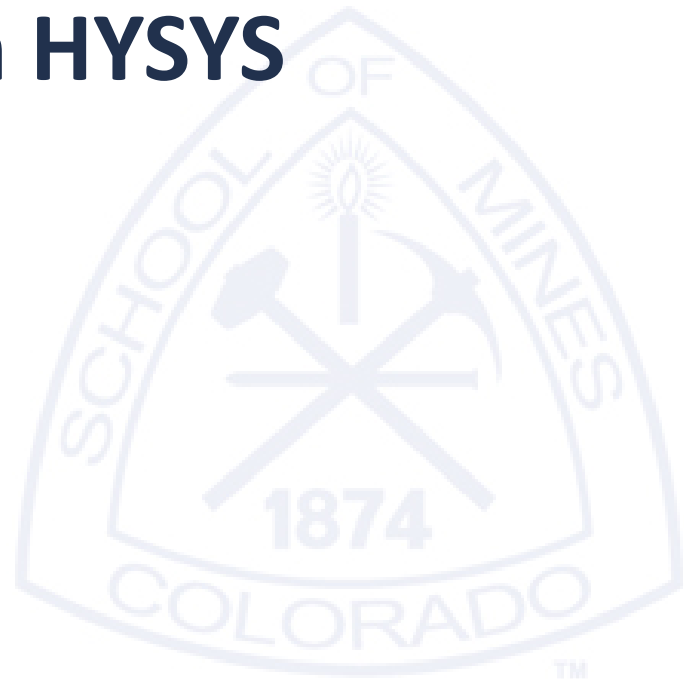


Process Engineering Simulation with Aspen HYSYS



Process Engineering Simulation

Core chemical engineering doctrine – mass & energy balances

Modes

- Steady state simulation
- Dynamic simulation

Simulation program features

- Components / chemical species
 - Pure component data library
 - Non-library components
- Property models & methods
 - Thermodynamic models
 - Physical & transport properties
- Chemical reaction models & methods
- Unit operation models
- Flowsheet capabilities
 - Recycle loops
- Graphical interface

Updated: July 5, 2017

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HYSYS as Process Engineering Tool

Owned & marketed by Aspen Tech

- Developed by Hyprotech.
- Initially DOS-based -- HYSIM

Core calculations for steady state mass & energy balances

- Dynamic capabilities as add-on package

Historical orientation towards the oil & gas industry

- Components
 - Extensive pure component database of hydrocarbons
 - Generate pseudo-components from crude oil assay information
- Property models
 - Consistent with hydrocarbon systems – relatively non-ideal mixtures
 - Capabilities for presence of typical non-hydrocarbons
 - Simplified methods for mixtures with water
 - Acid gas components – CO₂ & H₂S
- Unit operation models
 - Towers with pumparounds, side strippers, ...
- Reaction system models
 - CatCracker, Hydrocracker, Reformer

Composition

Pure component database

- Typically use a small number of light hydrocarbons ($C_1 - nC_5$), CO_2 , H_2S , & H_2O

Pseudo/hypothetical components

- Narrow boiling point fractions from distillation analysis
- Assumption that all components in range will have the same split between vapor & liquid
 - Not a good assumption if chemical structure plays a big part in separation or reaction
- Correlations to generate “average” properties for the fraction
 - Empirical correlations based on boiling point, specific/API gravity, molecular weight
 - Group contribution methods

Electrolyte mixtures may require explicit definition of ionic species

Pure Components

hysys atm column example.hsc - Aspen HYSYS V9 - aspenONE

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Component List - 1x

Source Databank: HYSYS

Select: **Pure Components** Filter: **All Families**

Search for: Search by: **Full Name/Synonym**

Component	Type	Group
H2O	Pure Component	
Methane	Pure Component	
Ethane	Pure Component	
Propane	Pure Component	
i-Butane	Pure Component	
n-Butane	Pure Component	
i-Pentane	Pure Component	
n-Pentane	Pure Component	
NBP[0]55*	Oil Hypothetical	Blend-1 Hypos
NBP[0]85*	Oil Hypothetical	Blend-1 Hypos
NBP[0]120*	Oil Hypothetical	Blend-1 Hypos
NBP[0]155*	Oil Hypothetical	Blend-1 Hypos
NBP[0]187*	Oil Hypothetical	Blend-1 Hypos
NBP[0]226*	Oil Hypothetical	Blend-1 Hypos
NBP[0]260*	Oil Hypothetical	Blend-1 Hypos
NBP[0]294*	Oil Hypothetical	Blend-1 Hypos
NBP[0]329*	Oil Hypothetical	Blend-1 Hypos

