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

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 – CO_2 & H_2S
- Unit operation models
  - Towers with pumparounds, side strippers, …
- Reaction system models
  - CatCracker, Hydrocracker, Reformer

Updated: July 5, 2017

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Composition

Pure component database

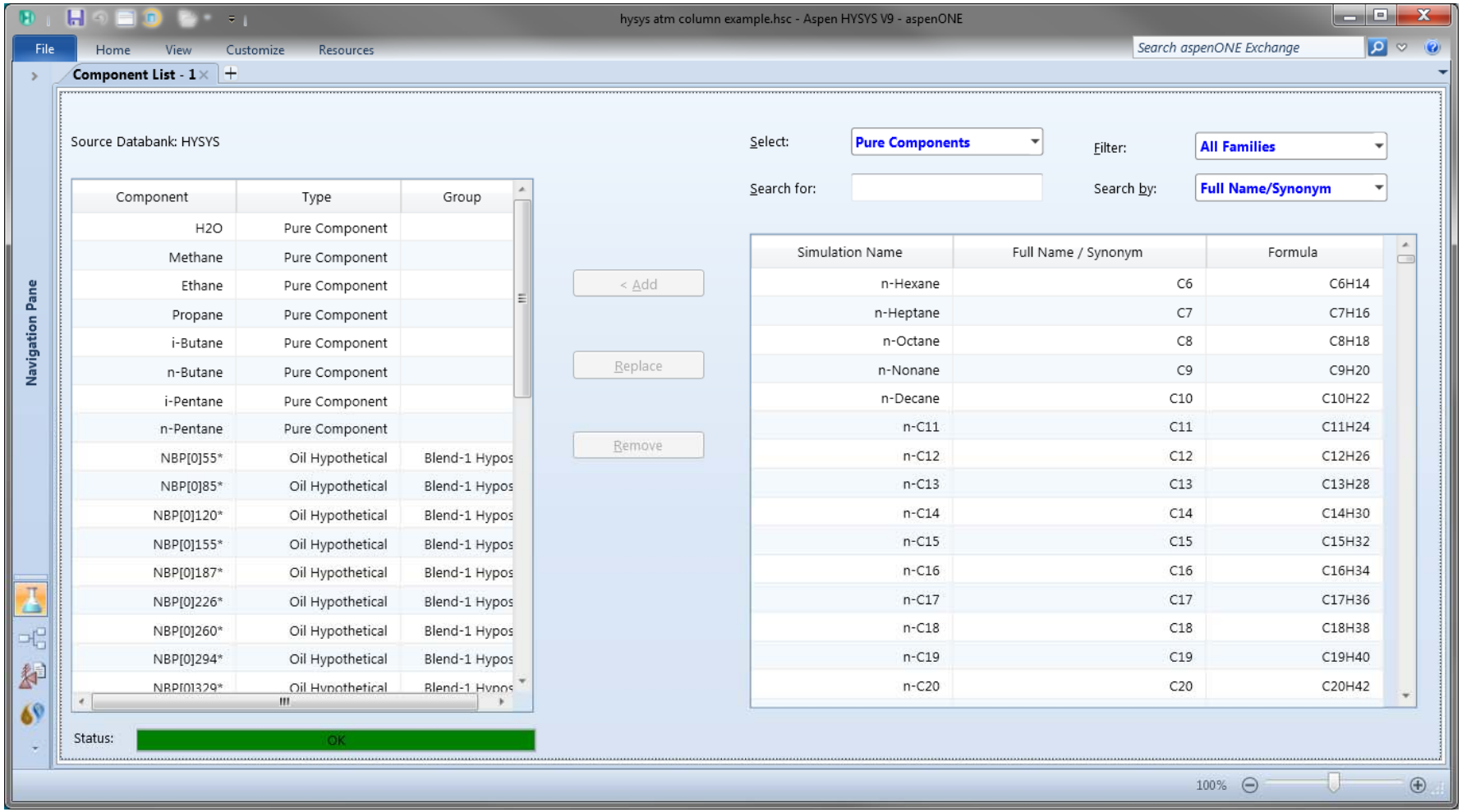
- Typically use a small number of light hydrocarbons (C_1 – nC_5), CO_2, H_2S, & H_2O

