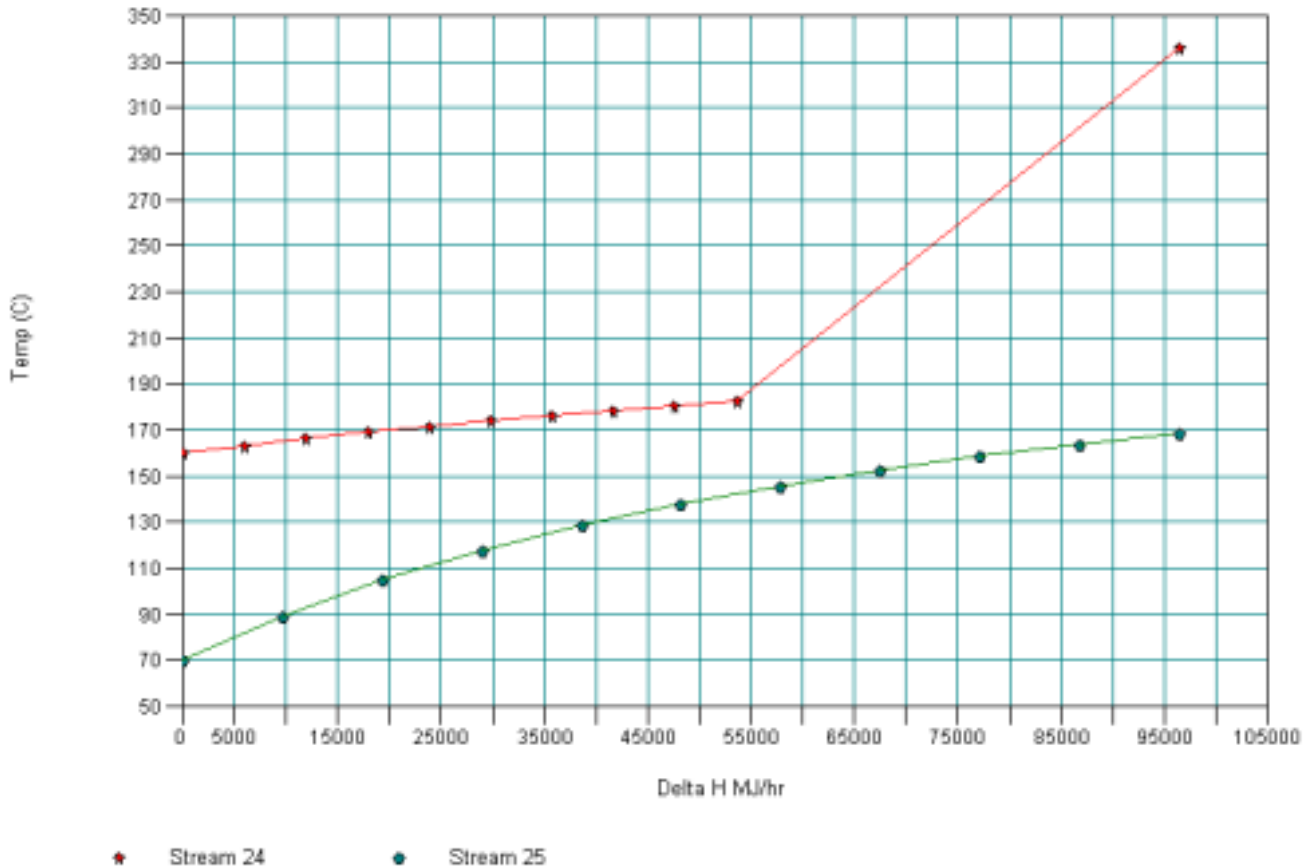
DESCRIPTION:

Real life technology to make 3:1 H2/N2 syngas has been shown. It involves processes such as methane conversion with steam and air, CO to CO2 conversion (the Shift reaction), and the methanation reaction. The flowsheet includes multiple recycle loops.

CHEMCAD 5's Equilibrium Reactor and Gibbs Reactor models are perfectly fit to rigorously calculate reactions involved in syngas manufacture. The Equilibrium Reactor has equilibrium constants for methanation/shift reaction built-in, so it does not require any intervention from the user.