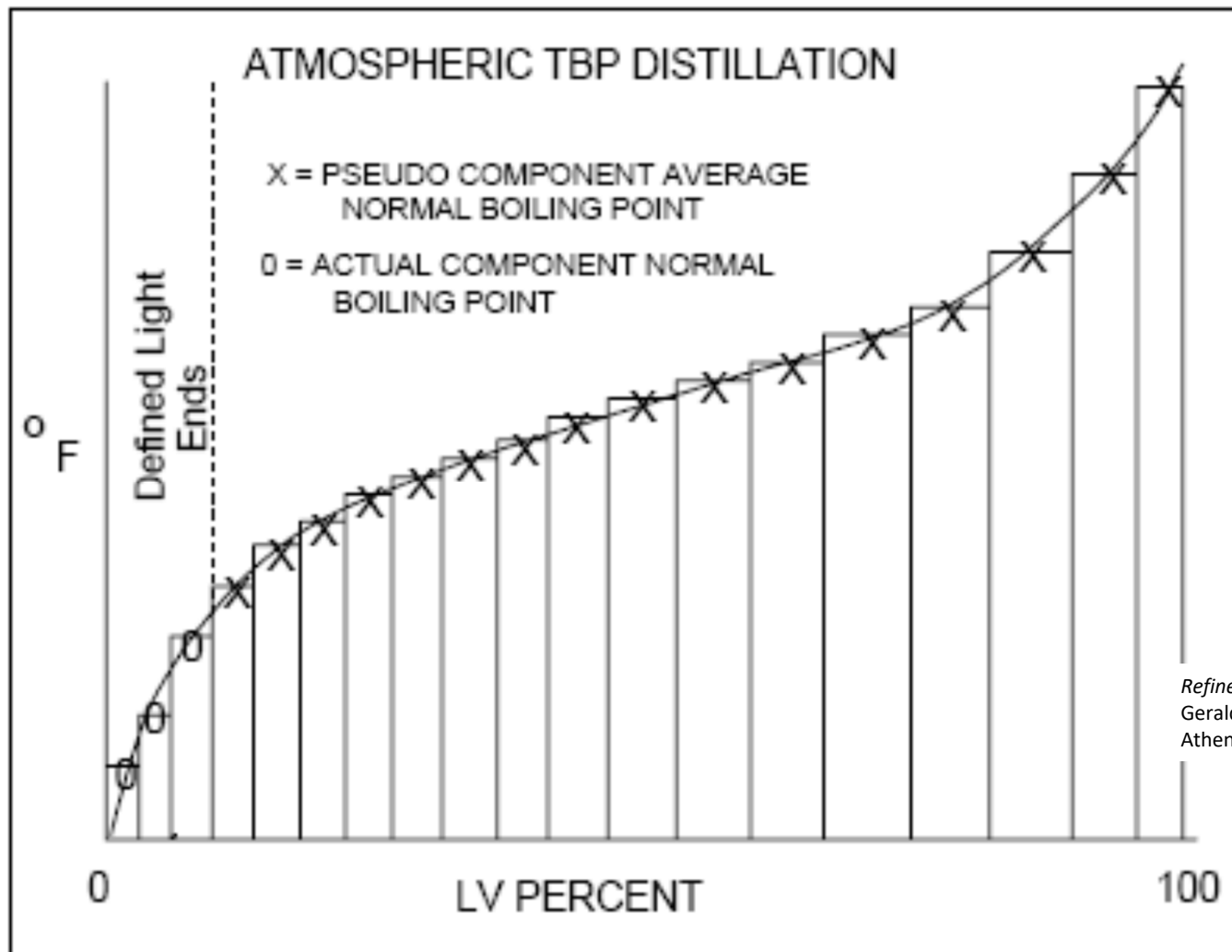
< Add Replace Remove

Simulation Name	Full Name / Synonym	Formula
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22
n-C11	C11	C11H24
n-C12	C12	C12H26
n-C13	C13	C13H28
n-C14	C14	C14H30
n-C15	C15	C15H32
n-C16	C16	C16H34
n-C17	C17	C17H36
n-C18	C18	C18H38
n-C19	C19	C19H40
n-C20	C20	C20H42