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

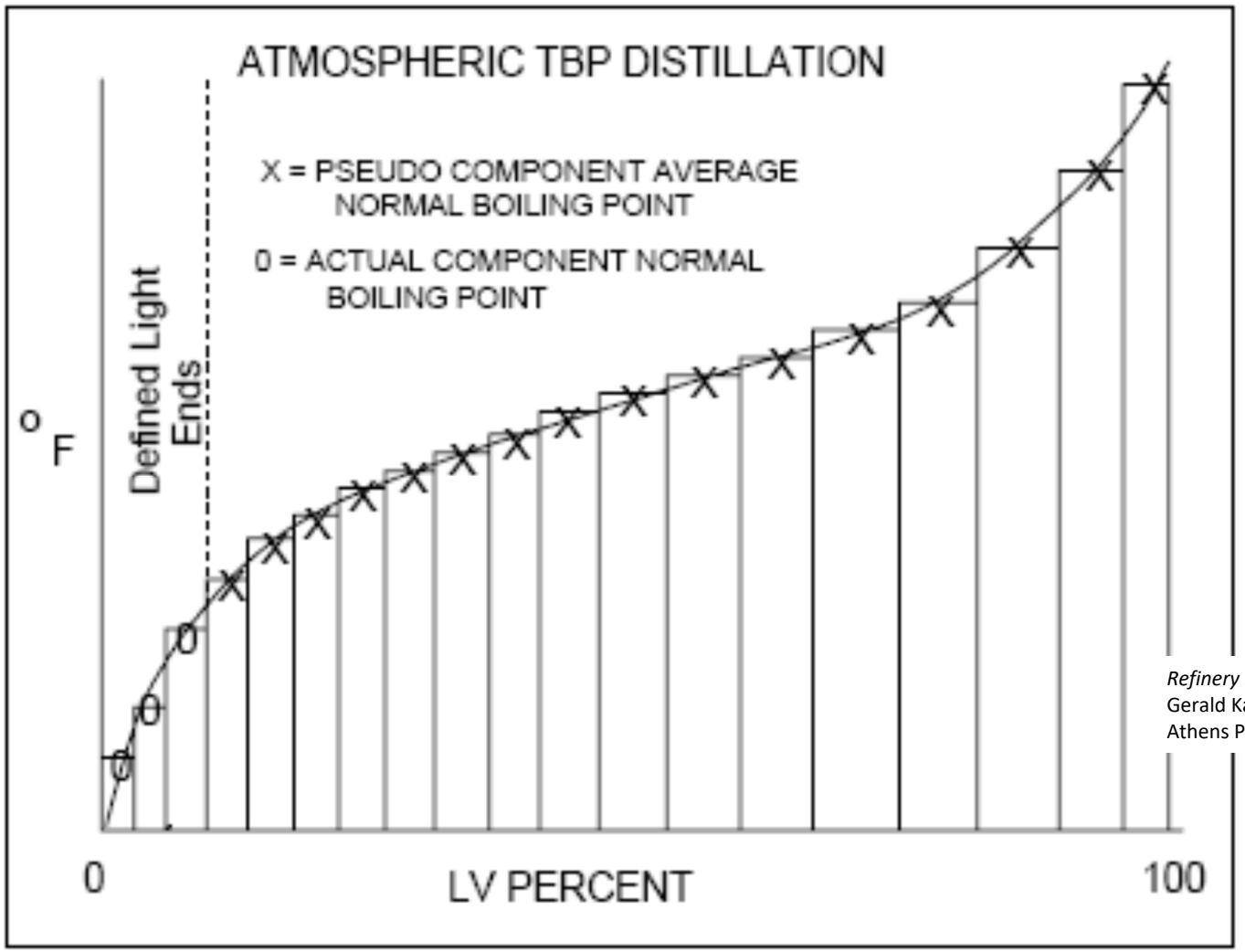
Electrolyte mixtures may require explicit definition of ionic species