CHEMCAD 5 is very useful in everyday plant operation. Once the plant has been modeled with a flowsheet (even a simplified one), it is very easy to find out the process bottlenecks, units with excessive utility consumption, etc. Very often, it is enough to change some process parameters to save substantial money and to make better product with existing equipment. Sometimes a small revamp would be adequate. When the story is the heat exchanger, the additional module CC-THERM can help to rate existing exchanger, make modifications in the heat exchanger, or design a new one. It has been proven that the savings achieved with CHEMCAD and CC-THERM can exceed many times the initial license cost.

Wet Desulfurization of Flue Gas
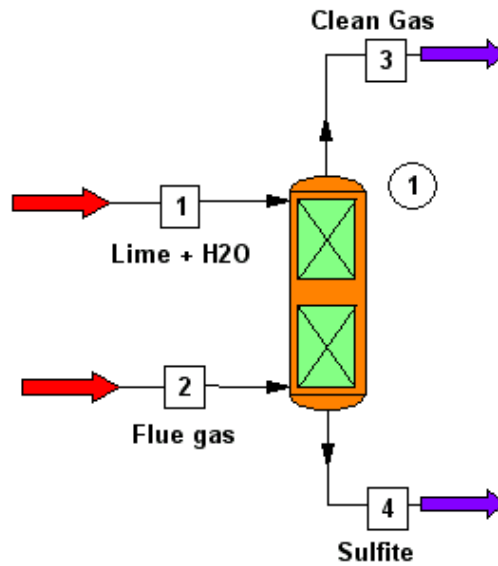

DESCRIPTION:

One of methods to clean up flue gas is the wet process. Aqueous lime suspension is introduced onto the top of a spray tower, and flue gas counter-currently contacts liquid droplets. Sulfur dioxide is converted into sulfites, and CO2 is released.

Enhanced electrolyte package being an integral portion of CHEMCAD 5 makes this sort of calculations feasible. The unique True Species Approach treats electrolyte species as they were regular components, so the calculation results reflect true distribution of material into molecules and ions. The Electrolyte Expert tool helps setting up the electrolyte system very effectively; this action is almost transparent to the user.

```
Job Name: wet-sox

Stream No.                          1              2              3              4
Stream Name                 Lime + H2O       Flue gas      Clean Gas        Sulfite
Temp   C                      20.0000*        40.0000*       15.2654        15.1076
Pres   bar                     1.1000*         1.1000*        1.0000         1.0000
Enth   MJ/hr              -8.5824E+005   -1.5906E+006   -1.9039E+006   -5.4498E+005
Vapor mole fraction           0.00000         1.0000         1.0000        0.00000
Ph value                      10.1498         0.0000         0.0000         6.2584
Ionic strength molal           0.0006         0.0000         0.0000         3.2546
Total kmol/hr              2828.0085     61882.0478     62976.8497      1755.4089
Total kg/hr              55296.2303   1800000.0139   1819076.1812     36219.9106
Total std L m3/h             50.9465      2221.7423      2241.5958        31.2470
Total std V m3/h          63385.98      1387002.41     1411540.89       39345.12
Flowrates in kmol/hr
Sulfur Dioxide                0.0000        28.0965         0.0005         0.0000
Carbon Dioxide                0.0000      4089.9795      4114.8903         0.0824
CalciumCarbonate             52.9916         0.0000         0.0000        27.6882
Water                      2774.9948         0.0000      1098.0072      1673.8902
Nitrogen                      0.0000     57764.0000     57764.0000         0.0214
H+                            0.0000         0.0000         0.0000         0.0000
OH-                           0.0051         0.0000         0.0000         0.0000
CO3--                         0.0033         0.0000         0.0000         0.0008
HCO3-                         0.0051         0.0000         0.0000         0.3176
HSO3-                         0.0000         0.0000         0.0000         5.8884
SO3--                         0.0000         0.0000         0.0000        22.2080
Ca++                          0.0084         0.0000         0.0000        25.3118
```

