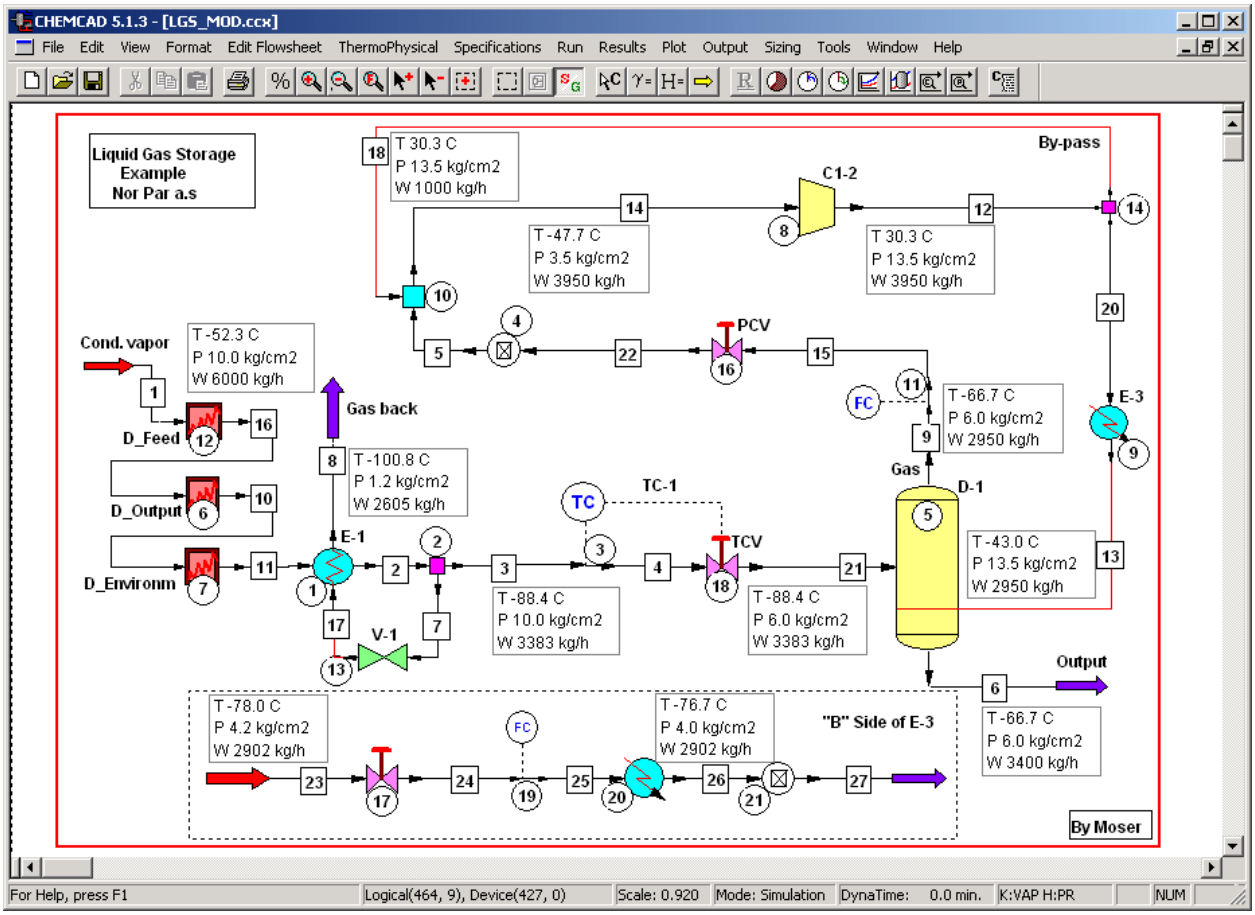
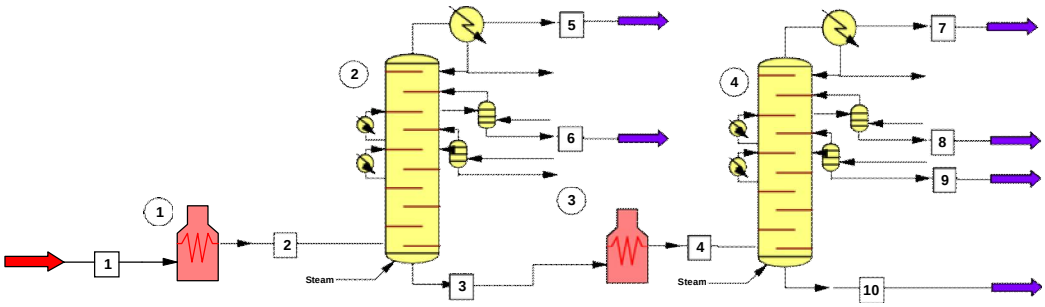
CHEMCAD™



Steady State and Dynamics

Oil Refining and Petrochemicals

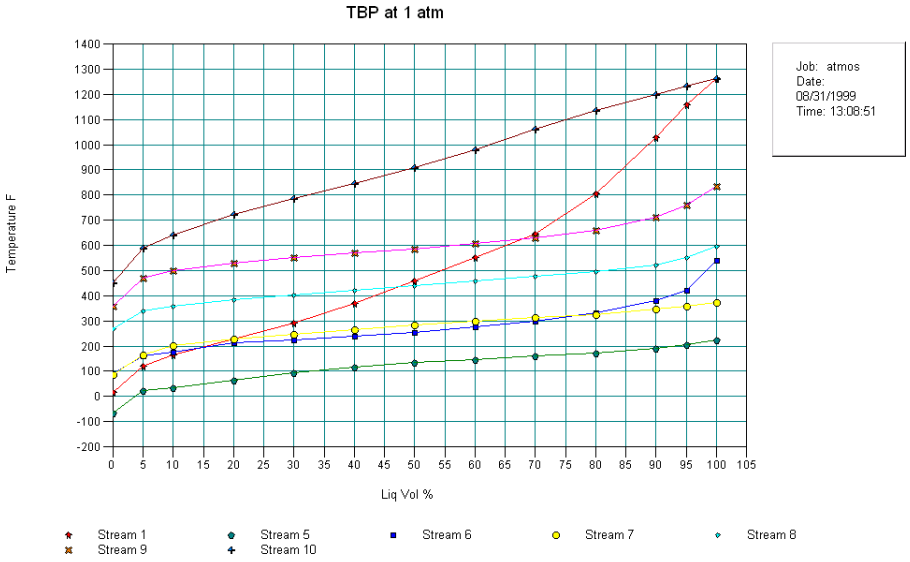
Atmospheric Distillation of Crude Oil



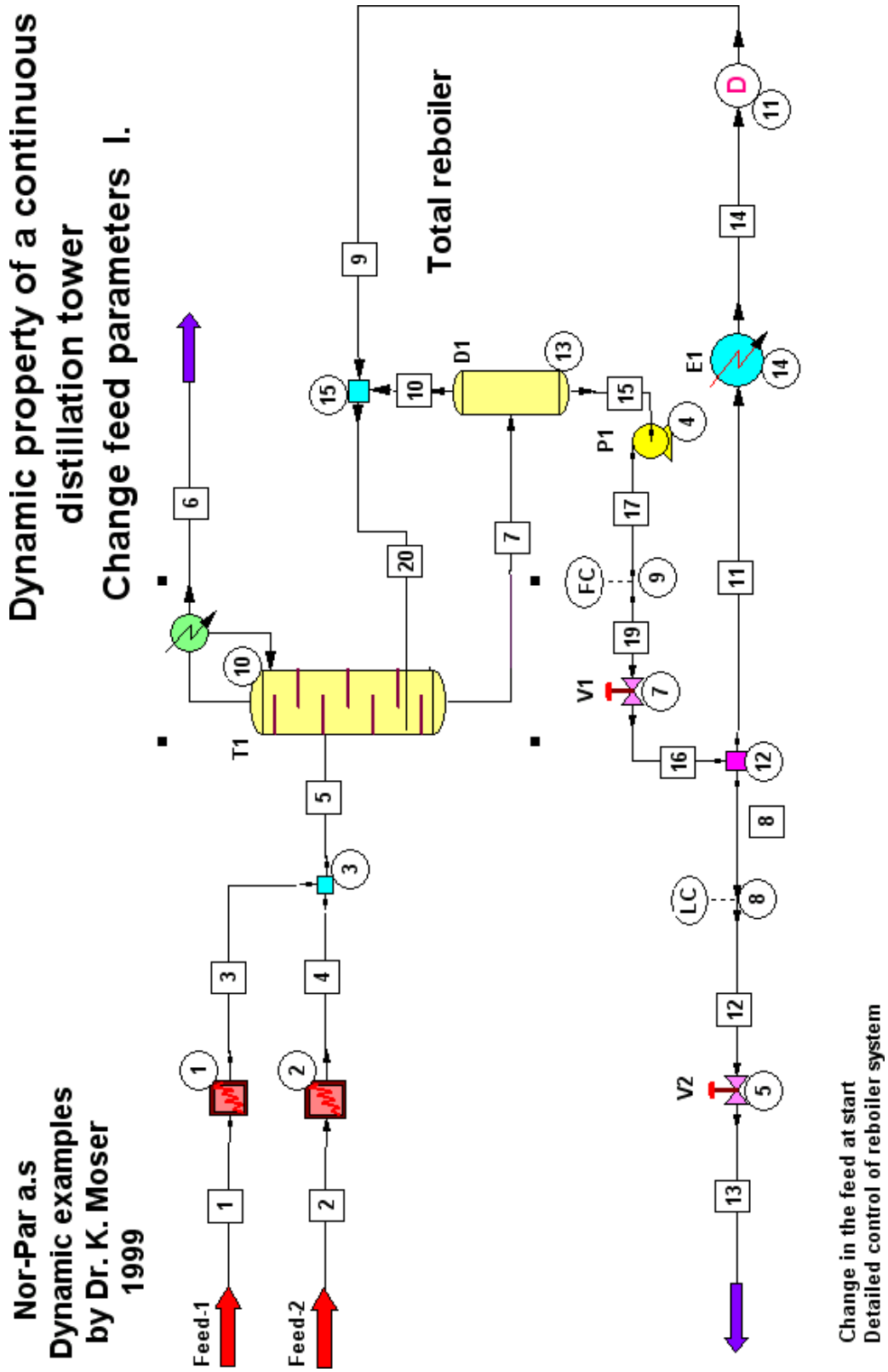
DESCRIPTION:

Crude oil is heated in process furnace to 400 F. Then, it enters the tower T-1001 near to the tower bottom. The tower is equipped with 12 stages, a condenser, one side stripper for naphtha, one side heat exchanger, and one pump around. 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 heatexchanger, and one pump around.