Status: OK

100%

Pseudo Components from Assay



Refinery Process Modeling
Gerald Kaes
Athens Printing Company., 2000, pg. 32

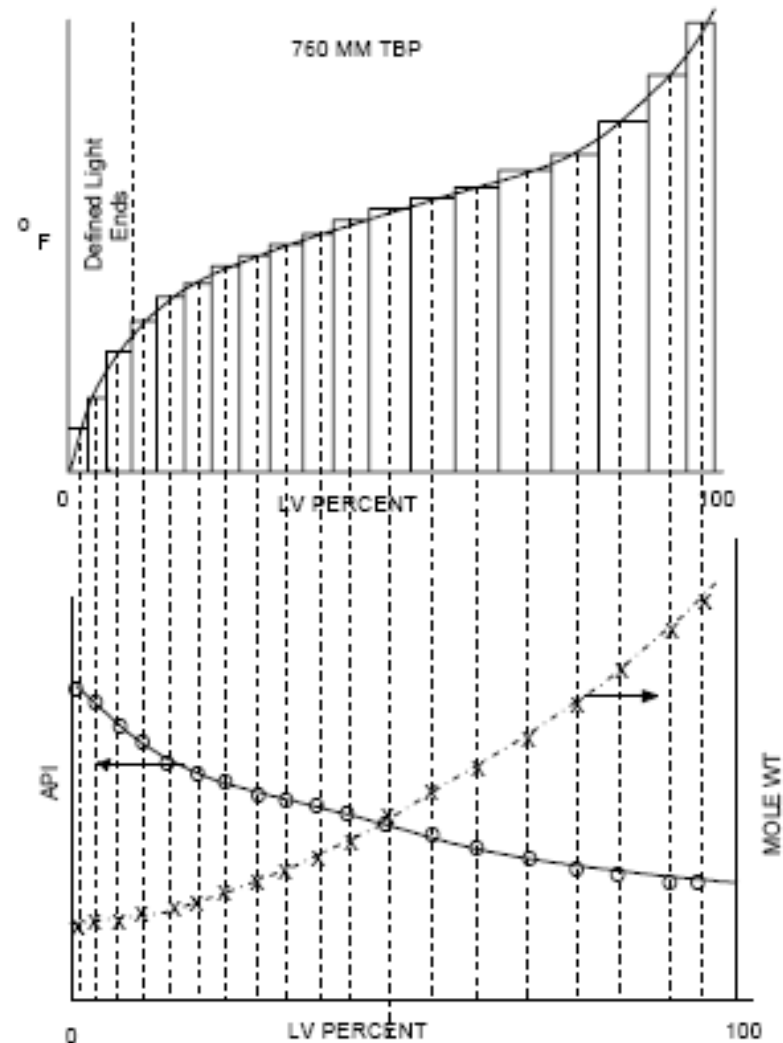
Pseudo Components from Assay

Split the yield curve into boiling point ranges

Use the property curves to generate consistent with measured data

Use correlations to estimate unmeasured & unmeasurable properties

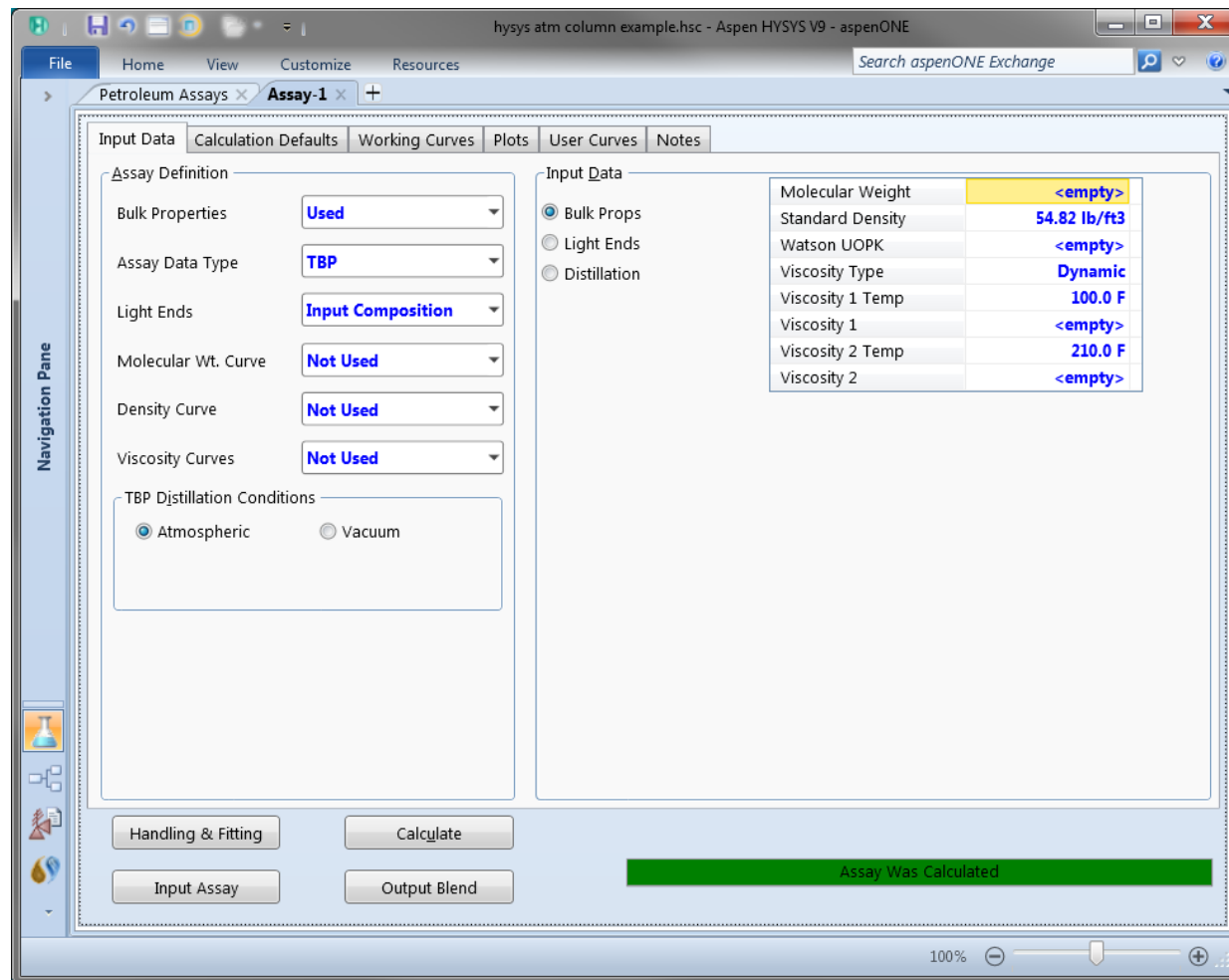
- Critical properties
- Accentric factor
- Binary interaction coefficients



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Pseudo Components from Assay



Pseudo Components from Assay

hysys atm column example.hsc - Aspen HYSYS V9 - aspenONE

File Home View Customize Resources Search aspenONE Exchange

Petroleum Assays x **Assay-1** x +

Input Data Calculation Defaults Working Curves Plots User Curves Notes

Assay Definition

Bulk Properties **Used**

Assay Data Type **TBP**

Light Ends **Input Composition**

Molecular Wt. Curve **Not Used**

Density Curve **Not Used**

Viscosity Curves **Not Used**

TBP Distillation Conditions

☒ Atmospheric ☐ Vacuum

Input Data

☐ Bulk Props ☒ Light Ends ☐ Distillation

Light Ends Basis **Liquid Volume %**

Light Ends	Composition	NBP [F]
H2O	0.0000	212.0
Methane	6.500e-003	-258.7
Ethane	2.250e-002	-127.5
Propane	0.3200	-43.78
i-Butane	0.2400	10.89
n-Butane	0.8200	31.10
i-Pentane	0.0000	82.18
n-Pentane	0.0000	96.91

Percent of Light Ends in Assay **1.4090**

Handling & Fitting Calculate

Input Assay Output Blend

Assay Was Calculated

100%

Pseudo Components from Assay

The image shows the Aspen HYSYS V9 interface with the 'Assay-1' configuration window open. The 'Assay Input Table' dialog is also visible, showing a table of assay data points.

Assay Input Table Data:

Assay Percent [%]	Temperature [F]
0.0000	15.00
4.500	90.00
9.000	165.0
14.50	240.0
20.00	310.0
30.00	435.0
40.00	524.0
50.00	620.0
60.00	740.0
70.00	885.0
76.00	969.0
80.00	1015
85.00	1050
<empty>	<empty>

Assay-1 Configuration Window:

- Assay Definition:**
 - Bulk Properties: **Used**
 - Assay Data Type: **TBP**
 - Light Ends: **Input Composition**
 - Molecular Wt. Curve: **Not Used**
 - Density Curve: **Not Used**
 - Viscosity Curves: **Not Used**
 - TBP Distillation Conditions: **Atmospheric** (selected), Vacuum
- Input Data:**
 - Assay Basis: **Liquid Volume**
 - Input Data Table (same as Assay Input Table):

Buttons and Status:

- Buttons: **Handling & Fitting**, **Calculate**, **Input Assay**, **Output Blend**, **Edit Assay...**
- Status: **Table is Ready**, **Assay Was Calculated**

Pseudo Components from Assay

The screenshot displays the Aspen HYSYS V9 - aspenONE interface. The left sidebar shows the 'Properties' section with 'Blend-1' selected under 'Output Blend'. The main window shows the 'Component Physical Properties' table for 'Blend-1'. The table includes columns for 'Comp Name', 'NBP [F]', 'Mole Wt.', 'Density [lb/ft3]', 'Viscosity1 [cP]', and 'Viscosity2 [cP]'. The table lists 20 pseudo-components, with 'NBP_55' highlighted. Below the table are buttons for 'Install Oil', 'Output Blend', and 'Input Assay'. A green status bar at the bottom indicates 'Blend Was Calculated'.