CO$_2$ Removal by the Benfield Process
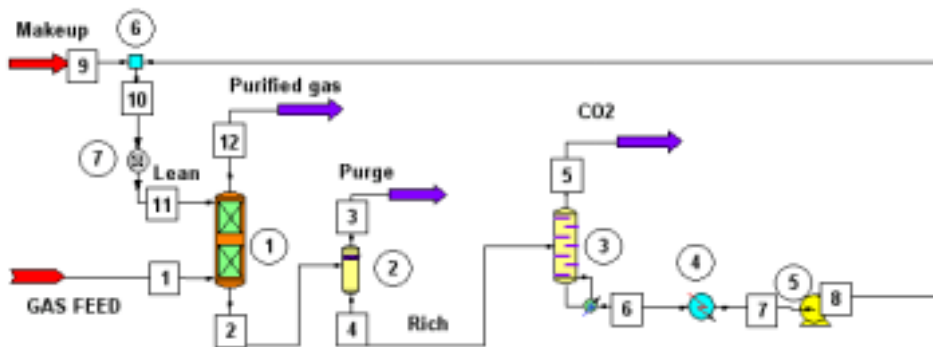
Stream No.	1	12	3	5
Name	GAS FEED	Purified gas	Purge	CO2
- - Overall - -				
Temp C	30.80	83.70	86.35	93.70
Pres bar	22.20	21.50	1.50	1.00
Actual vol m3/h	1866.10	2157.94	129.55	7192.02
Std vap 0 C m3/h	28668.52	26527.91	146.49	8923.21
Component mole fractions				
Ethylene	0.1939	0.2060	0.3009	0.0007
Oxygen	0.0483	0.0479	0.0166	0.0009
Carbon Dioxide	0.0582	0.0080	0.0503	0.3792
Water	0.0086	0.0170	0.2709	0.6198
Nitrogen	0.0248	0.0262	0.0054	0.0009
Argon	0.0889	0.0943	0.0394	0.0009
Methane	0.6086	0.6047	0.3151	0.0002
Ethane	0.0036	0.0038	0.0015	0.0009

| Stream No.	11	4
Name	lean	Rich
- - Overall - -		
Molar flow kmol/hr	6923.38	6895.29
Mass flow kg/hr	163428.52	168078.61
Temp C	83.49	86.35
Pres bar	28.50	1.50
- - Liquid only - -		
PH value	11.19	10.03
Flowrates in kmol/hr		
Carbon Dioxide	0.01	0.16
Water	5550.93	5407.38
K Carbonate	0.00	0.00
H+	0.00	0.00
OH-	2.32	0.30
CO3--	432.08	317.09
HCO3-	35.78	267.78
K+	902.26	902.26

DESCRIPTION:

What you can see in the picture above is the simulation of an existing plant to remove CO2 from a process stream by absorption/regeneration with a hot potassium carbonate solution. CO2 is absorbed by chemical reaction, and it is the type of calculations CHEMCAD 5 Electrolyte Package has been made for.

This sort of simulation requires applying the True Species Approach, where regular components and electrolyte species are treated equally.

CHEMCAD 5 has a database of ionic reactions built-in. Many industrially important systems have been covered. In case some reaction data are missing, CHEMCAD 5 would try to calculate equilibrium coefficients. Electrolyte Regression facility is also available.