The bottoms of both towers as well as all strippers are fed with live steam.

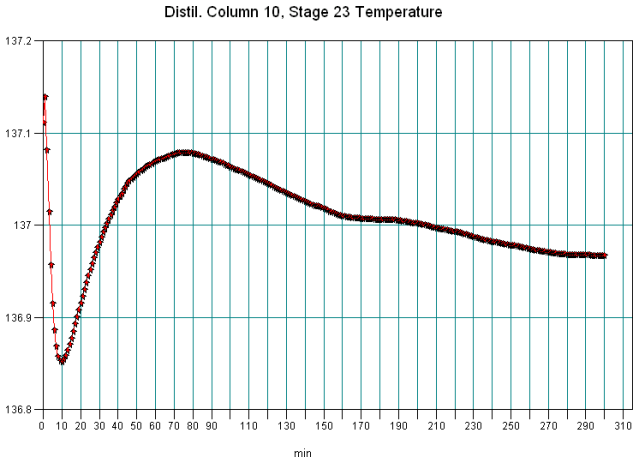


This example explains usage of the Tower Plus distillation model and the way of performing crude oil characterization.


Dynamic property of a continuous distillation tower
Change feed parameters I.
Nor-Par a.s
Dynamic examples
by Dr. K. Moser
1999
Total reboiler
Feed-1
Feed-2
T1
D1
P1
E1
V1
V2
FC
LC
D
Change in the feed at start
Detailed control of reboiler system

Dynamics: Properties of Continuous Distillation Column

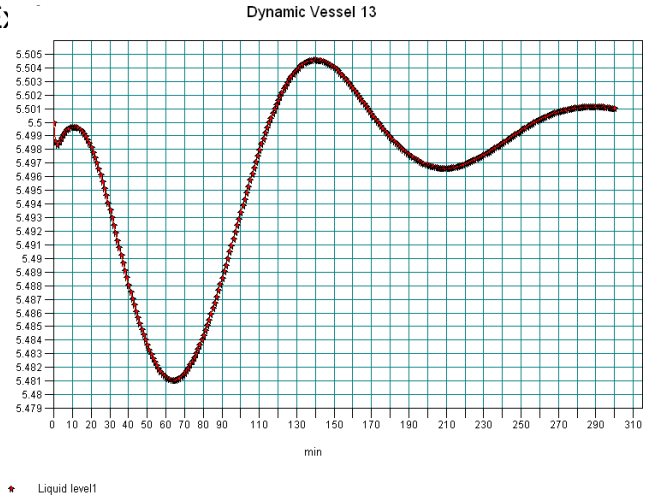
DESCRIPTION:



This example makes use of CHEMCADDynamics.

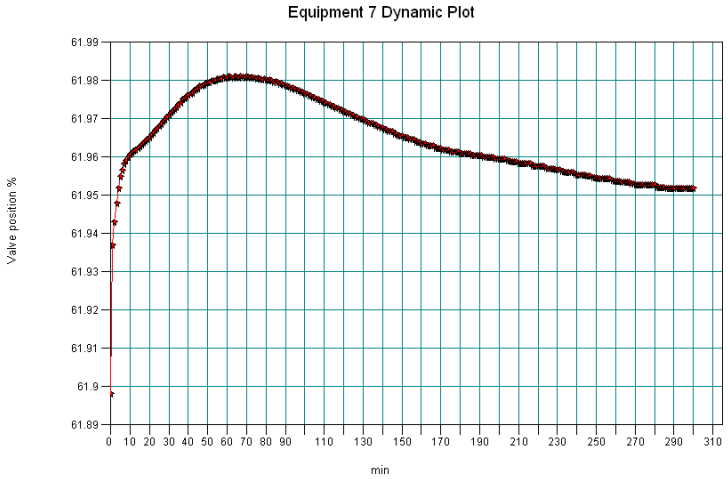
The calculation begins at steady state. At the very beginning of the dynamic simulation, the feed streams are switched with Ramp Controllers, what creates a distortion to steady state. The control system at the reboiler has to maintain possibly constant recirculation flow rate through the heat exchanger and constant level in the column's bottom.

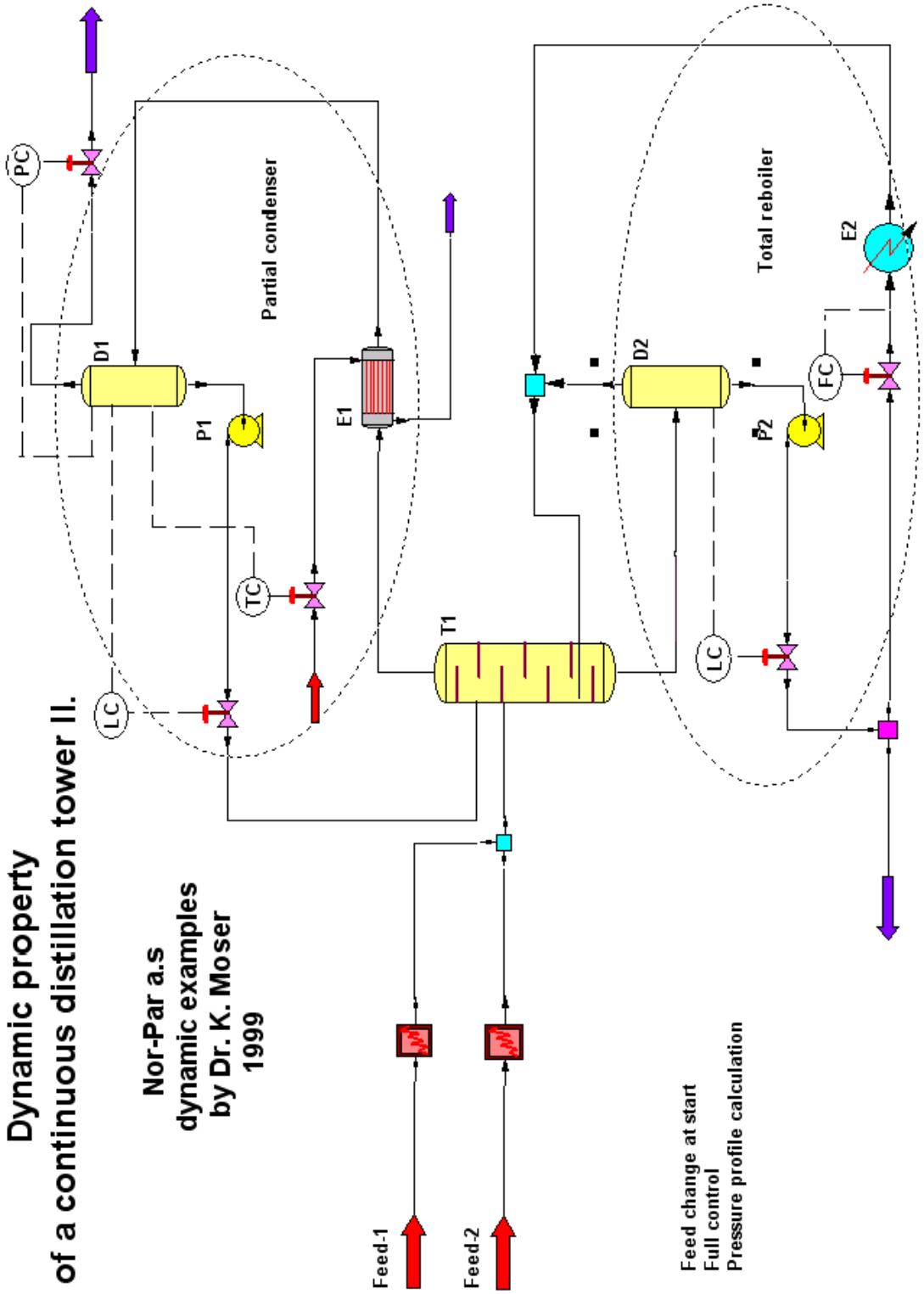
The distillation tower has been modeled with CC-DCOLM module, and a detailed model for the total reboiler has been made as combination of a Dynamic Vessel, PID Controllers, Control Valves, Time Delay, and steady state units such as Heat E



You can study various time dependent parameters, such as for instance compositions, temperature or pressure in thecolumn, pressure or level in the column bottom, output signals of controllers, valve positions, and even dependence of reboiler'sheat duty against time.

Dynamic capabilities of CHEMCAD are invaluable tool for process and control engineers, as appropriate controller settingscan be found for given process.

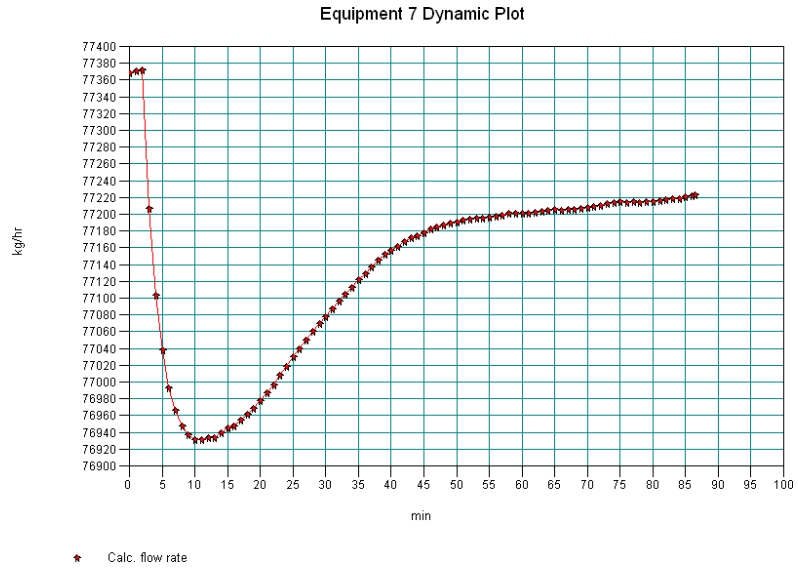

Equipment 7 Dynamic Plot
Valve position %
61.99
61.98
61.97
61.96
61.95
61.94
61.93
61.92
61.91
61.9
61.89
0 10 20 30 40 50 60 70 80 90 110 130 150 170 190 210 230 250 270 290 310
min