Pure Components



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



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

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

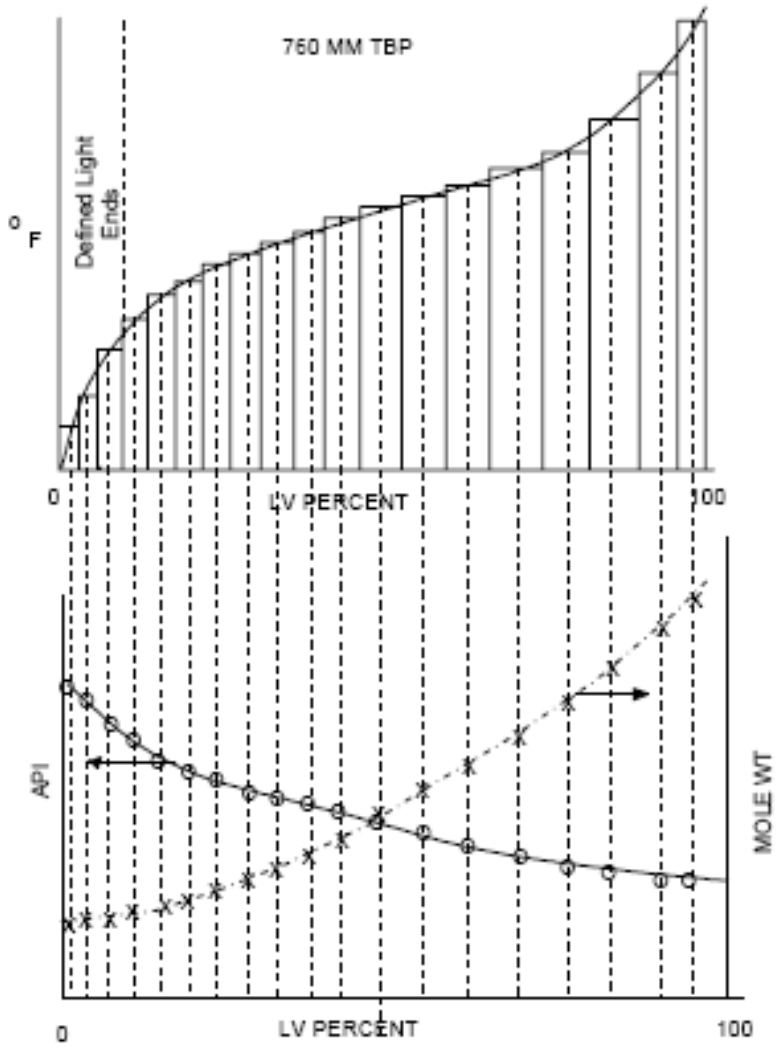
Pseudo Components from Assay

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

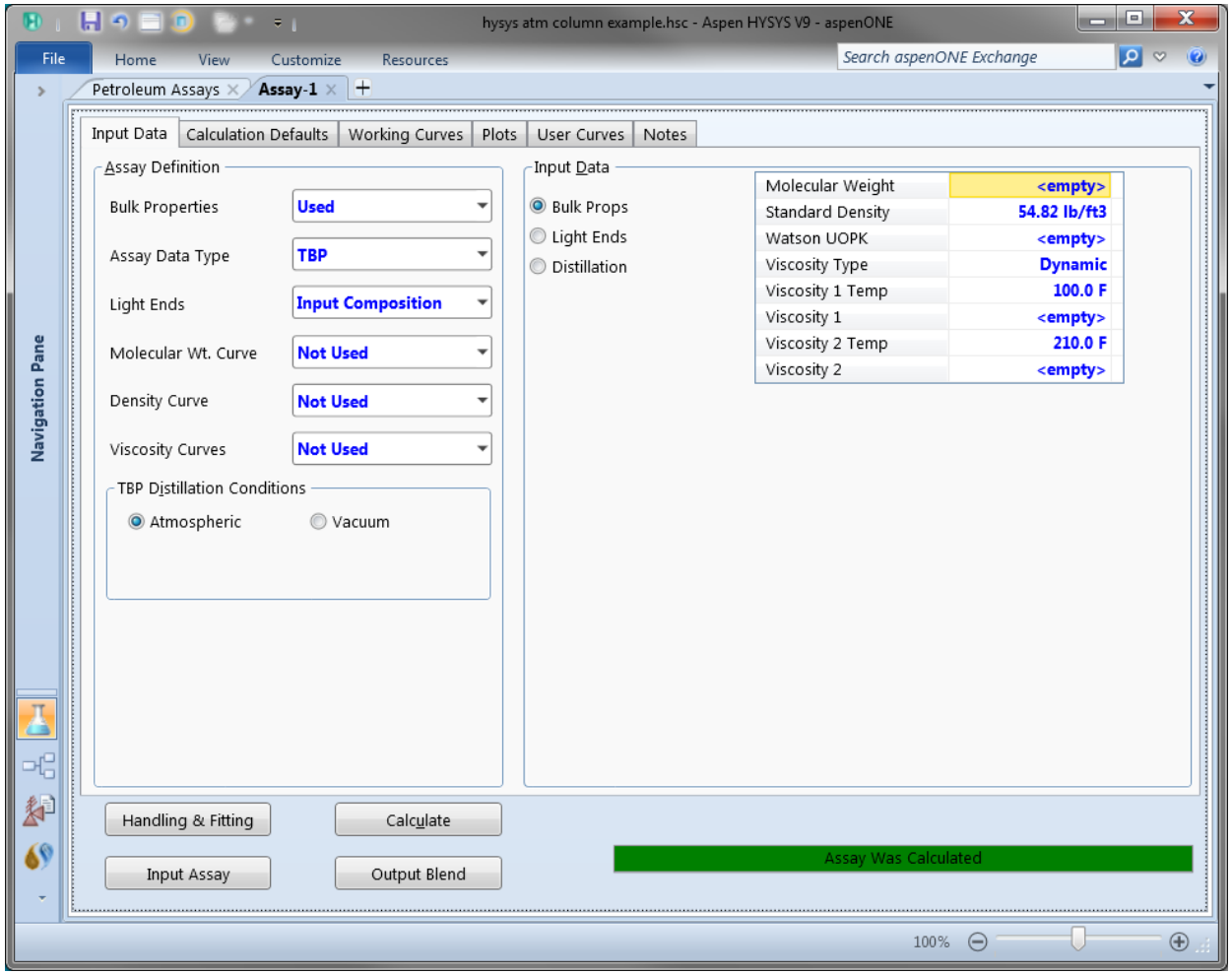
- Critical properties
- Accentric factor
- Binary interaction coefficients