Selective H₂S Removal with MDEA
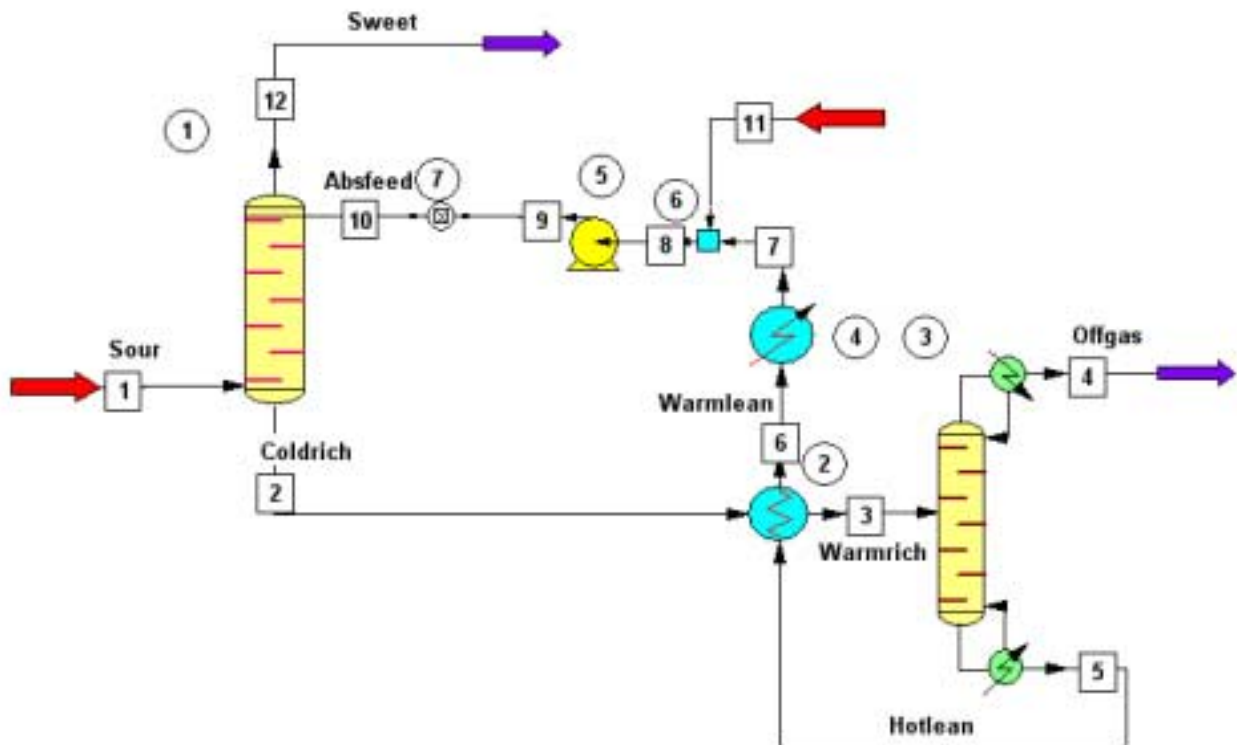
DESCRIPTION:

This example is a selective H2S removal by using 50 weight % MDEA in a 10 tray absorber.

This problem was calculated by the Apparent Component electrolyte method, where 'visible' components are separated from the ionic species.

The constants for the MDEA process have been taken from the CHEMCAD's ionic reaction library.

CHEMCAD 5 includes enhanced SCDS distillation/absorption model. It allows specifying stage efficiencies for individual column trays, as well as stage efficiencies for individual components. In this example, the CO2 absorption is controlled by mass transfer, so individual stage efficiencies for carbon dioxide have been applied.

Ref: Jou, F. Y. F.D. Otto and A. E. Mather, "Solubility of Mixtures of H2S and CO2 in a Methyldiethanolamine Solution". Paper #140b AIChE Annual Meeting, Miami Beach, FL (Nov 2-7,1986)

Gas Turbine Simulation
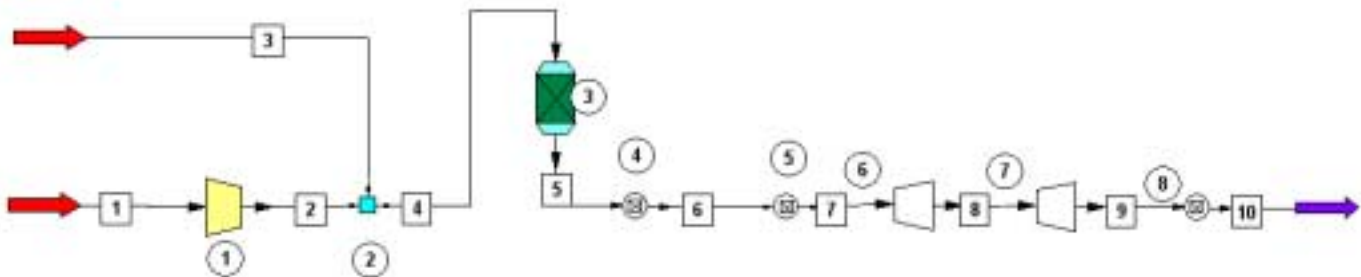
DESCRIPTION:

A typical gas turbine consists of an axial compressor, fuel combustion chamber and an expander which drives the compressor and any external load or loads. For modeling purposes only, the work to drive the compressor and external loads are considered separately. The design or rating of a turbine system depends on how the controls are configured. CHEMCAD 5 can define the theoretical work requirements and fuel for a defined load or frame size.