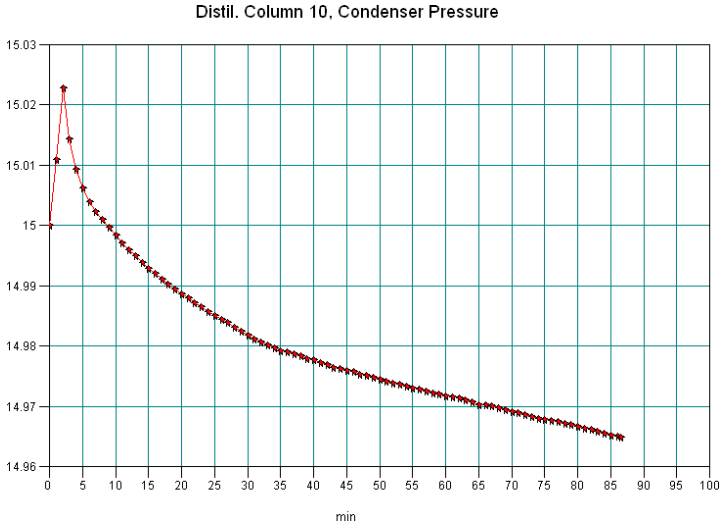

Dynamic property
of a continuous distillation tower II.
Nor-Par a.s
dynamic examples
by Dr. K. Moser
1999
Partial condenser
Total reboiler
D1
D2
P1
P2
E1
E2
T1
PC
TC
LC
FC
Feed-1
Feed-2
Feed change at start
Full control
Pressure profile calculation

Dynamics: Full Control Model of Continuous Distillation Column

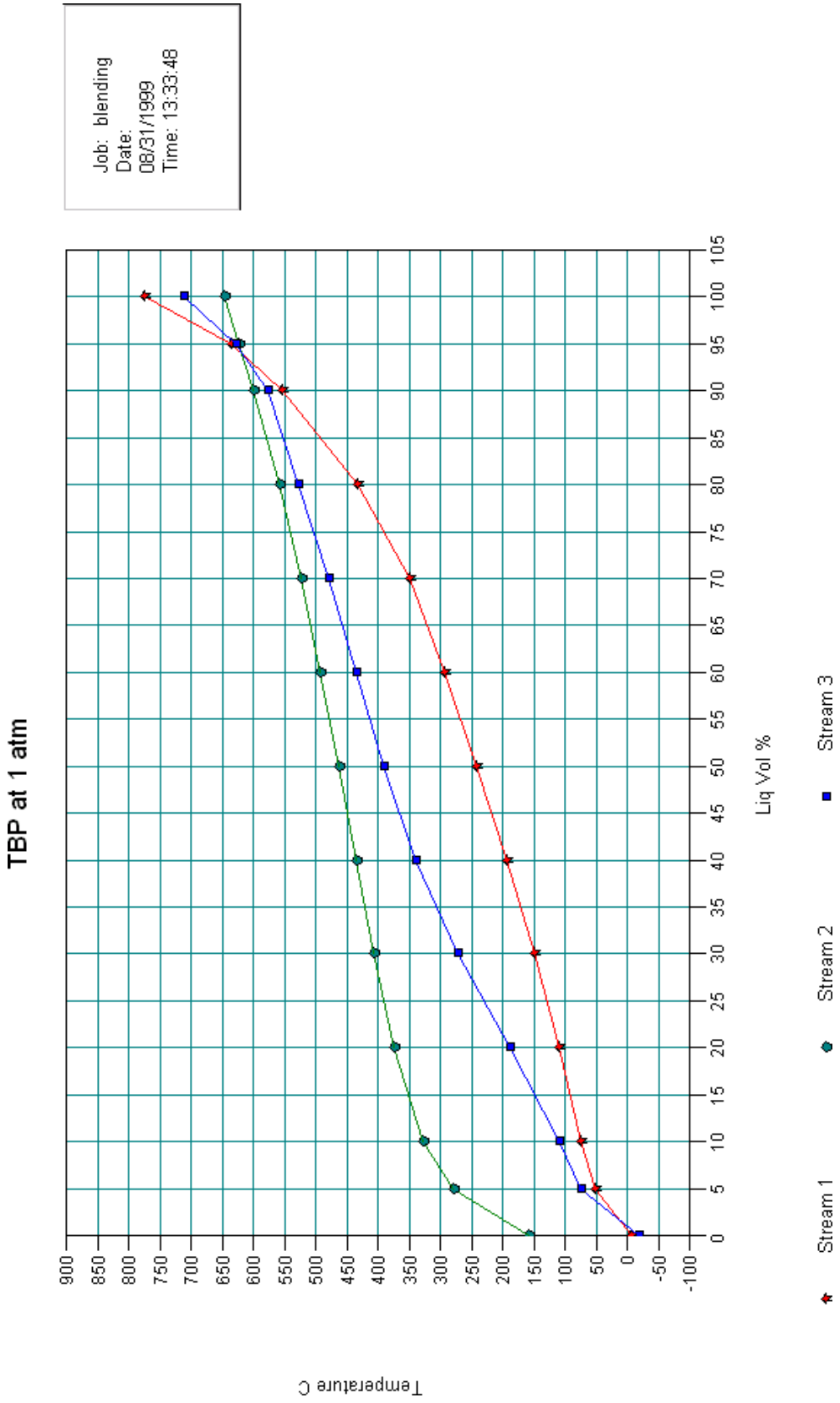
DESCRIPTION:

This example solves control of both reboiler and condenser. Full pressure profiles are calculated both in the Dynamic Column and in Dynamic Vessels. In the condenser, temperature, pressure and level control is applied, whereas level and flow rate control has been designed for the reboiler.

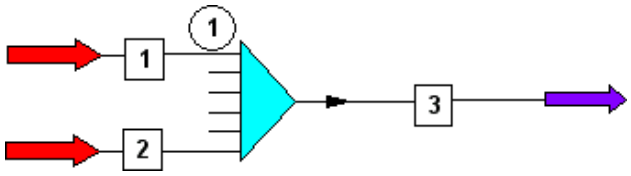




CHEMCAD give the engineer freedom to make design or analysis selections. You can use an integrated DCOLM model at the very beginning to get the steady state and dynamic solution fast. Later, you can develop your model by building reboiler, condenser, side streams, etc., from individual unit operations and applying respective controllers and control valves.


Job: blending
Date:
08/31/1999
Time: 13:33:48
TBP at 1 atm
Temperature C
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
Liq Vol %
Stream 1
Stream 2
Stream 3

Blending of Crude Oil



DESCRIPTION:

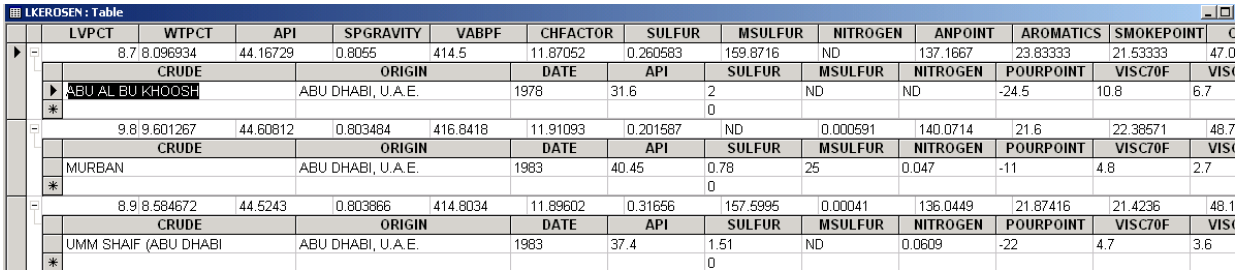
CHEMCAD 5 has the ability to generate crude oil pseudo-components according to user provided distillation curves. CHEMCAD 5 supports the following blending options:

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 flow sheet 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 yourreports using your favorite office software.

CHEMCAD has now Crude Oil Database as well. This contains properties of around 250 crude oils including the properties of all oil fractions:



LKEROSEN : Table

LVPCT	WTPCT	API	SPGRAVITY	VABPF	CHFACTOR	SULFUR	MSULFUR	NITROGEN	ANPOINT	AROMATICS	SMOKEPOINT
8.7	8.096934	44.16729	0.8055	414.5	11.87052	0.260583	159.8716	ND	137.1667	23.83333	21.53333

CRUDE	ORIGIN	DATE	API	SULFUR	MSULFUR	NITROGEN	POURPOINT	VISC70F
ABU AL BU KHOOSH	ABU DHABI, U.A.E.	1978	31.6	2	ND	ND	-24.5	10.8

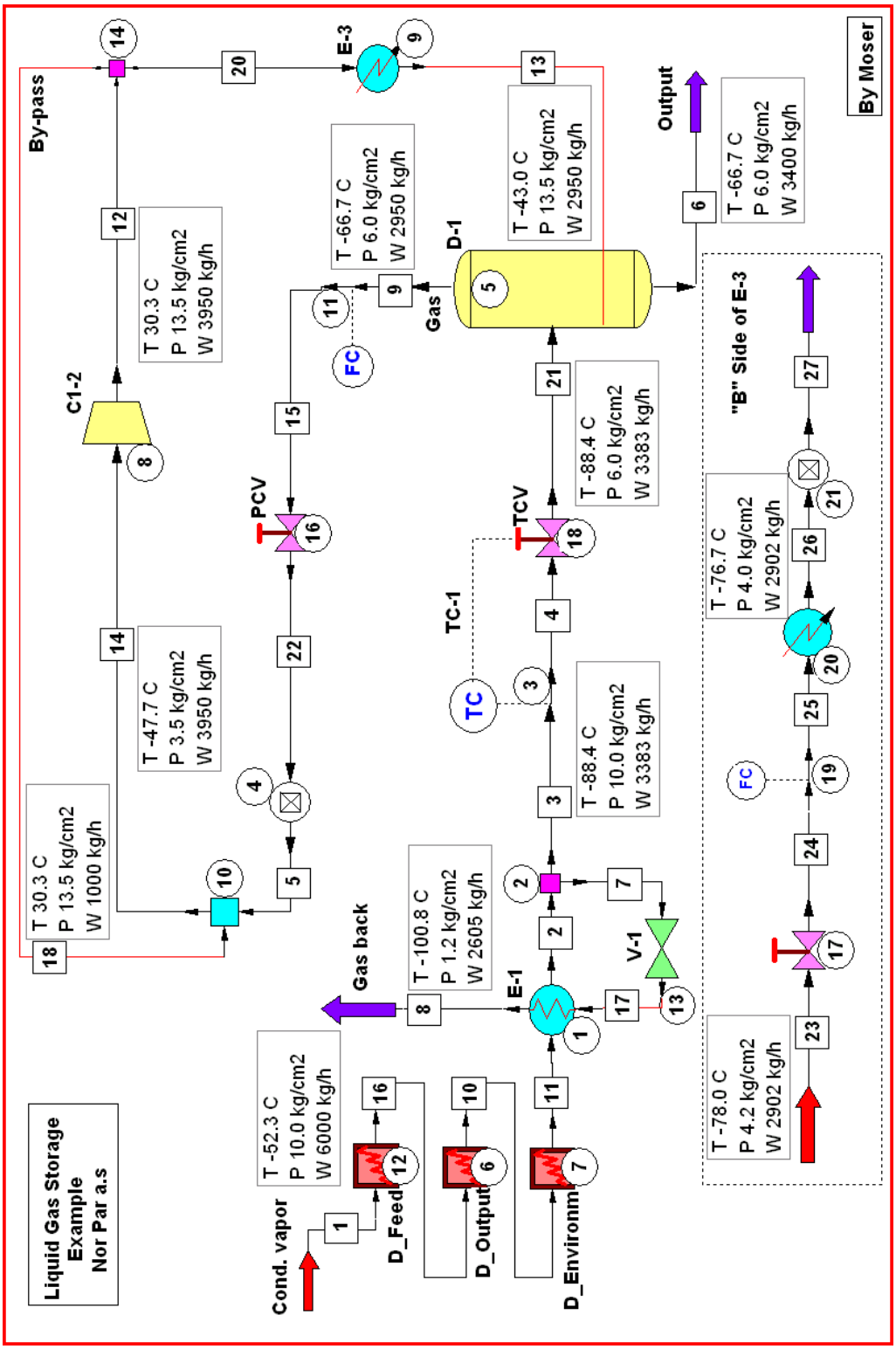
LVPCT	WTPCT	API	SPGRAVITY	VABPF	CHFACTOR	SULFUR	MSULFUR	NITROGEN	ANPOINT	AROMATICS	SMOKEPOINT
9.8	9.601267	44.60812	0.803484	416.8418	11.91093	0.201587	ND	0.000591	140.0714	21.6	22.38571