Comp Name	NBP [F]	Mole Wt.	Density [lb/ft3]	Viscosity1 [cP]	Viscosity2 [cP]
NBP_55	55.30	59.32	42.94	0.27184	0.13911
NBP_85	84.89	65.04	43.80	0.31160	0.16239
NBP_120	119.9	72.73	44.73	0.33529	0.18111
NBP_155	155.4	81.30	45.65	0.31188	0.18882
NBP_187	186.9	89.25	46.51	0.35605	0.21344
NBP_226	226.2	97.36	47.16	0.40271	0.23734
NBP_260	259.5	107.2	47.94	0.47264	0.27177
NBP_294	294.3	117.6	48.73	0.56178	0.31413
NBP_329	329.3	128.5	49.48	0.66733	0.36300
NBP_364	364.3	140.3	50.21	0.80047	0.42308
NBP_399	399.4	153.2	50.94	1.0020	0.49600
NBP_435	435.0	167.4	51.68	1.2874	0.59005
NBP_469	469.4	182.4	52.40	1.6733	0.70557
NBP_504	503.8	198.0	53.05	2.1747	0.84096
NBP_538	538.4	214.2	53.68	2.8484	1.0039
NBP_573	573.4	231.4	54.29	3.8004	1.2080
NBP_608	608.2	249.3	54.89	5.1529	1.4618
NBP_643	643.2	267.7	55.47	7.1293	1.7822
NBP_678	678.2	286.4	56.04	10.139	2.1974
NBP_713	713.0	304.5	56.60	14.831	2.7384
NBP_748	748.0	322.8	57.14	22.320	3.4471

Pseudo Components from Assay

The screenshot displays the Aspen HYSYS V9 - aspenONE software interface. The main window shows the 'Component Physical Properties' table for the 'Blend-1' assay. The table lists various pseudo-components (NBP_55, NBP_85, etc.) and their physical properties (Critical Temp, Critical Press, Accentric Fac, Watson K). The 'Table Control' on the left indicates that the 'Main Properties' are selected for the 'Blend-1' assay. A green status bar at the bottom of the table area reads 'Blend Was Calculated'.

Comp Name	Critical Temp [F]	Critical Press [psia]	Accentric Fac	Watson K
NBP_55	365.25	581.67	0.13755	11.629
NBP_85	397.25	545.87	0.17300	11.617
NBP_120	438.23	527.22	0.21170	11.612
NBP_155	482.25	508.30	0.23726	11.608
NBP_187	521.97	488.10	0.25193	11.584
NBP_226	564.05	448.53	0.28616	11.650
NBP_260	600.68	422.91	0.31409	11.643
NBP_294	638.29	398.74	0.34385	11.637
NBP_329	675.36	376.37	0.37470	11.635
NBP_364	712.01	355.95	0.40641	11.632
NBP_399	748.31	337.28	0.43906	11.626
NBP_435	784.73	320.26	0.47282	11.616
NBP_469	819.68	305.31	0.50634	11.603
NBP_504	853.77	290.84	0.54153	11.599
NBP_538	887.39	276.99	0.57840	11.599
NBP_573	920.95	263.90	0.61694	11.600
NBP_608	953.87	251.78	0.65641	11.602
NBP_643	986.60	240.30	0.69745	11.605
NBP_678	1019.1	229.63	0.73964	11.606
NBP_713	1051.2	219.73	0.78271	11.608
NBP_748	1083.0	210.34	0.82708	11.610

Property Models & Methods

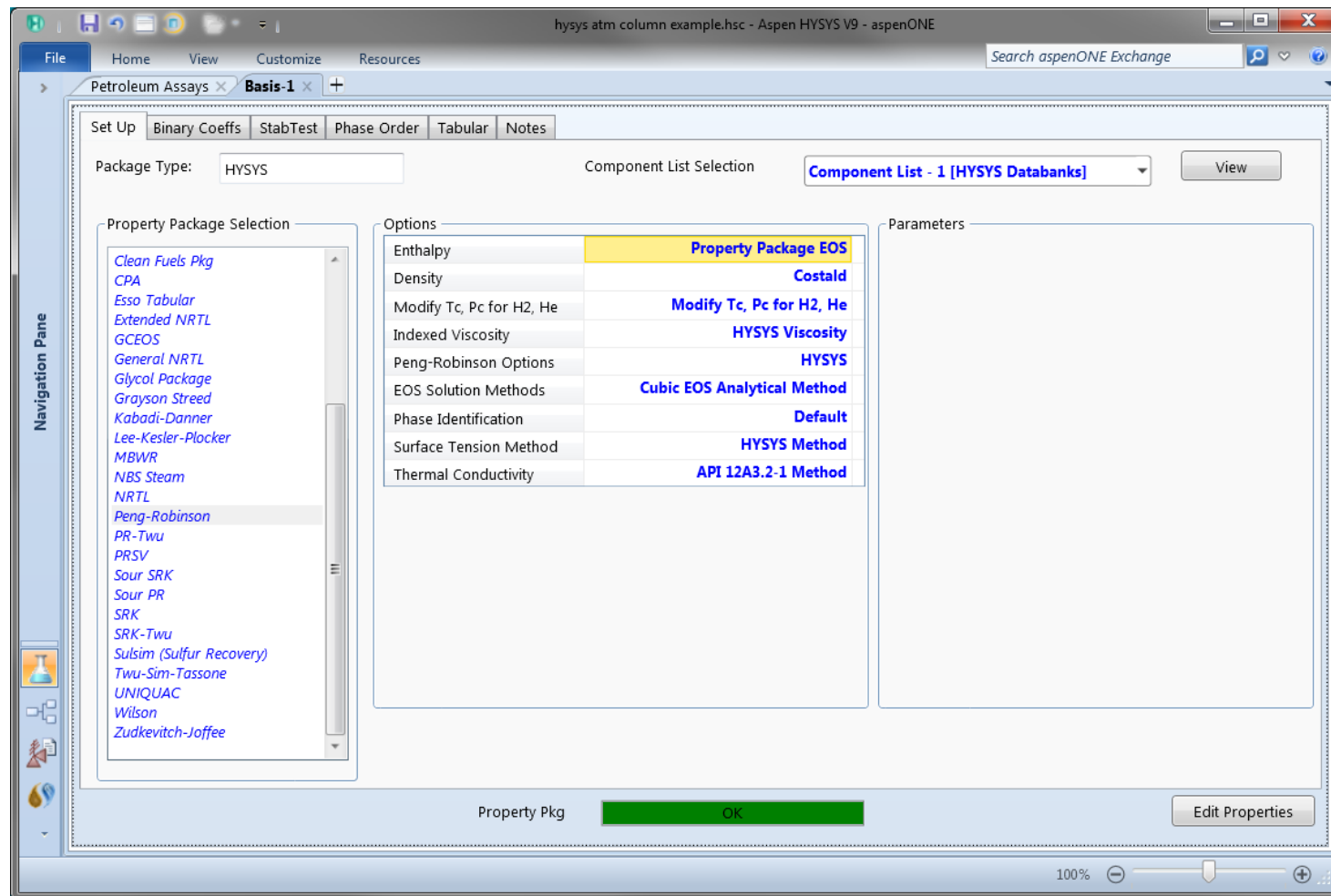
Typically use an equation of state (EOS) for properties