This example defines the air and fuel requirements for a turbine, which drives an electrical generator under combustion conditions, as defined by excess air requirement.

The flowsheet is a close representation of a SOLAR Saturn turbine operating at conditions typical of a co-generation installation.

Power Plant Steam Balance

DESCRIPTION:

CHEMCAD 5 is an invaluable tool for balancing a powerplant. In this example, general balance of a three-stage turbine powerplant block was calculated. This block was aimed at electricity production. Special care was taken to balance the condensate tank. When water is the only component in the system, using the "Ideal Vapor pressure" thermo model makes CHEMCAD use digital steam tables, thus ensuring high accuracy of steam/water calculations.
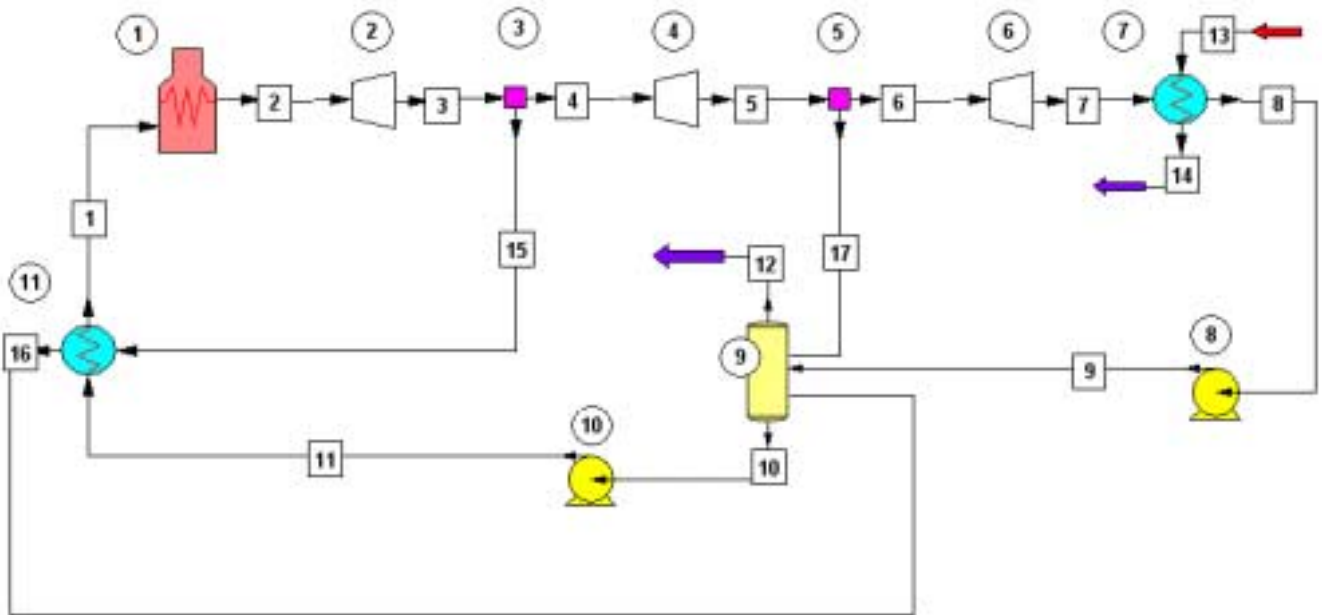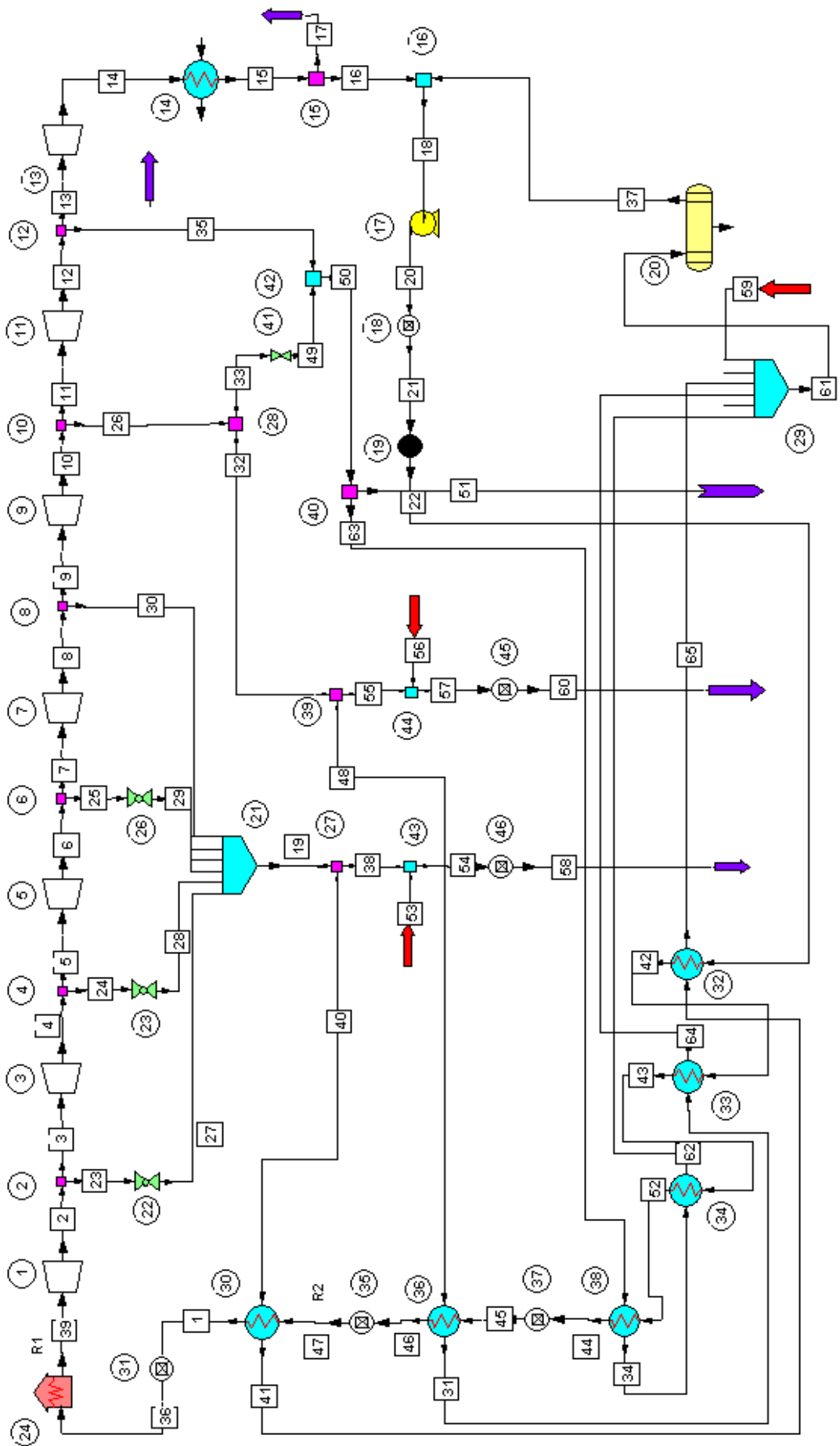
# Detailed Model of an Industrial Power Plant.