Updated: July 5, 2017

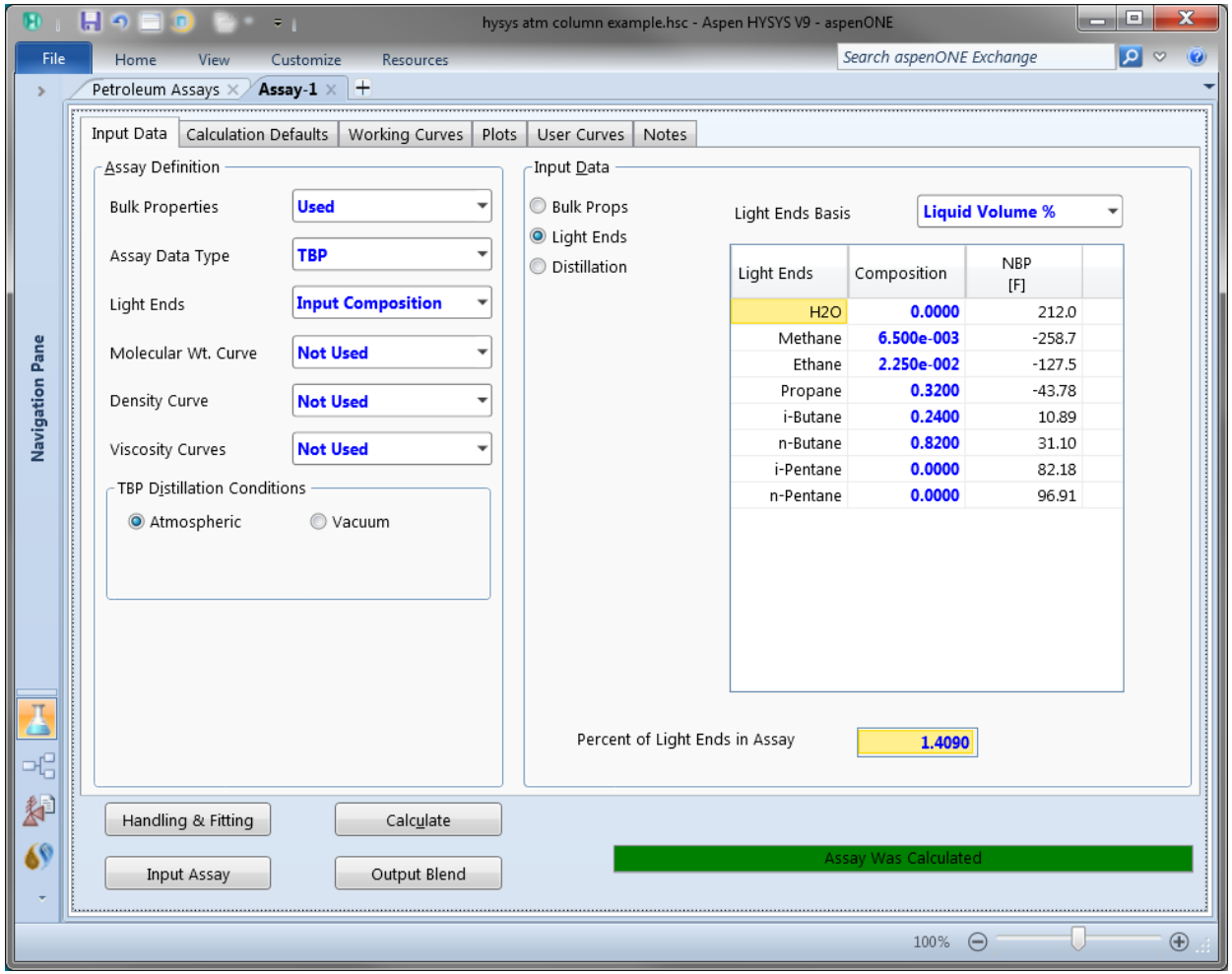
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