- Consistent properties for vapor, liquid, & transitions between
- Thermodynamic properties from the same set of equations
 - Equilibrium coefficients (fugacity)
 - Enthalpy
 - Entropy
 - Density
- Non-ideal behavior from binary interaction coefficients
 - Major effect on equilibrium coefficients
 - Very small effect on other properties

May use other properties for other thermodynamic properties

- Lee-Kesler for enthalpy
- COSTALD for liquid density

Property Models & Methods



Updated: July 5, 2017

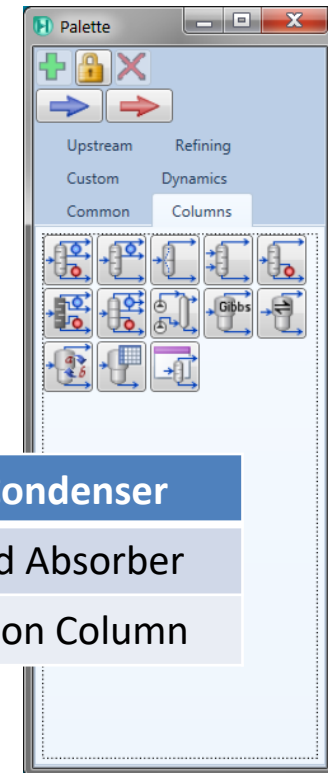
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Unit Operation Models

“Typical” unit operation models

- Valve
- Separators
- Heat exchangers
- Pumps
- Compressors
- Reactors – CSTR & plug flow
- Towers – with & without condenser & reboiler

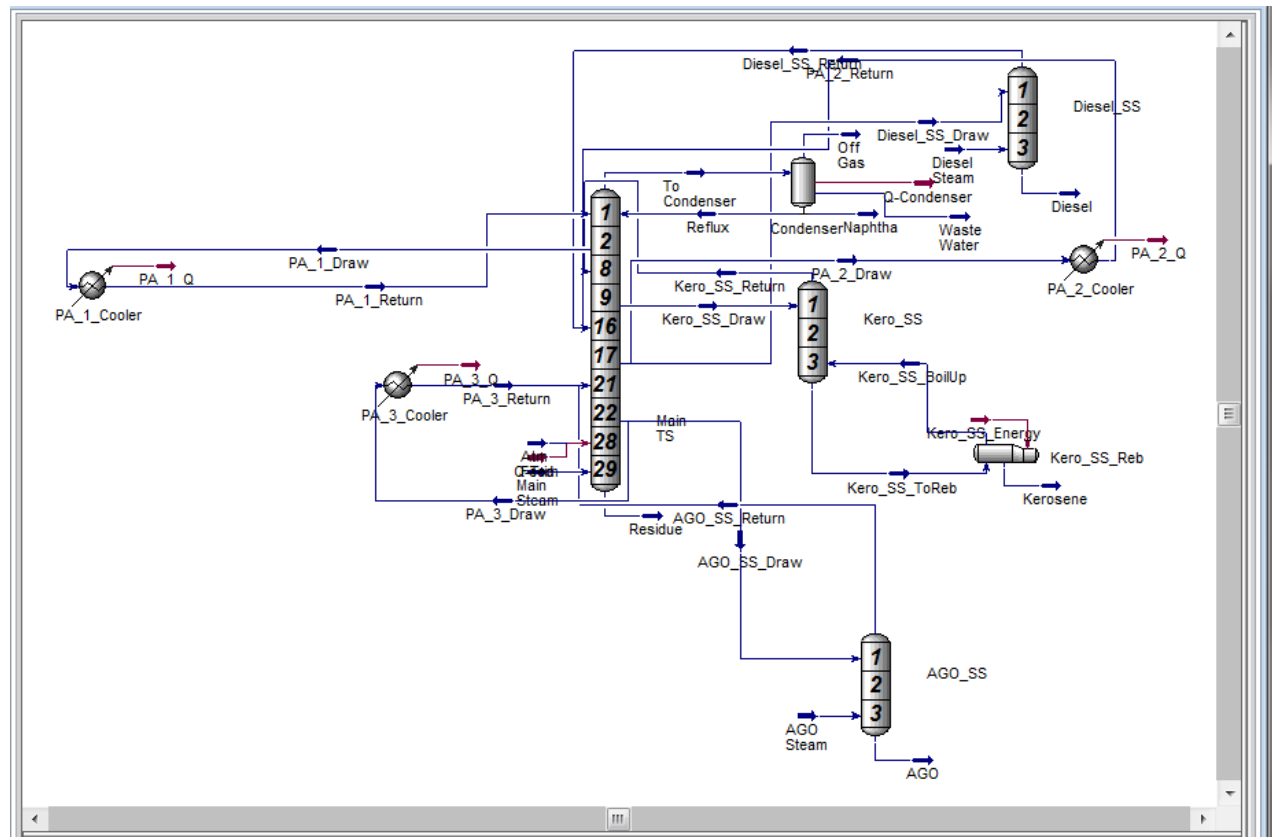
	Without Condenser	With Condenser
Without Reboiler	Absorber	Refluxed Absorber
With Reboiler	Reboiled Absorber	Distillation Column



Unit Operation Models for Refining

Complex tower configurations

- Pumparounds
- Side draws
- Side strippers
- Condenser with water draw
- Complex specifications
 - ASTM temperature spec