CRUDE	ORIGIN	DATE	API	SULFUR	MSULFUR	NITROGEN	POURPOINT	VISC70F
MURBAN	ABU DHABI, U.A.E.	1983	40.45	0.78	25	0.047	-11	4.8

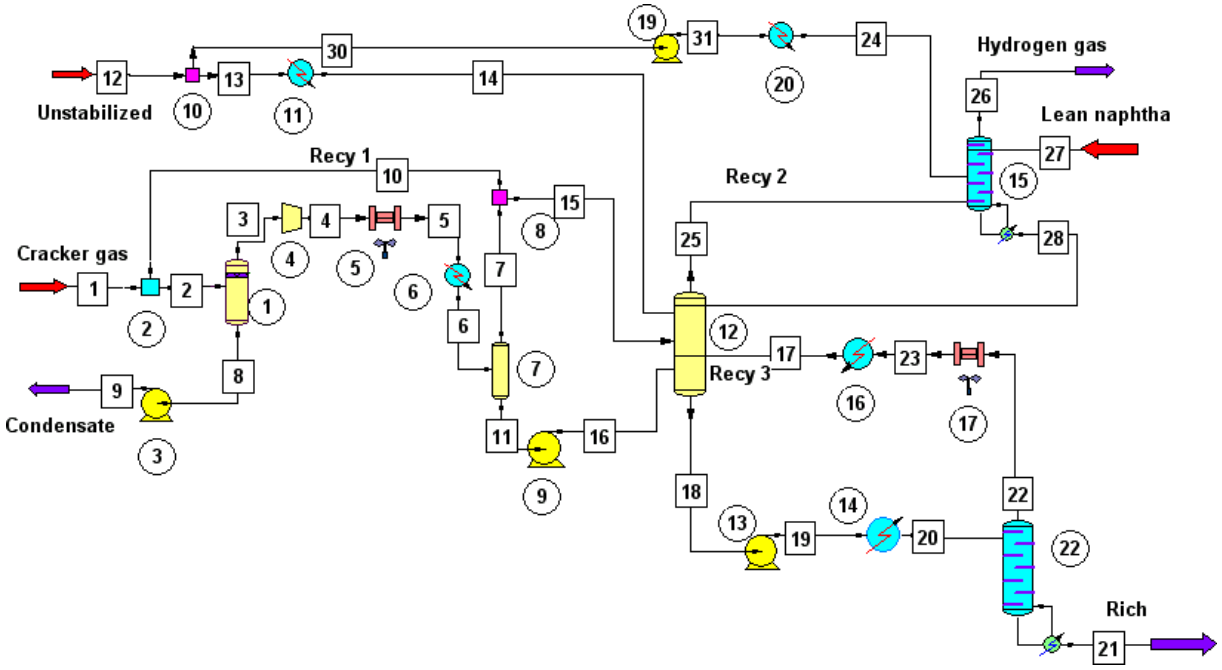
LVPCT	WTPCT	API	SPGRAVITY	VABPF	CHFACTOR	SULFUR	MSULFUR	NITROGEN	ANPOINT	AROMATICS	SMOKEPOINT
8.9	8.584672	44.5243	0.803866	414.8034	11.89602	0.31656	157.5995	0.00041	136.0449	21.87416	21.4236

CRUDE	ORIGIN	DATE	API	SULFUR	MSULFUR	NITROGEN	POURPOINT	VISC70F
UMM SHAIF (ABU DHABI	ABU DHABI, U.A.E.	1983	37.4	1.51	ND	0.0609	-22	4.7

Dynamics: Liquefied Ethylene Storage Simulation



Cat-Cracker Gas Separation

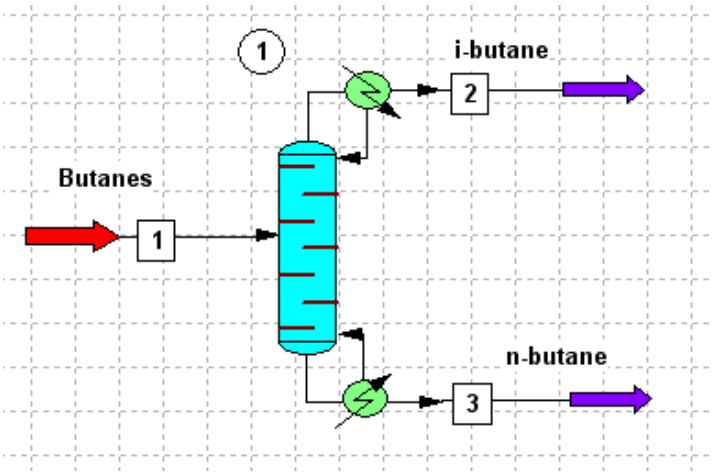


DESCRIPTION:

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 after cooler, 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 withboth 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 flow sheet 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

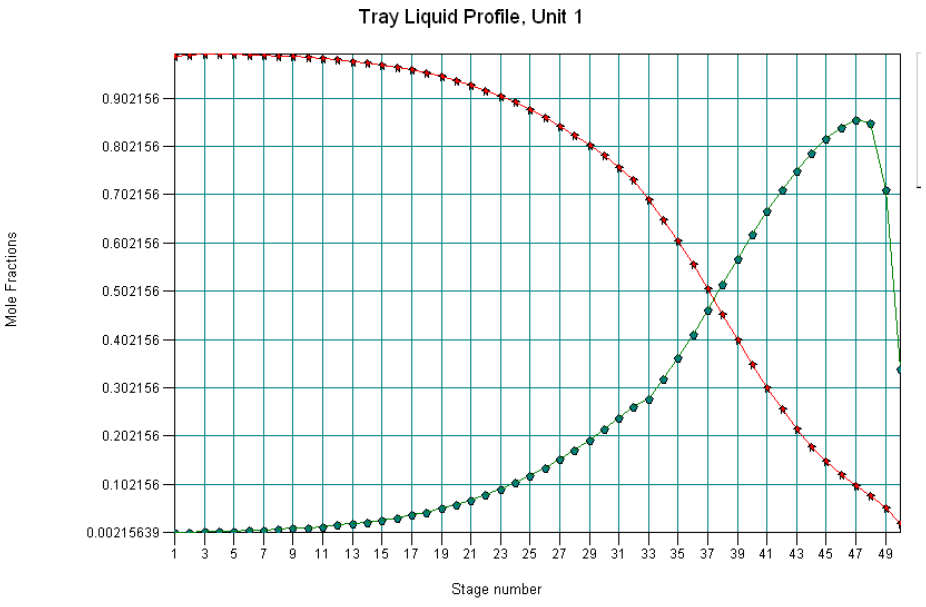


DESCRIPTION:

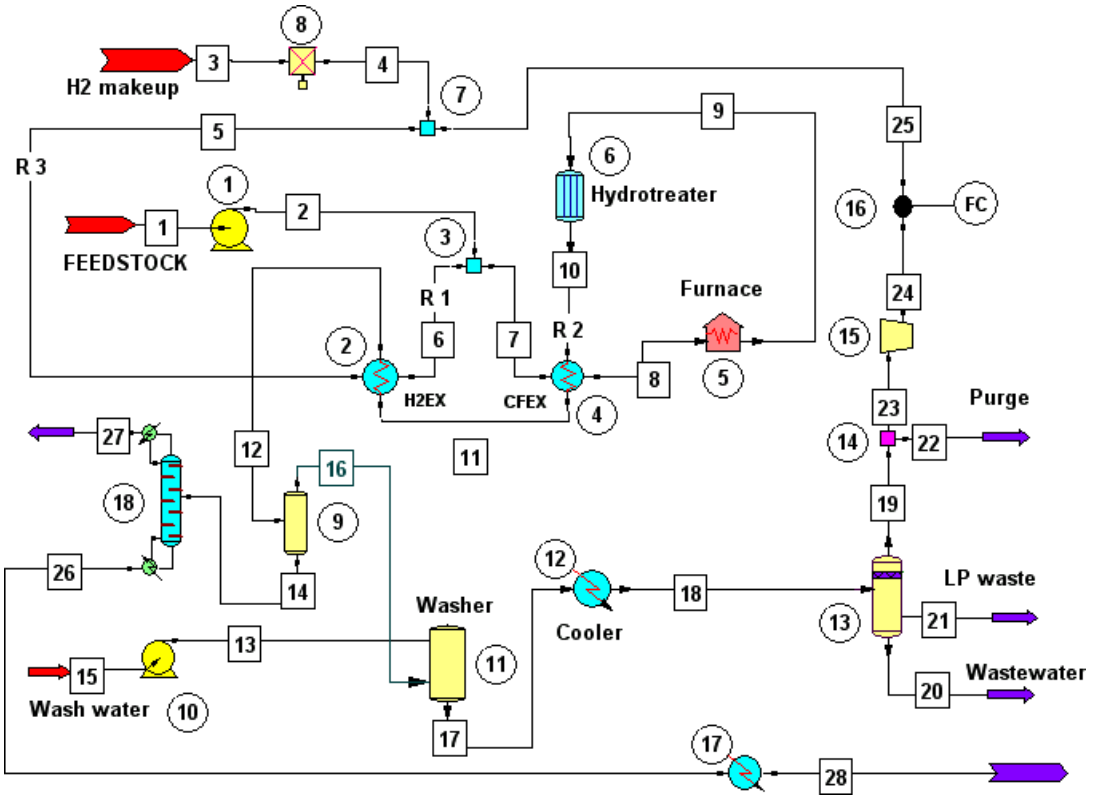
This example demonstrates how to make a preliminary design of a i-butane/n-butane splitter.