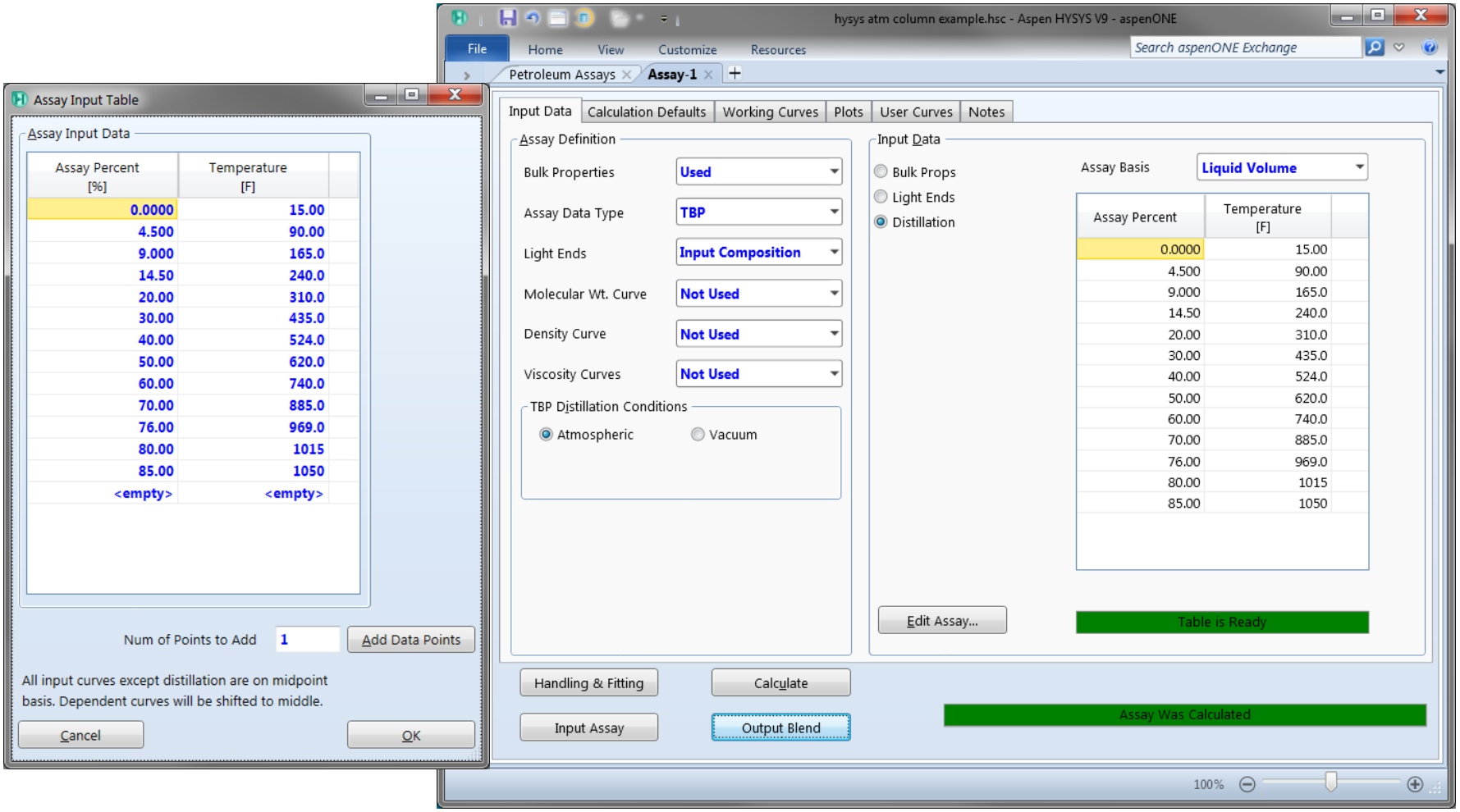
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



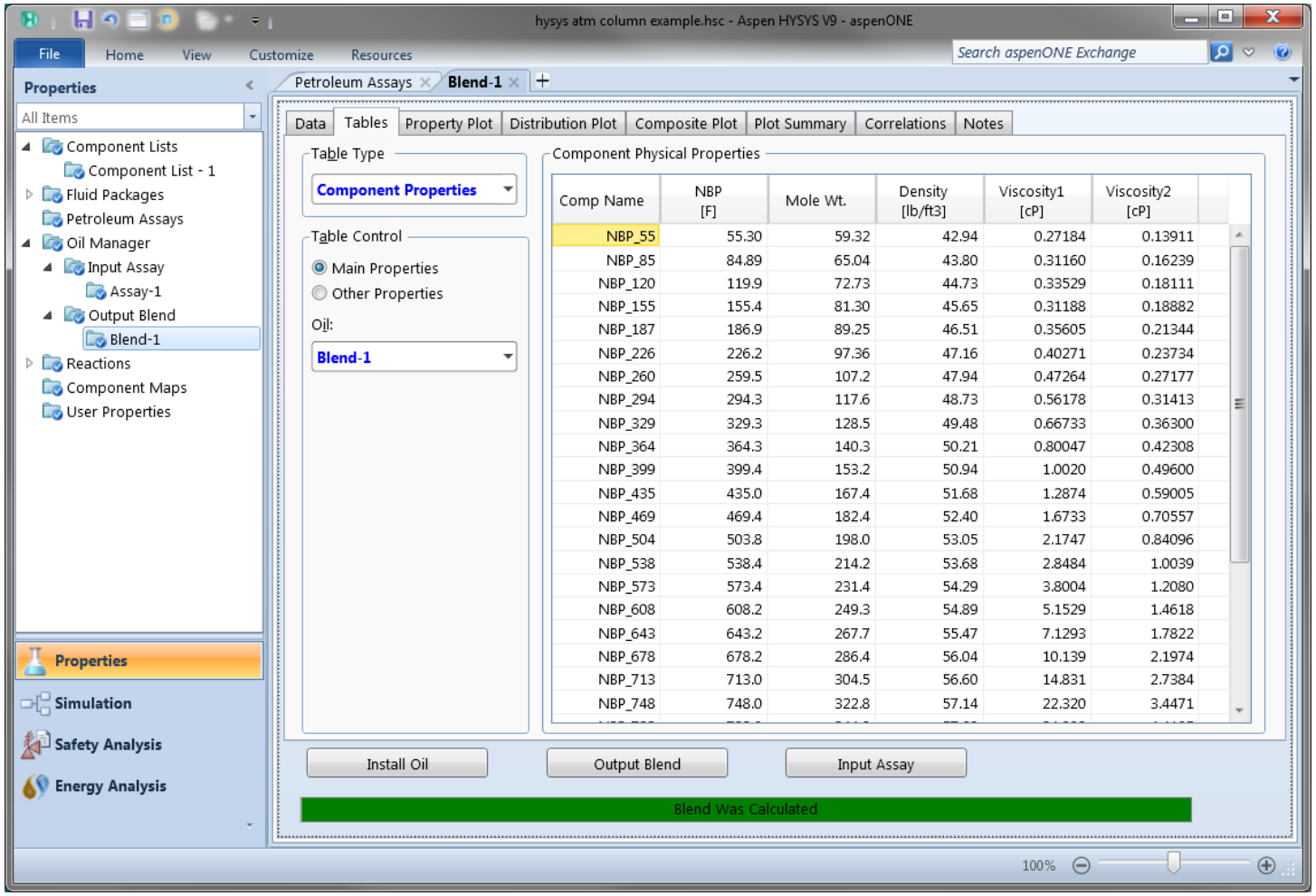
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