Typical Overall Efficiencies

Column Service	Typical No. of Actual Trays	Typical Overall Efficiency	Typical No. of Theoretical Trays
Simple Absorber/Stripper	20 – 30	20 – 30	
Steam Side Stripper	5 – 7		2
Reboiled Side Stripper	7 – 10		3 – 4
Reboiled Absorber	20 – 40	40 – 50	
Deethanizer	25 – 35	65 – 75	
Depropanizer	35 – 40	70 – 80	
Debutanizer	38 – 45	85 – 90	
Alky DeiC4 (reflux)	75 – 90	85 – 90	
Alky DeiC4 (no reflux)	55 – 70	55 – 65	
Naphtha Splitter	25 – 35	70 – 75	
C2 Splitter	110 – 130	95 – 100	
C3 Splitter	200 – 250	95 – 100	
C4 Splitter	70 – 80	85 – 90	
Amine Contactor	20 – 24		4 – 5
Amine Stripper	20 – 24	45 – 55	9 – 12
Crude Distillation	35 – 50	50 – 60	20 – 30
Stripping Zone	5 – 7	30	2
Flash Zone – 1 st draw	3 – 7	30	1 – 2
1 st Draw – 2 nd Draw	7 – 10	45 – 50	3 – 5
2 nd Draw – 3 rd Draw	7 – 10	50 – 55	3 – 5
Top Draw – Reflux	10 – 12	60 – 70	6 – 8
Vacuum Column (G.O. Operation)			
Stripping	2 – 4		1
Flash Zone – HGO Draw	2 – 3		1 – 2
HGO Section	3 – 5		2
LGO Section	3 – 5		2
FCC Main Fractionator	24 – 35	50 – 60	13 – 17
Quench Zone	5 – 7		2
Quench – HGO Draw	3 – 5		2 – 3
HGO – LCGO	6 – 8		3 – 5
LCGO – Top	7 – 10		5 – 7

Refinery Process Modeling

Gerald Kaes, Athens Printing Company., 2000, pg. 32

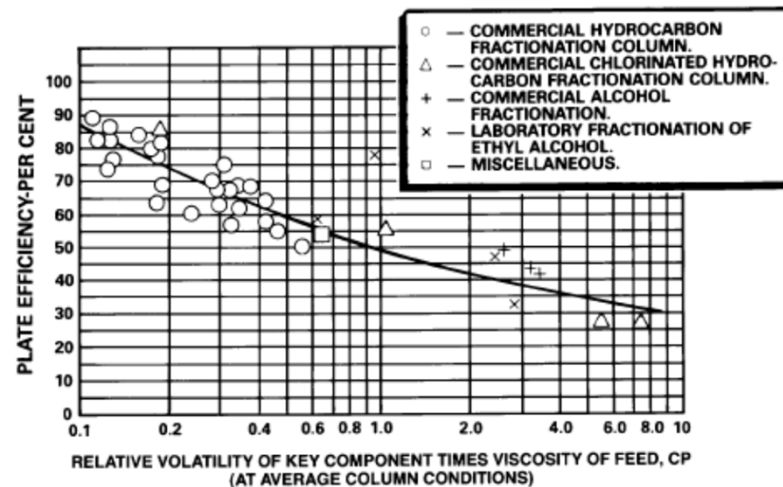
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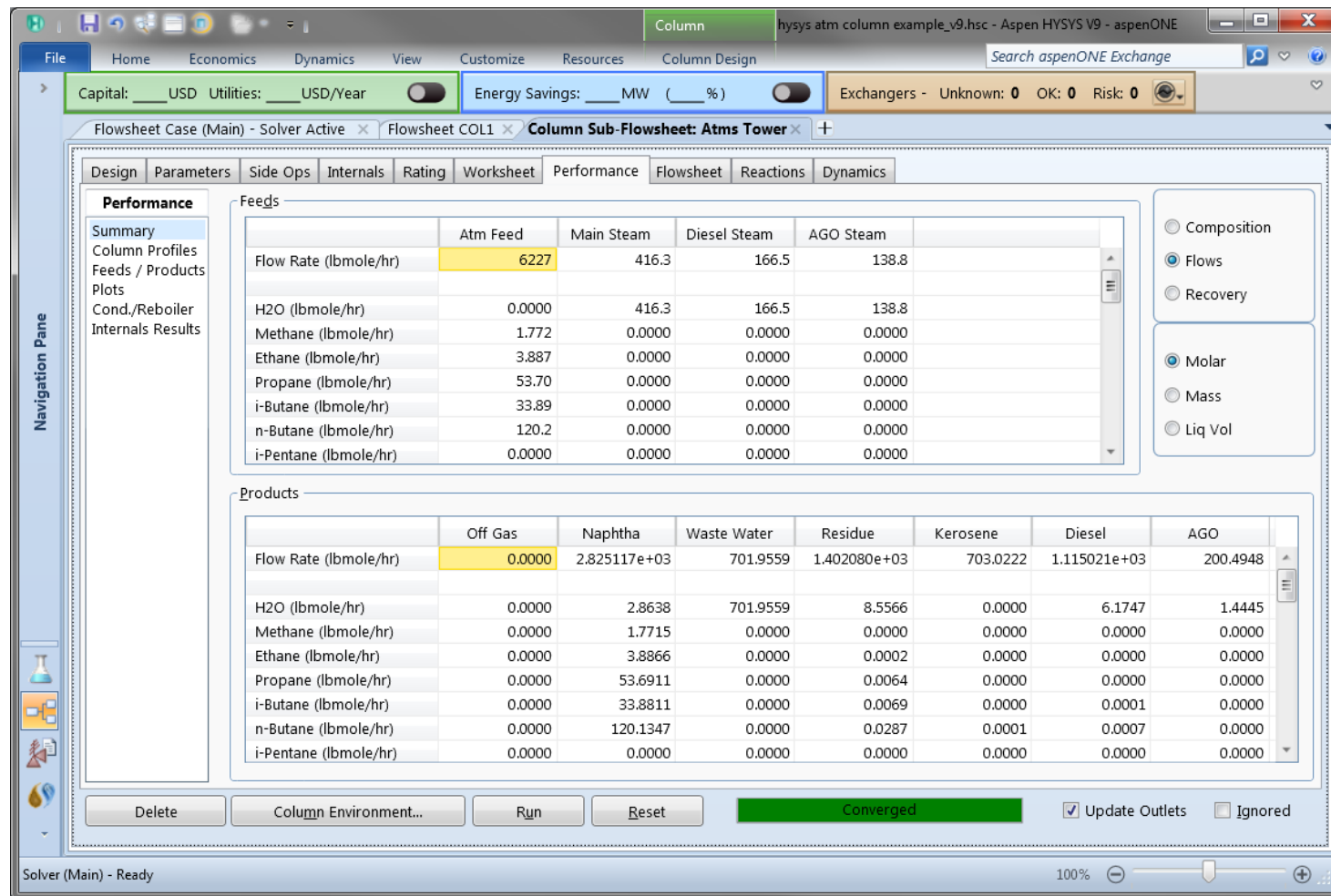
Viscosity	Maxwell	Drickamer & Bradford in Ludwig
cP	Ave Viscosity of liquid on plates	Molal Ave Viscosity of Feed
0.05	...	98
0.10	104	79
0.15	86	70
0.20	76	60
0.30	63	50
0.40	56	42
0.50	50	36
0.60	46	31
0.70	43	27
0.80	40	23
0.90	38	19
1.00	36	17
1.50	30	7
1.70	28	5