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 calculatepressure drop through a packed column, including a modern and accurate correlation of Mackowiak.

The CC-Thermmodule can do a rigorous



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.

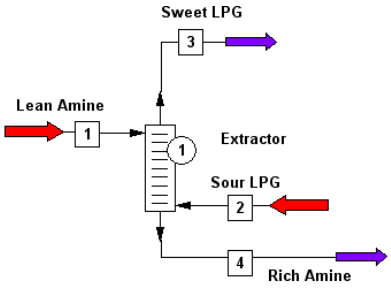
The feedstock is pumped from tank age and mixed with recycle hydrogen gas. Then it is preheated withhot reactor product gas in the CFEX heat exchanger. The reactor feed is then heated near to the reaction temperature in a process furnace, and introduced to the adiabatic hydrogenation reactor.

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 theCFEX exchanger.

Heat is further recovered in the H2EX heat exchanger, where the recycled hydrogen is preheated. Thecooled 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.

LLE Desulfurization of Liquefied Petroleum Gas



Extractor Summary	
Equip. No.	1
Name	Extractor
No. of Stages:	5
1st feed stage	1
2nd feed stage	5

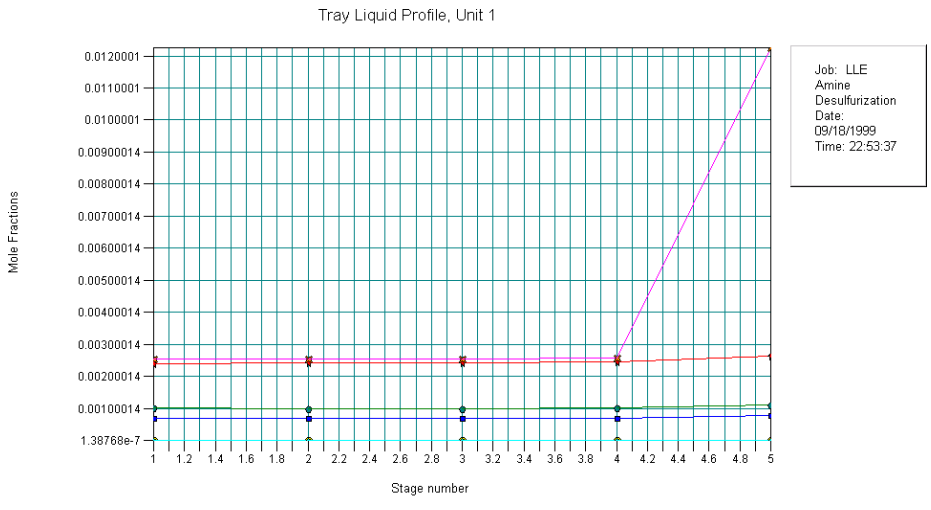
Stream No.	1	2	3	4
Name	Lean Amine	Sour LPG	Sweet LPG	Rich Amine
- - Overall - -				
Molar flow kmol/hr	745.0	132.8	120.4	757.4
Mass flow kg/hr	16124.5	6768.8	6308.0	16585.3
Temp C	39.0	39.0	38.7	43.5
Pres kg/cm2	20.0	20.0	20.0	20.0
Vapor mole fraction	0.0000	0.0000	0.0000	0.0000
Actual vol m3/h	16.0	13.5	12.6	16.9
Std liq m3/h	15.8	12.3	11.6	16.6
Std vap 0 C m3/h	16698.8	2976.0	2699.3	16975.4
Component mole %				
Methane	0.00	0.83	0.56	0.06
Ethane	0.00	4.88	4.57	0.13
Propane	0.00	28.87	30.16	0.26
I-Butane	0.00	35.20	38.11	0.11
N-Butane	0.00	24.28	26.28	0.08
I-Pentane	0.00	0.20	0.22	0.00
N-Pentane	0.00	0.01	0.02	0.00
Hydrogen Sulfide	0.25	5.57	0.00	1.23
Water	95.63	0.17	0.08	94.09
Diethanolamine	4.12	0.00	0.00	4.05

DESCRIPTION:

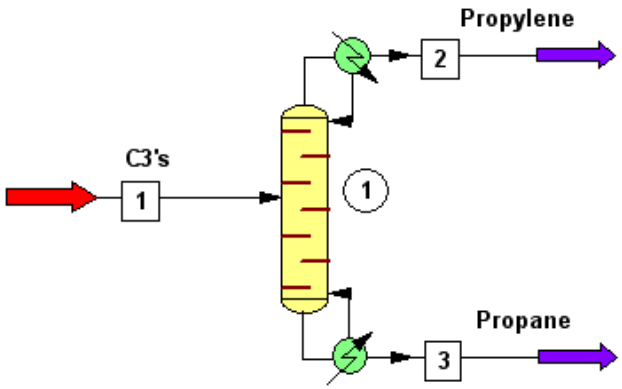
Traditional way of gas desulfurization involved absorption process, where H2S was being removed with aqueous solution of mono- or diethanolamine. The new technology, becoming popular, is liquid-liquid extraction of liquefied petroleum gas (LPG).

CHEMCAD includes modified both AMINe thermodynamic model of CHEMCAD as well as the modifiedEXTRactor model able to simulate the new process possible.

CHEMCAD is a technology- and market-driven product, so market demands of common interest are implemented in the program. This example shows how to set up the flow sheet to make use of the special methods.