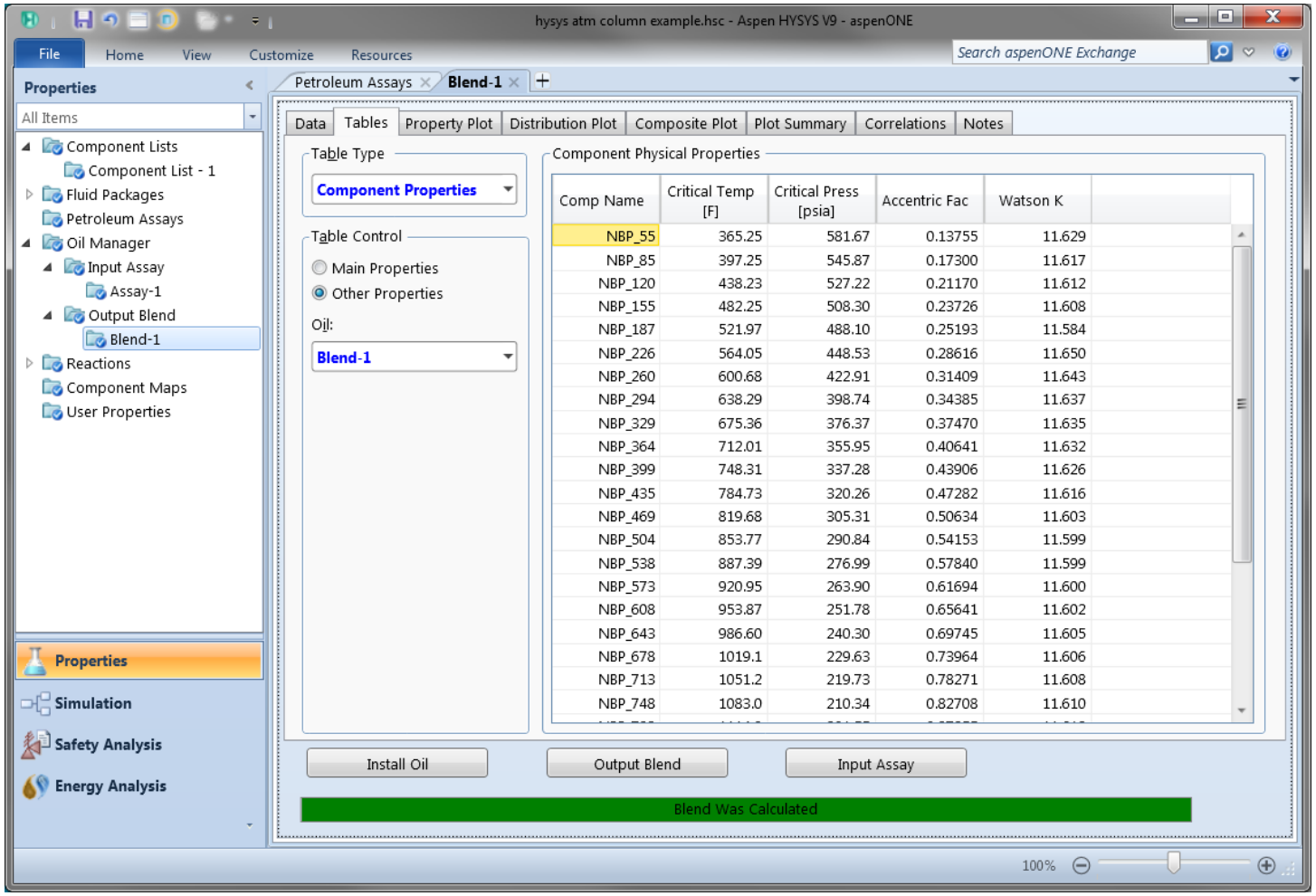
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Pseudo Components from Assay