DESCRIPTION:

CHEMCAD 5 can be used for optimizing operation of an existing plant. This flowsheet presents a single block of a big industrial powerplant, producing simultaneously electricity and HP, MP, and LP steam for a chemical plant.

This block has seven turbine sections: six of non-condensing type and one of condensing operation. Depending on current demand, the powerplant manager can decide upon steam distribution in the system. Specific streams can be shut (actually one of steam outlets has been deliberately closed.) This flowsheet has been made non-optimal on purpose. A CHEMCAD user can play with controllers, especially with those responsible for operation of re-heaters, to increase overall thermal efficiency of the plant.

A very useful feature of CHEMCAD 5 is built-in interpreter of simple CHEMCAD Inline-C programming language. The users can write procedures representing their own calculation routines (Parser), or programs reading the data from the flowsheet, performing calculations, and writing the calculations results back to the flowsheet or to the report. For this specific example, both a parser and a calculator for determining the overall thermal efficiency of the plant have been written.

CHEMCAD 5 includes a dialog editor that allows building own data entry screens for Calculators.

Batch Distillation of Essential Oils (*CC-BATCH*)

Batch Column 1, Bottom
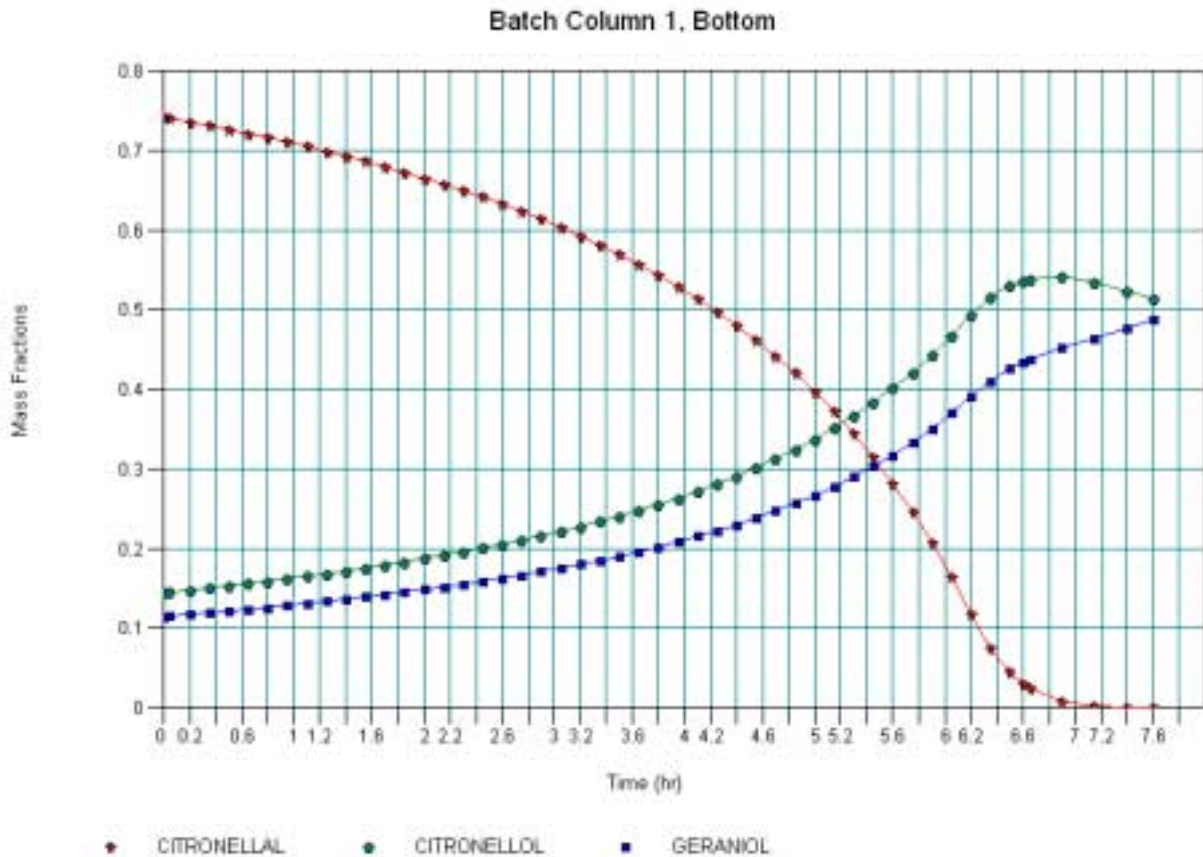
DESCRIPTION:

The CC-BATCH module is a package for rigorous calculations of batch distillation processes.

A new packed column, equivalent to 34 theoretical plates, was designed to separate Citronella oil into citronellal and mixture of citronellol and geraniol. The process had to be carried out under vacuum of order of 1 mmHg.

The properties of essential oil components have been calculated with prediction features of CHEMCAD.