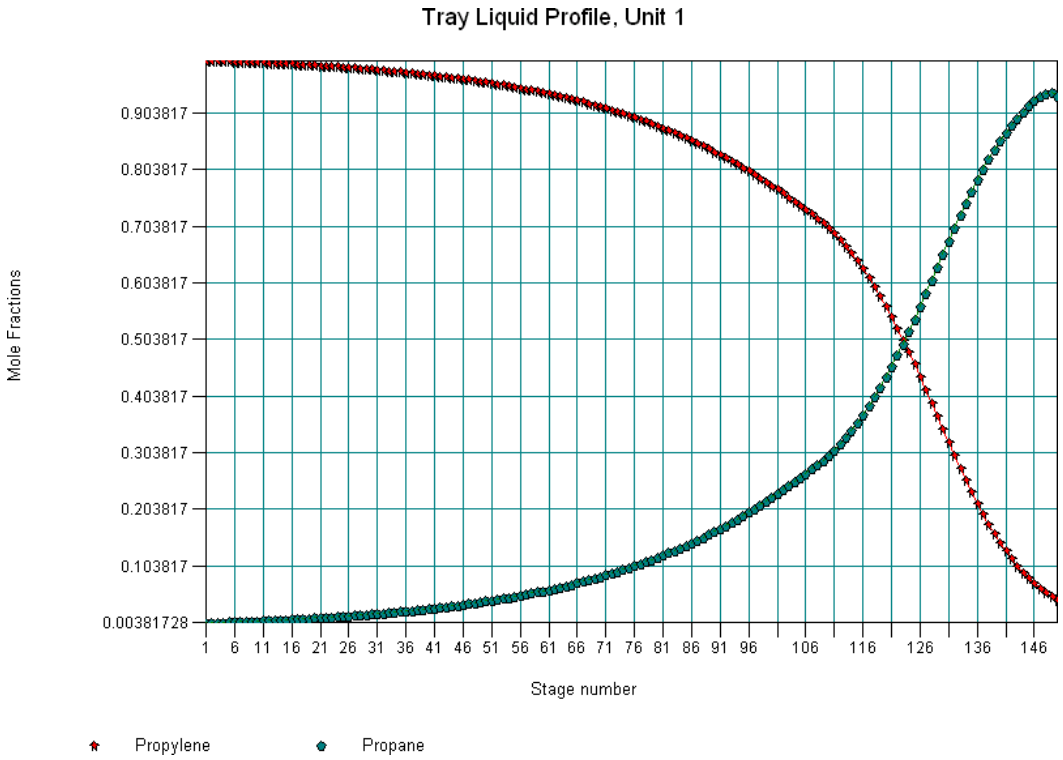
Propane-Propylene Splitter



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

Nor-Par a.s

Propane-Propylene Splitter

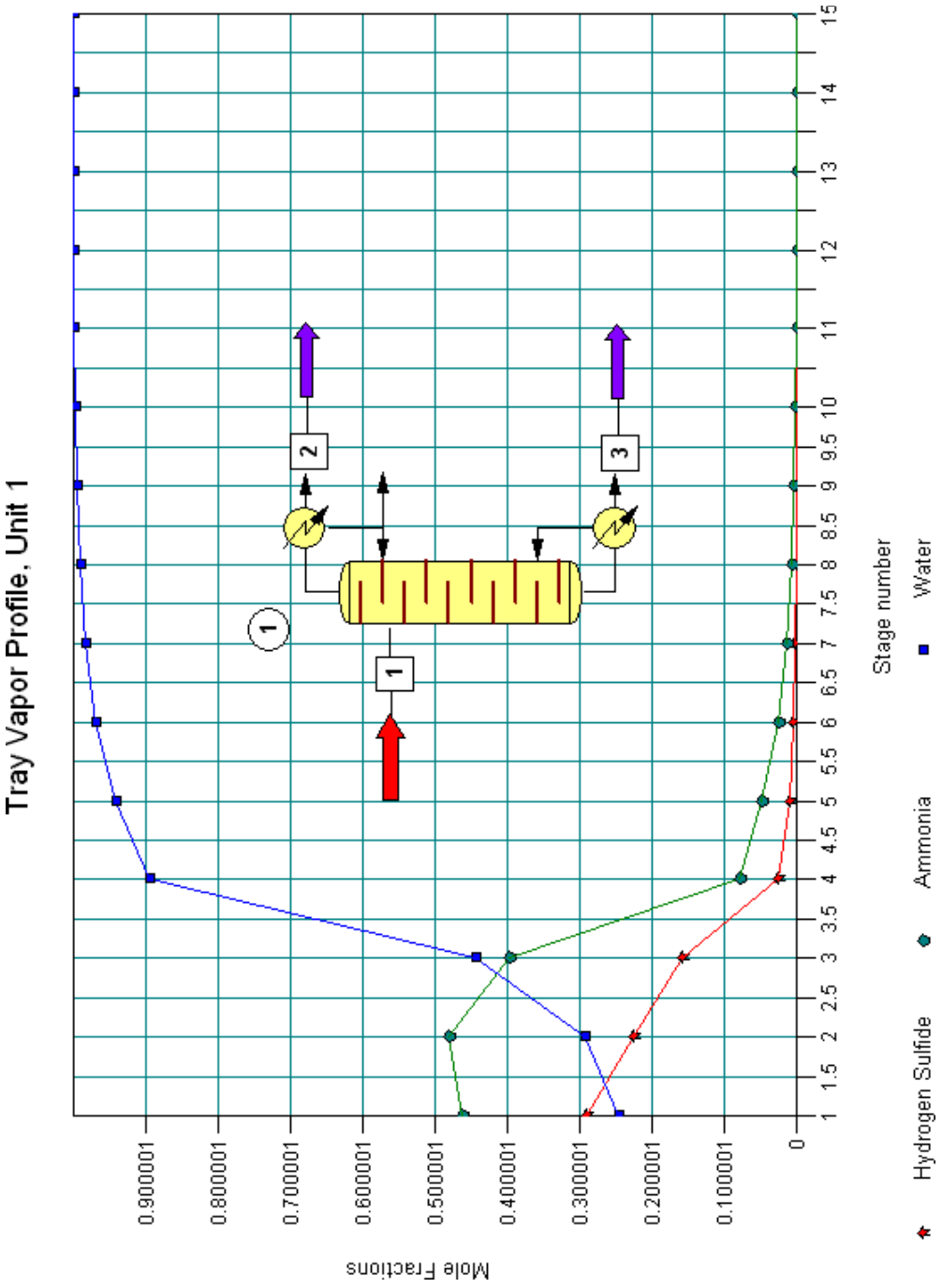


DESCRIPTION:

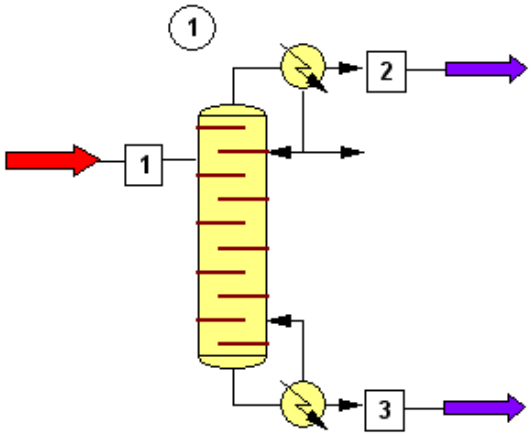
Propane and propylene are very difficult to separate one from another, as they are close-boiling components. Nonetheless, distillation at elevated pressure is a common technology, provided sufficientnumber of trays exists in the distillation column.

Calculations of a 148 actual-tray tower are presented in this example. The SCDS distillation model wasused 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
Mole Fractions
0.900001
0.800001
0.700001
0.600001
0.500001
0.400001
0.300001
0.200001
0.100001
0
Stage number
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
8
8.5
9
9.5
10
11
12
13
14
15
Water
Ammonia
Hydrogen Sulfide
1
2
3

Sour Water Stripper



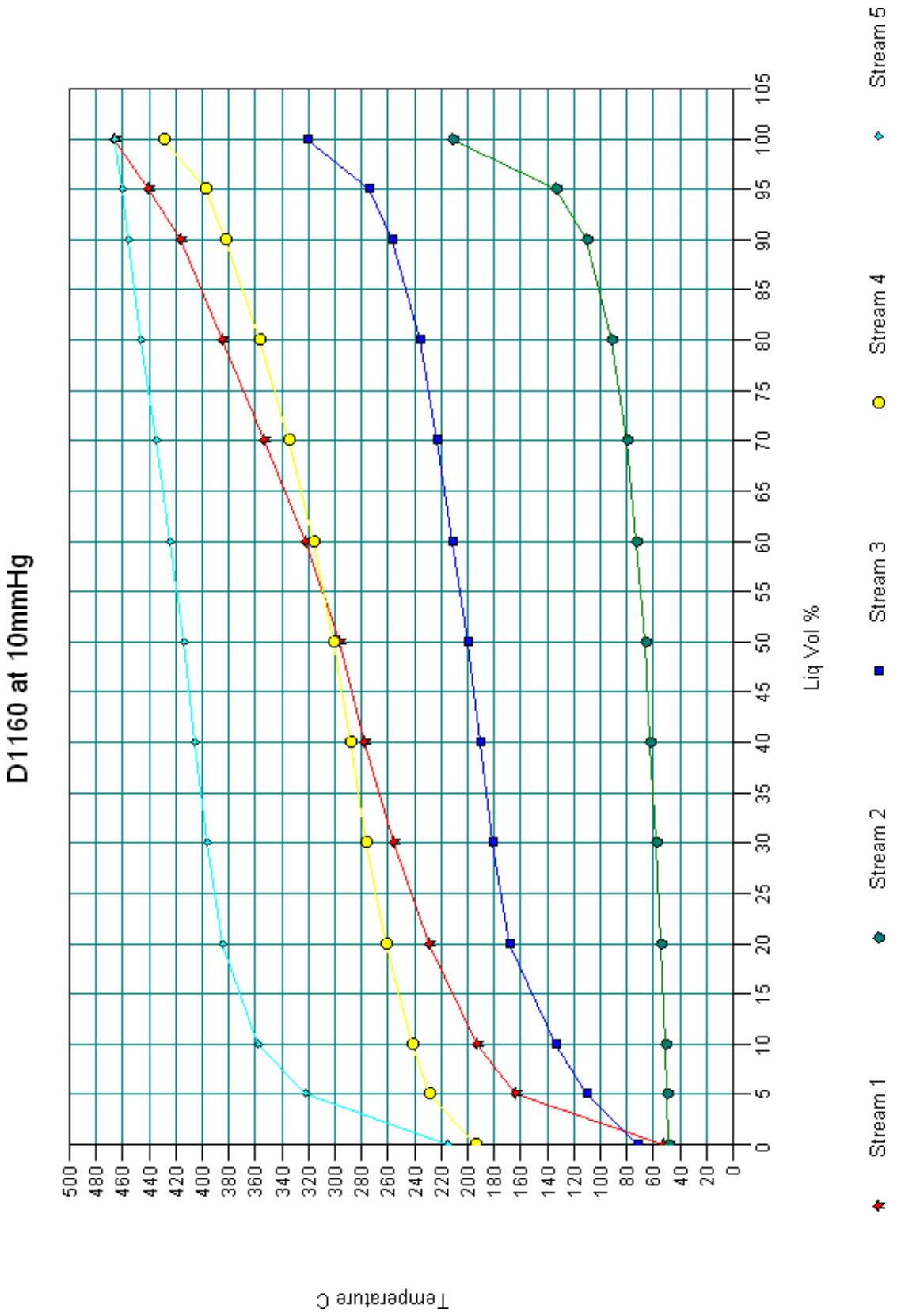
Stream No.	1	2	3
Name			
- - Overall - -			
Mass flow lb/hr	69503.7	343.2	69160.5
Temp F	140.0	148.1	218.7
Pres psia	56.9	14.4	16.8
Vapor mass fraction	0.0000	1.000	0.0000
Component mole fractions			
Hydrogen Sulfide	0.00	0.29	0.00
Ammonia	0.00	0.46	0.00
Water	1.00	0.25	1.00

DESCRIPTION:

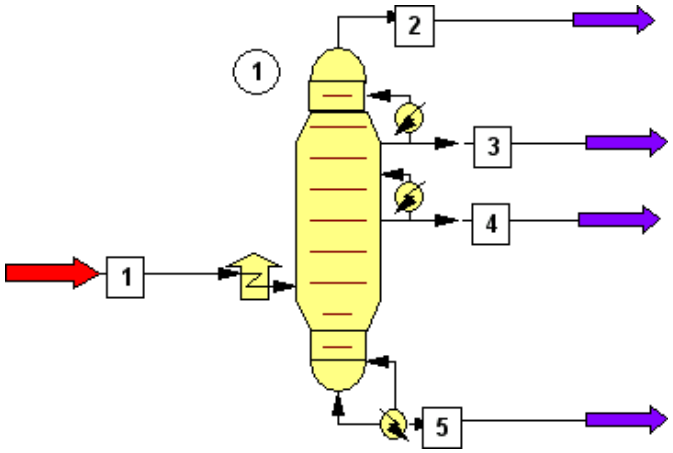
In this example, the Tower Plus (TPLS) model has been used to simulate stripping wastewater from Hydrogen Sulfide and Ammonia down to the level of 5 ppm. This is another application of the TPLS model, which is normally used to simulate atmospheric and vacuum distillation of crude oil.

The tower is equipped with a reboiler, and a pump around 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 Data boxes. CHEMCAD 5 allows placing Stream and Equipment Databoxes on a PFD, and you are free to select properties and the unitsof measure that would appear there.