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Property Models & Methods

Typically use an equation of state (EOS) for properties

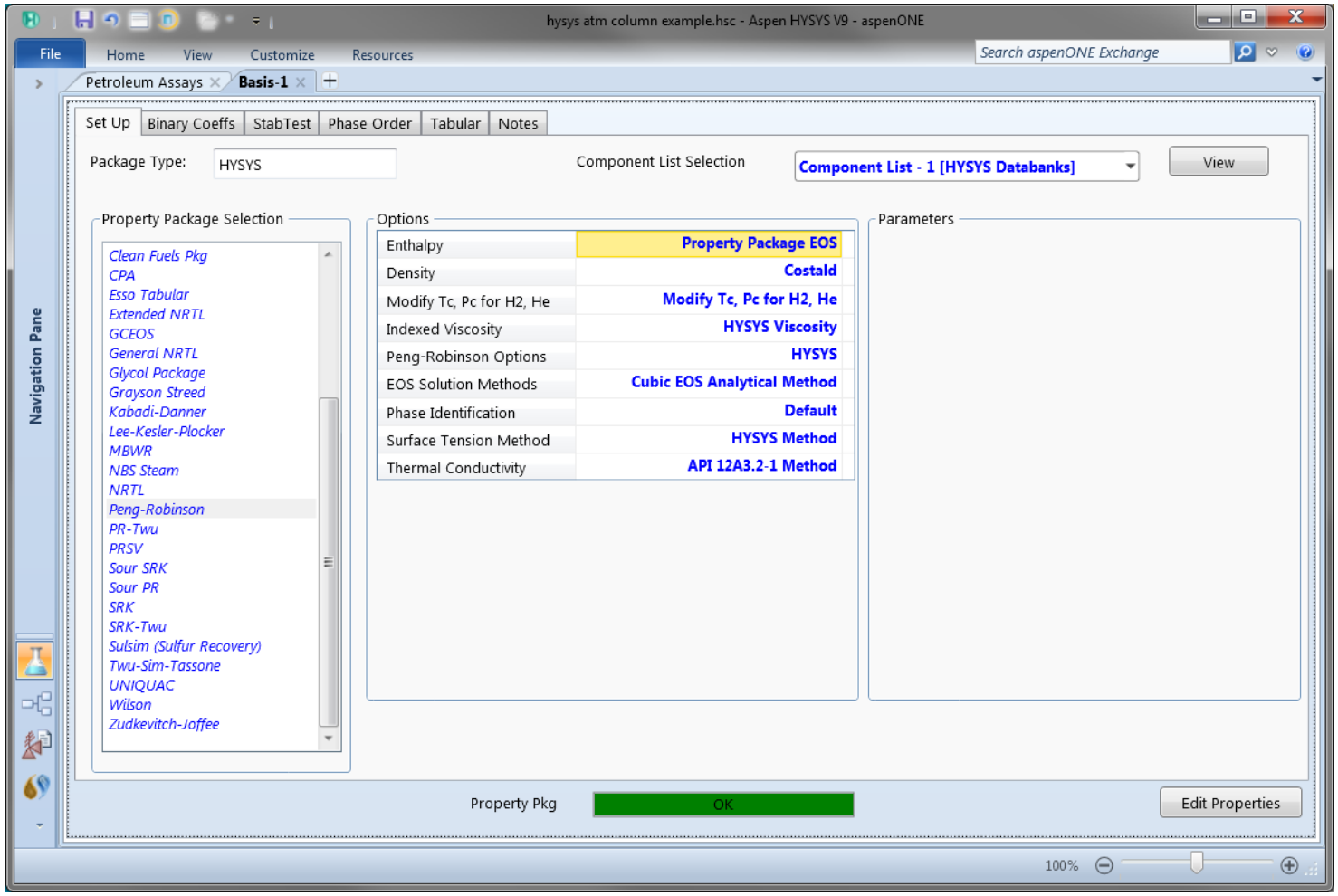
- Consistent properties for vapor, liquid, & transitions between
- Thermodynamic properties from the same set of equations
  - Equilibrium coefficients (fugacity)
  - Enthalpy
  - Entropy
  - Density
- Non-ideal behavior from binary interaction coefficients
  - Major effect on equilibrium coefficients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