Rules of Thumb for Chemical Engineers, 4th ed.
Carl Branan, Gulf Professional Publishing, 2005

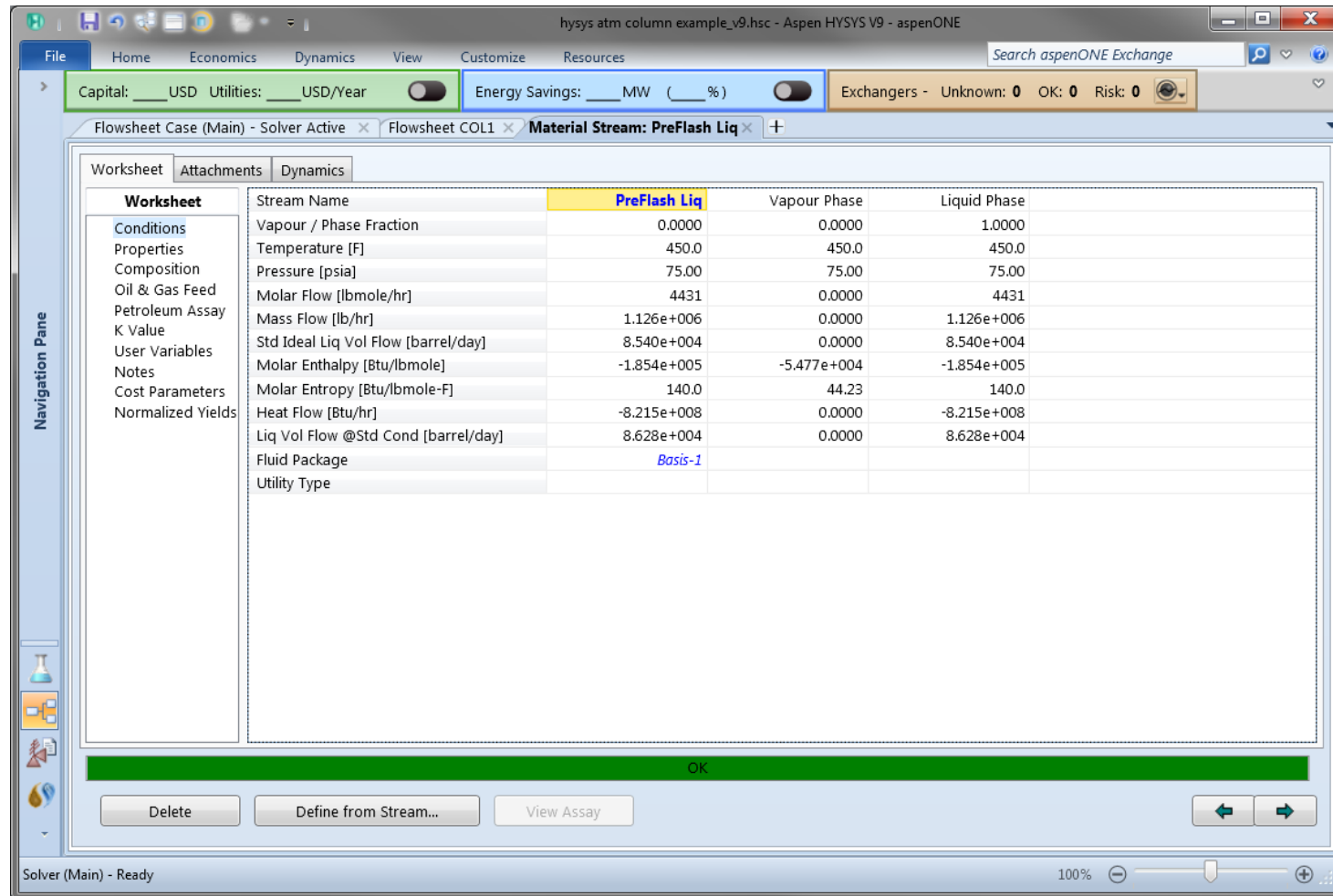
Engineering Data Book, 12th ed.
Gas Processors Association, 2004