D1160 at 10mmHg
Temperature C
Liq Vol %
Stream 1
Stream 2
Stream 3
Stream 4
Stream 5

Vacuum Tower with TBP Assay

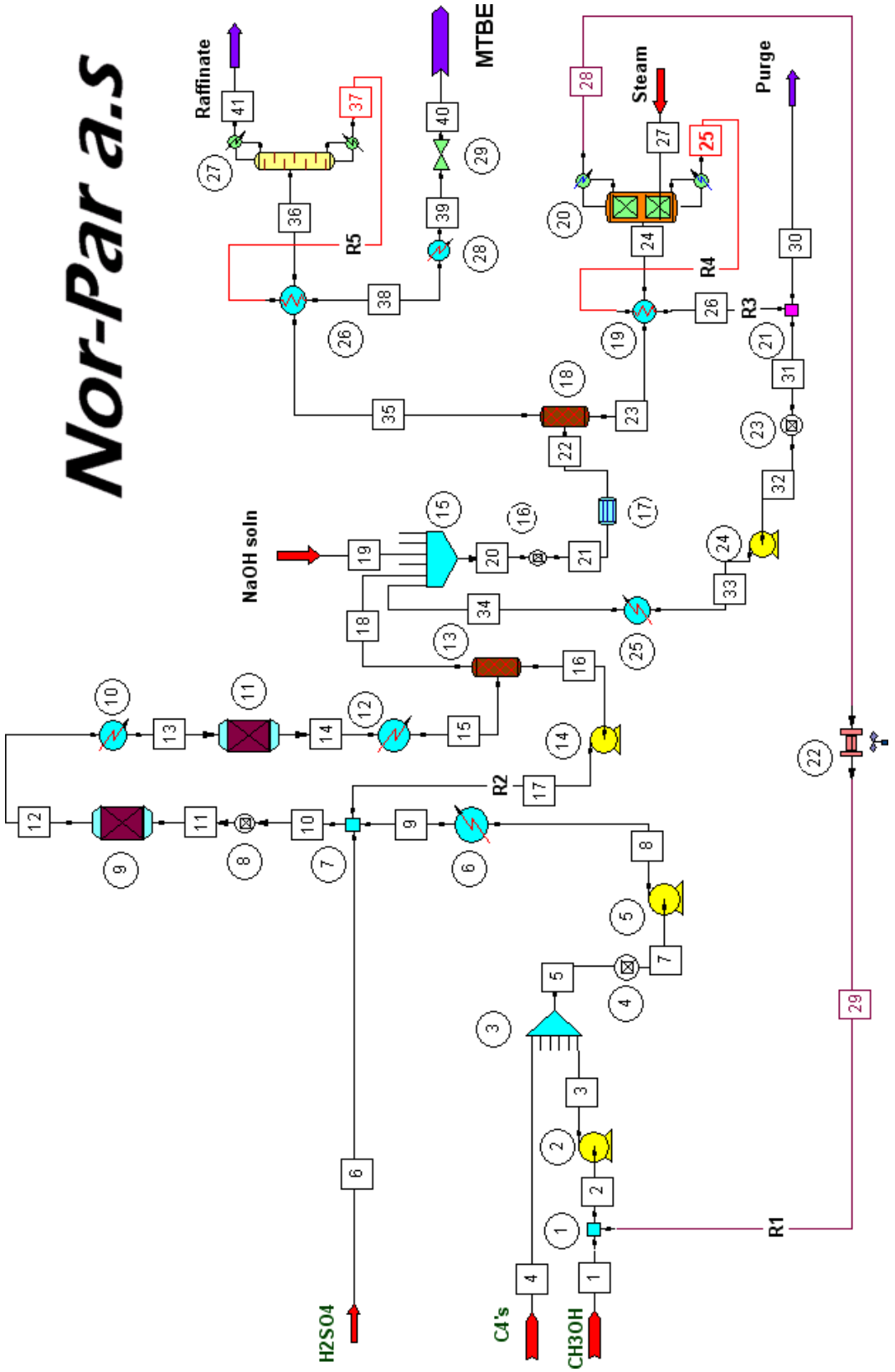


DESCRIPTION:

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 pump around 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 pump around, or the reboiler with side heat exchanger, if you need it.) It alsodemonstrates 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.


Nor-Par a.s
Raffinate
MTBE
Steam
Purge
NaOH soln
R1
R2
R3
R4
R5
H2SO4
C4's
CH3OH

MTBE Process with H_2SO_4 Catalyst

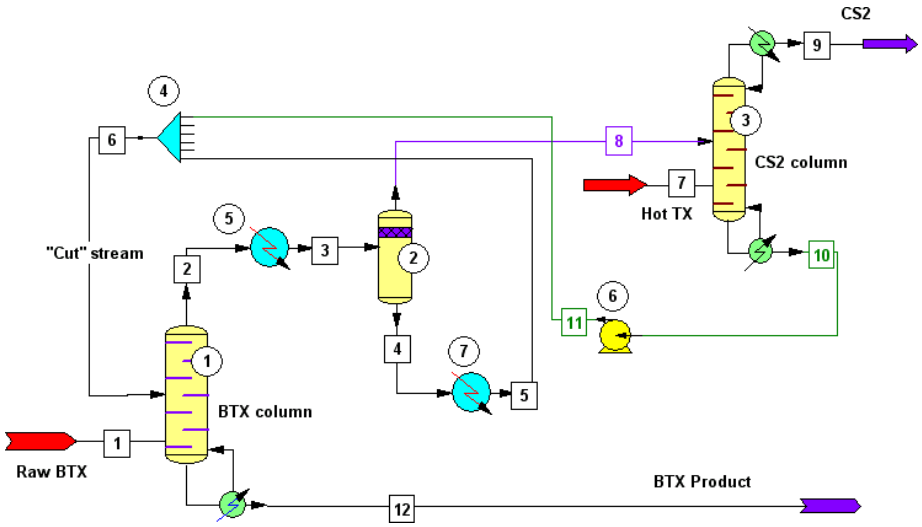
DESCRIPTION:

MTBE is made commercially by catalytic reaction between methanol and i-butylene. A widely used catalyst is an acidic ion exchange resin. This flow sheet shows the alternate route, where sulfuric acid is used as catalyst. The flow sheet 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.

CS_2 Removal from Carbochemical BTX Sensitivity Study, Optimization



DESCRIPTION:

Raw mixture of benzene, toluene and xylene derived from coal coking contains toxic and explosive carbon disulfide, which is removed in dual-column distillation system.

First column actually removes CS2 from BTX, and the second one serves as the regenerator, in attempt to minimize the losses of aromatics from the system.

Numerous process parameters influence CS2 recovery as well as the aromatics' losses, specifically theloss of benzene.

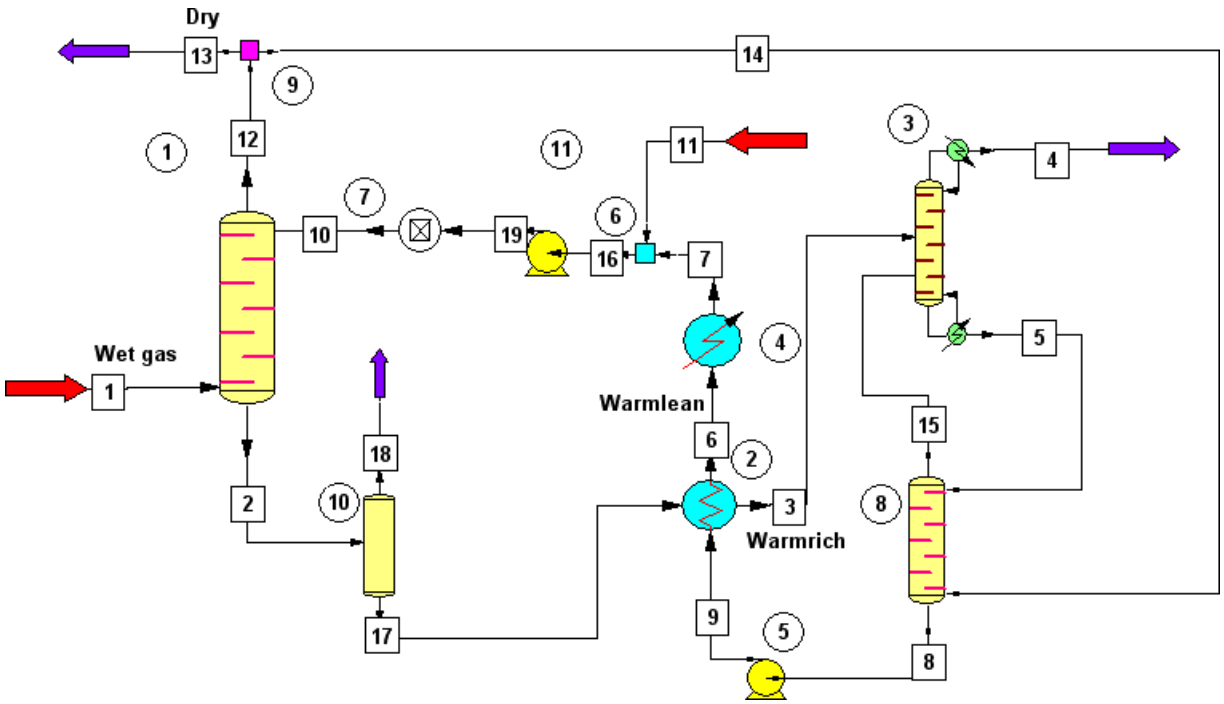
Sensitivity Study tool allows the user to vary up to 2 any process parameters during the flow sheet calculations, as well as recording up to 12 other parameters. The result of the analysis is the chart showing the influence of the varied parameters on the process performance.

In this specific case, we have studied influence of the Column 1 condenser specifications on the CS2 recovery, benzene losses, and necessary recycle flow rate.

Alternative tool available in CHEMCAD 5 is Optimization. You can define the Objective Function, up to
10 Independent Variables and apply Constraints. Optimization usually achieves the solution much faster than the Sensitivity Study does. You can combine Optimization with Costing tool and the Calculator to optimize Investment Cost and Total Manufacturing Cost.

Natural Gas Processing

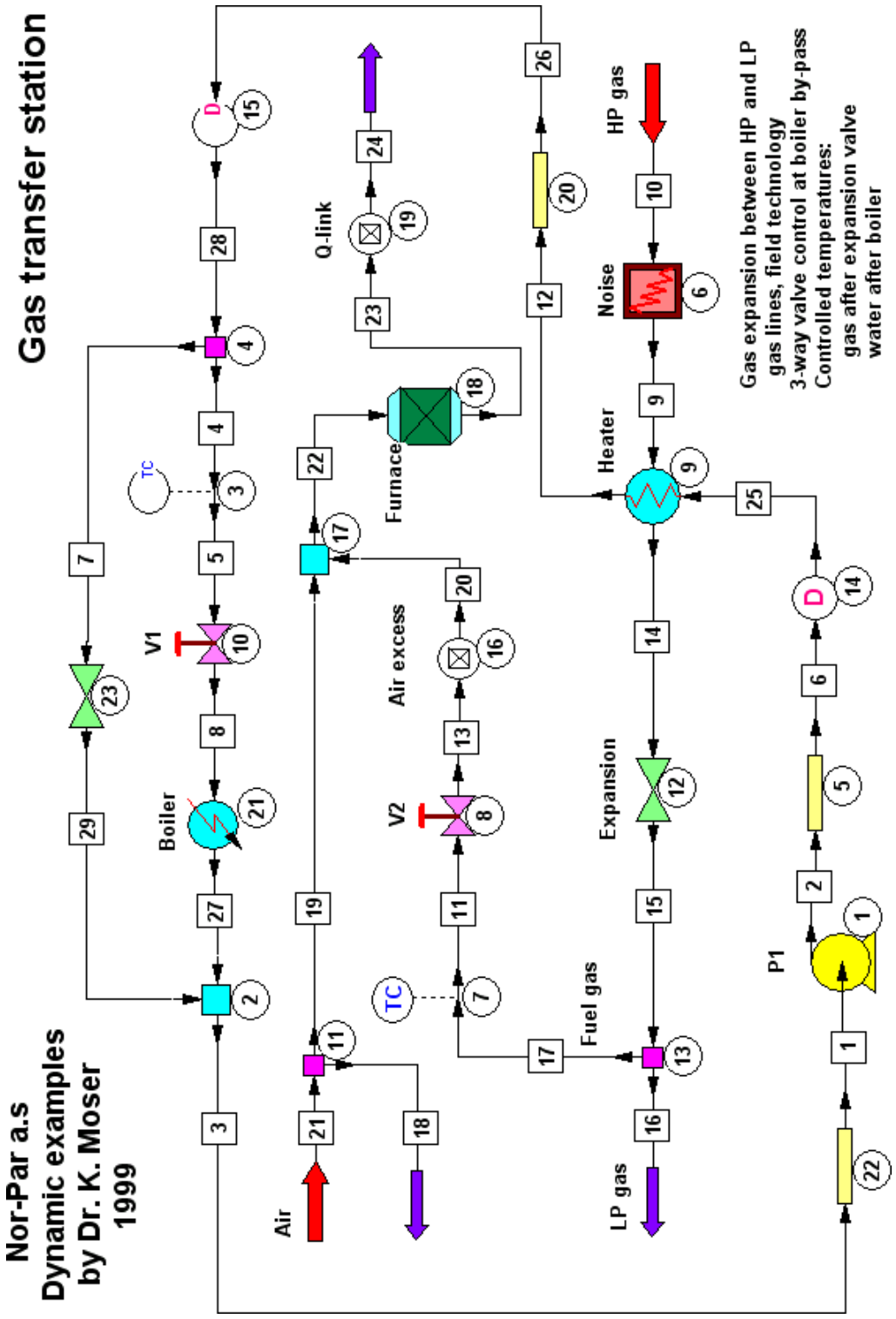
TEG Gas Dehydration–Regeneration



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 methodin CHEMCAD 5.

The flow sheet 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 flow sheet, the water removal from a process or natural gas stream as a function of operating variablesis calculated. The user may define circulating TEG flow, column pressures, flash pressure, stripping gas flow and heat exchanger performance.


Gas transfer station
Nor-Par a.s
Dynamic examples
by Dr. K. Moser
1999
Gas expansion between HP and LP
gas lines, field technology
3-way valve control at boiler by-pass
Controlled temperatures:
gas after expansion valve
water after boiler
HP gas
Noise
Heater
Expansion
Fuel gas
LP gas
Air
Air excess
Furnace
Q-link
Boiler
V1
V2
P1
TC

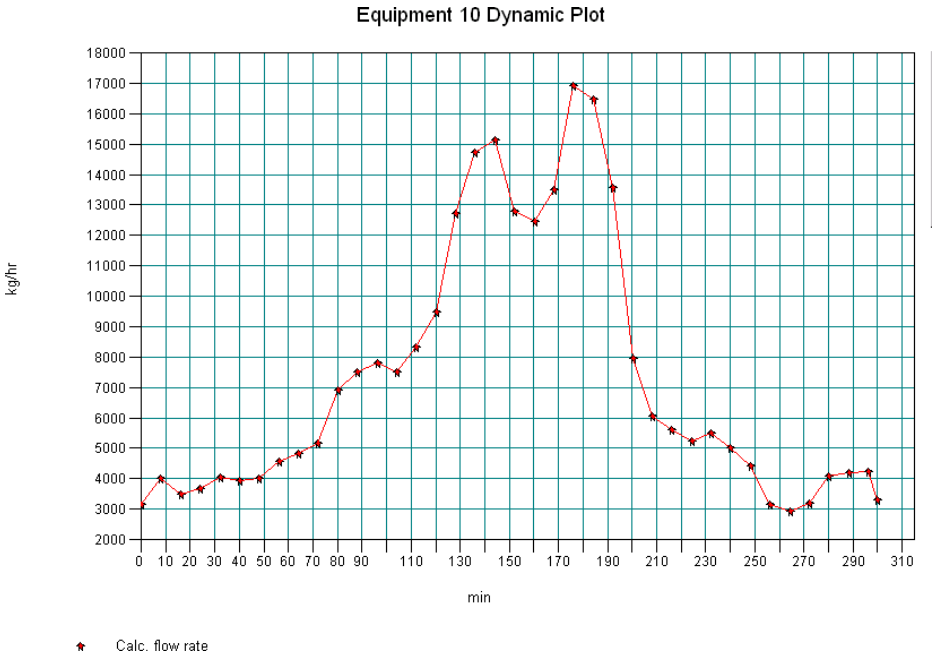
Dynamics: Natural Gas Transfer Station

DESCRIPTION:

This is a simulation of an existing technology. Natural gas at high pressure is reduced and distributed to a local community. As gas temperature decreases during the expansion, gas is heated up by circulating warm water, which in turn is heated up in a boiler. The boiler uses a part of gas as heating medium.

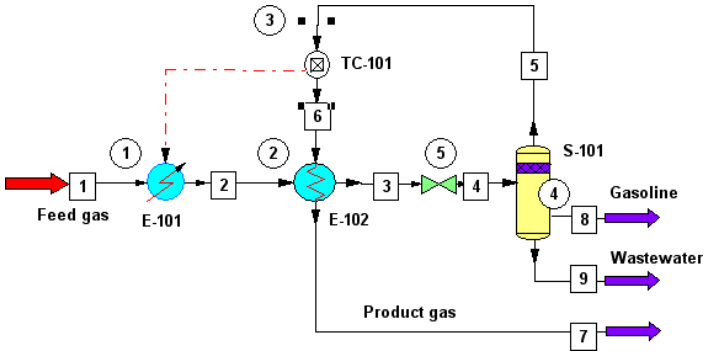
The demand for gas varies over time; therefore the process must be controlled.

The flowsheet was first solved in steady-state mode to determine initial state, then dynamics simulation has been run. Ramp controller simulates varying demand for the gas. Two control loops exist in the system: one to control water temperature after the boiler, and another to control gas supply to the boiler's burner.



Flow rate of water through the boiler over 5 hours

Natural Gas Expansion with Temperature Control

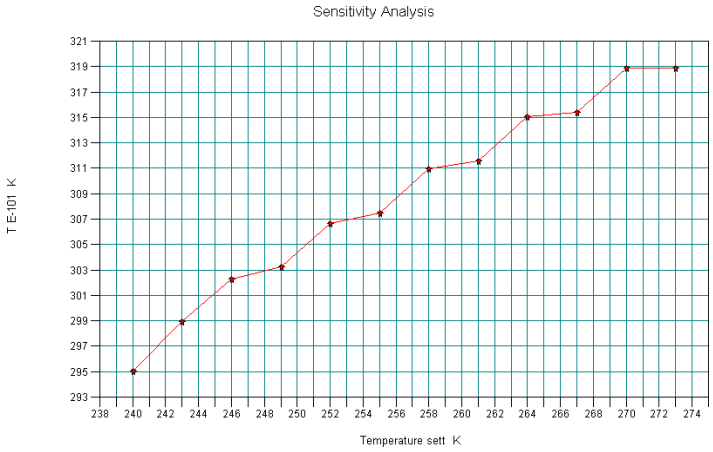


DESCRIPTION:

The flow sheet has been based on actual plant data. Natural gas at 100+ bar G and 283 K is heated in the E-101 exchanger, and then itself heats the product gas in exchanger E-102 to satisfy market requirements. The wet gasis then expanded with a valve, where the gas temperature decreases according to the Joule-Thompson effect. Gasoline and water condensate is knocked out in a flash drum, and further it is decanted. Cool product gas is re-heated in the E-102.

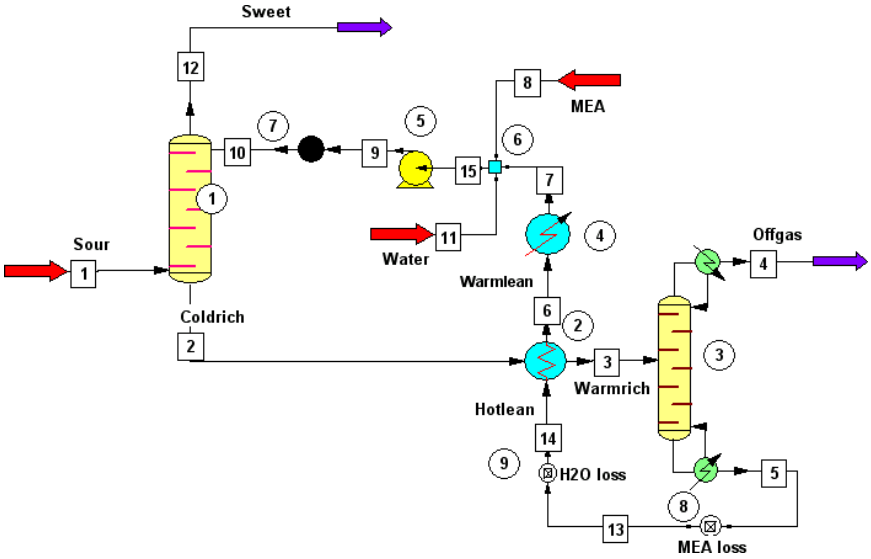
Temperature control is provided to prevent cooling the expanded gas below temperatures limited by material specifications. As gas composition and pressure at the wellhead changes in time, the automated flow sheet like this may serve for everyday field calculations and check-out. The behavior of the process can be also determined via Sensitivity Analysis.

CHEMCAD 5 can also help the gas engineer in predicting hydrate formation. Given stream composition,temperature and pressure, CHEMCAD 5 can tell whether a hydrate would form or not. It is possible to study the influence of inhibitor (methanol, EG, DEG, or TEG) on hydrate formation. Using Dynamics (CC-ReACS or CC- DCOLM module) you can study the behavior of the Control System when well capacity varies.



MEA Sour Gas Treatment Plant

DESCRIPTION:



A group of thermodynamic methods available in CHEMCAD 5 is intended for use with specific technical applications. This is the case with Amine model, which is capable to predict equilibrium for desulfurizationof gases with aqueous solutions of ethanolamines.

This flow sheet describes a typical monoethanolamine (MEA) sour gas treatment plant. Sour gas containing approx. 0.5 mole % of H2S and 2 mole % of CO2 enters the absorber unit at 900 psig and 90 F. Acid gases are removed in the absorber column by contact with lean MEA (15 wt. % aqueous solution). The rich MEA is then heated and regenerated in the stripper column at 26.2 psia. The regeneration column has a reboiler and a partial condenser. Regenerated MEA passes through heat exchanger to preheat the rich amine stream. It is then mixed with make-up MEA and water, boosted tothe absorption column's pressure, cooled, and directed onto the top of the absorber.