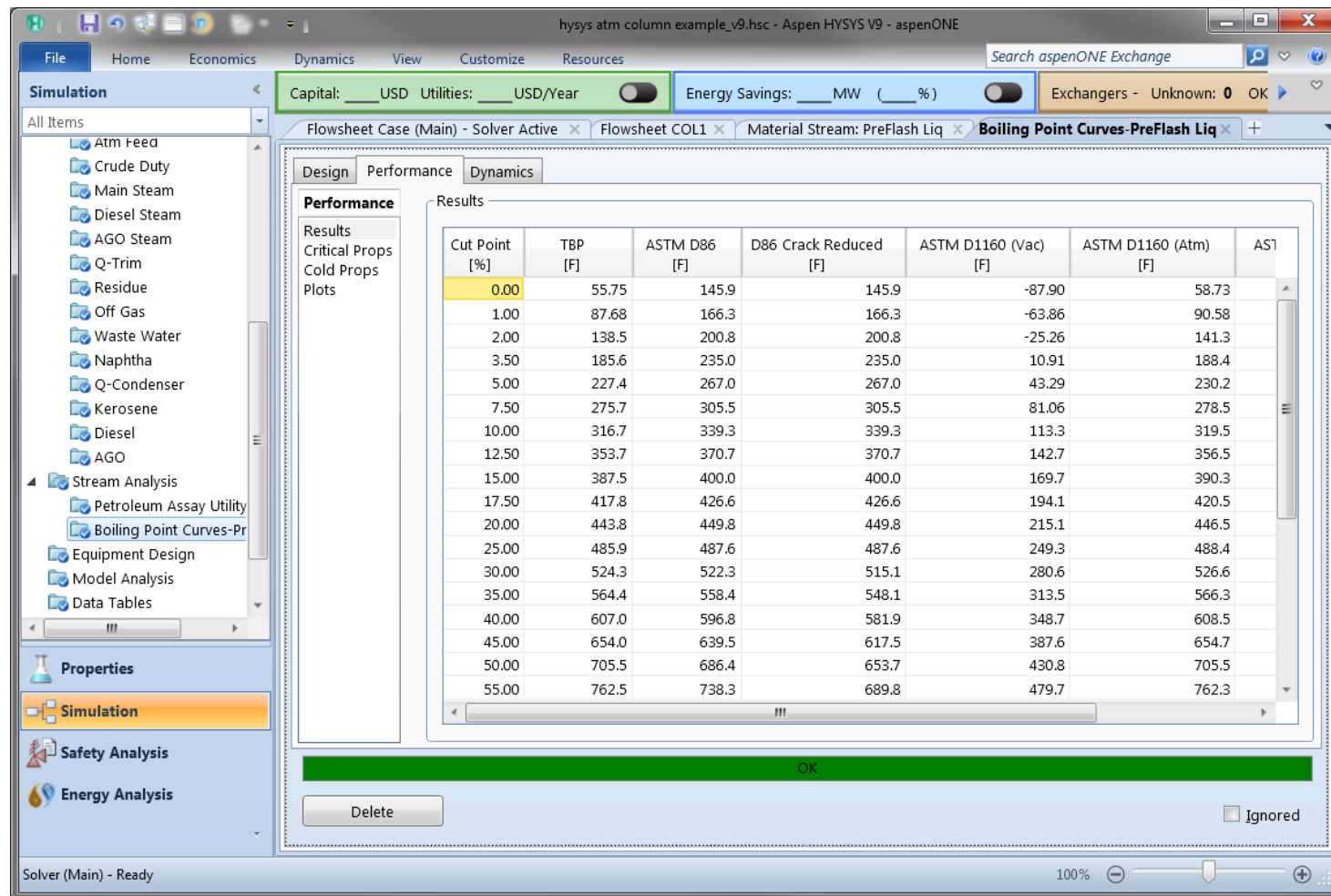
Unit Operations Results



Stream Results



Specialized Stream Reports



User Interface

Graphically build the flowsheet by dragging & dropping unit models

Calculations performed automatically as information is entered

Copy & paste capabilities

- Pasting in from other locations limited

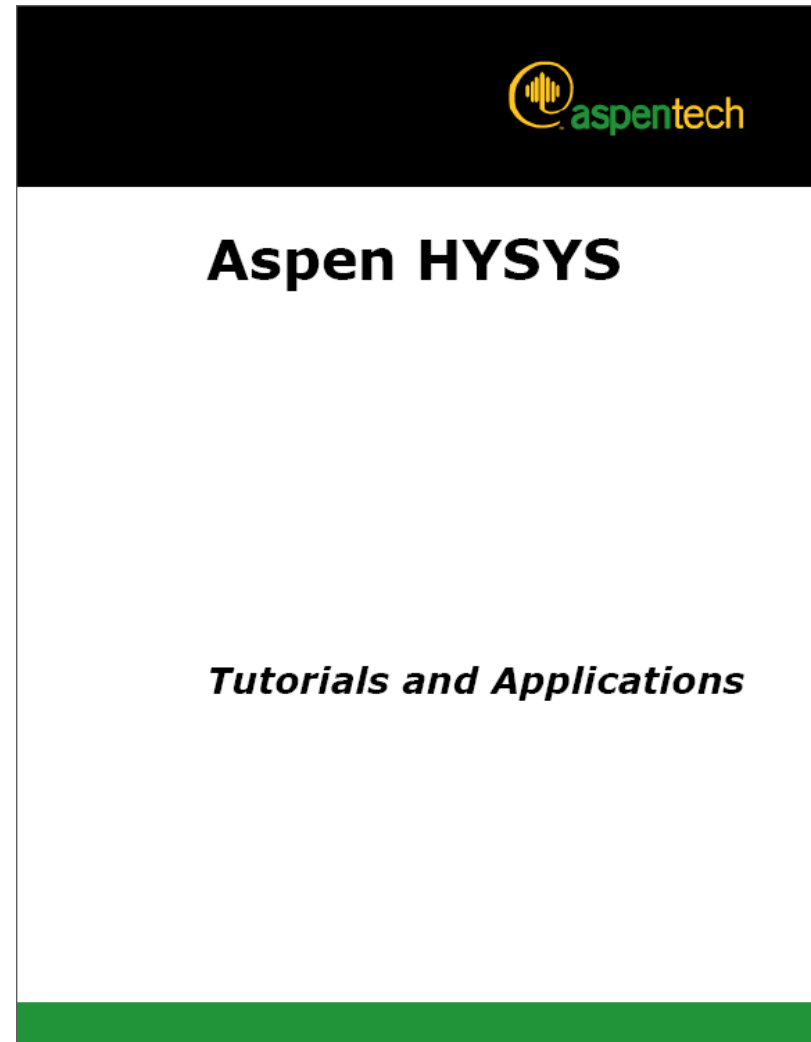
Aspen Simulation Workbook extends capabilities to put custom interface on top of simulation

HYSYS crude tower examples

Available from Aspen Tech web site

<http://support.aspentech.com/webteamasp/My/FrameDef.asp?/webteamasp/My/product.asp?id1=2674&id2=''&id3=all>

Additional problem developed specifically for this class.



Summary

HYSYS is a capable tool for performing mass & energy balances

Program features make it convenient for petroleum refining applications

- Pure component data library & psuedo-components from distillation analyses
- Property models & methods
- Thermodynamic, physical & transport property models appropriate for petroleum systems
- Chemical reaction models & methods
- Unit operation models
 - Specific configurations for complex equipment
- Flowsheet capabilities
- Unit operation & stream results
- Graphical interface