May use other properties for other thermodynamic properties

- Lee-Kesler for enthalpy
- COSTALD for liquid density

Updated: July 5, 2017

Property Models & Methods

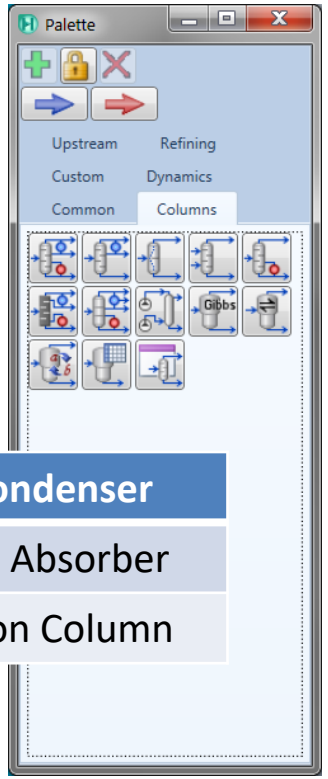


COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

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

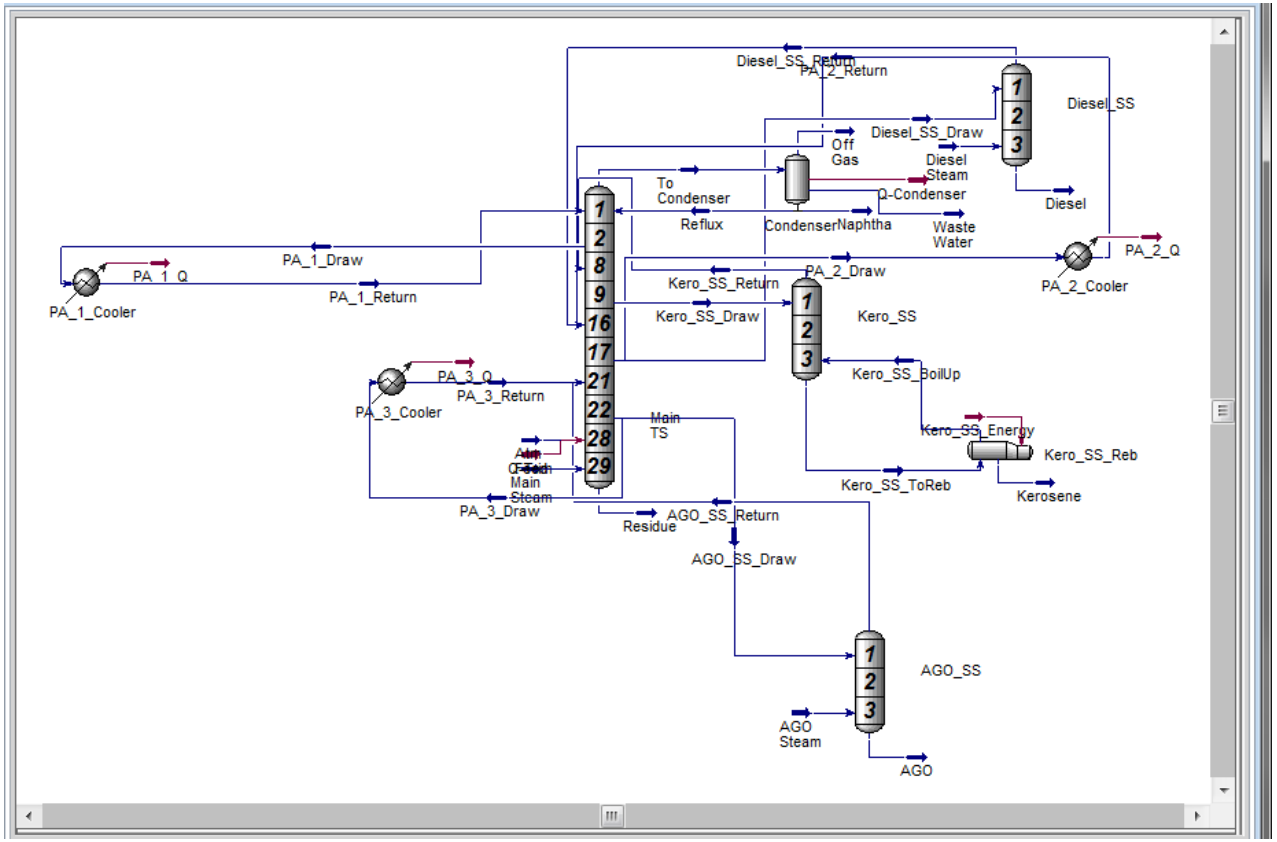
Updated: July 5, 2017

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Unit Operation Models for Refining

Complex tower configurations

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



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Typical Overall Efficiencies

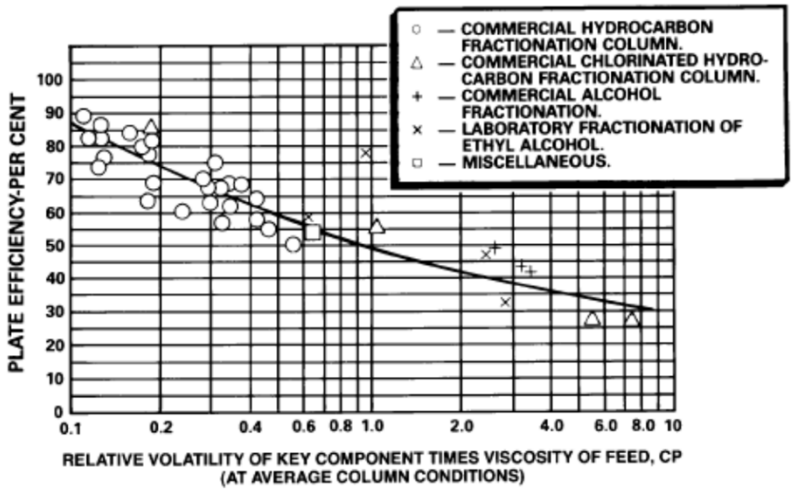
Column Service	Typical No. of Actual Trays	Typical Overall Efficiency	Typical No. of Theoretical Trays
Simple Absorber/Stripper	20 – 30	20 – 30	
Steam Side Stripper	5 – 7		2
Reboiled Side Stripper	7 – 10		3 – 4
Reboiled Absorber	20 – 40	40 – 50	
Deethanizer	25 – 35	65 – 75	
Depropanizer	35 – 40	70 – 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 – 1st draw	3 – 7	30	1 – 2
1st Draw – 2nd Draw	7 – 10	45 – 50	3 – 5
2nd Draw – 3rd 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

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

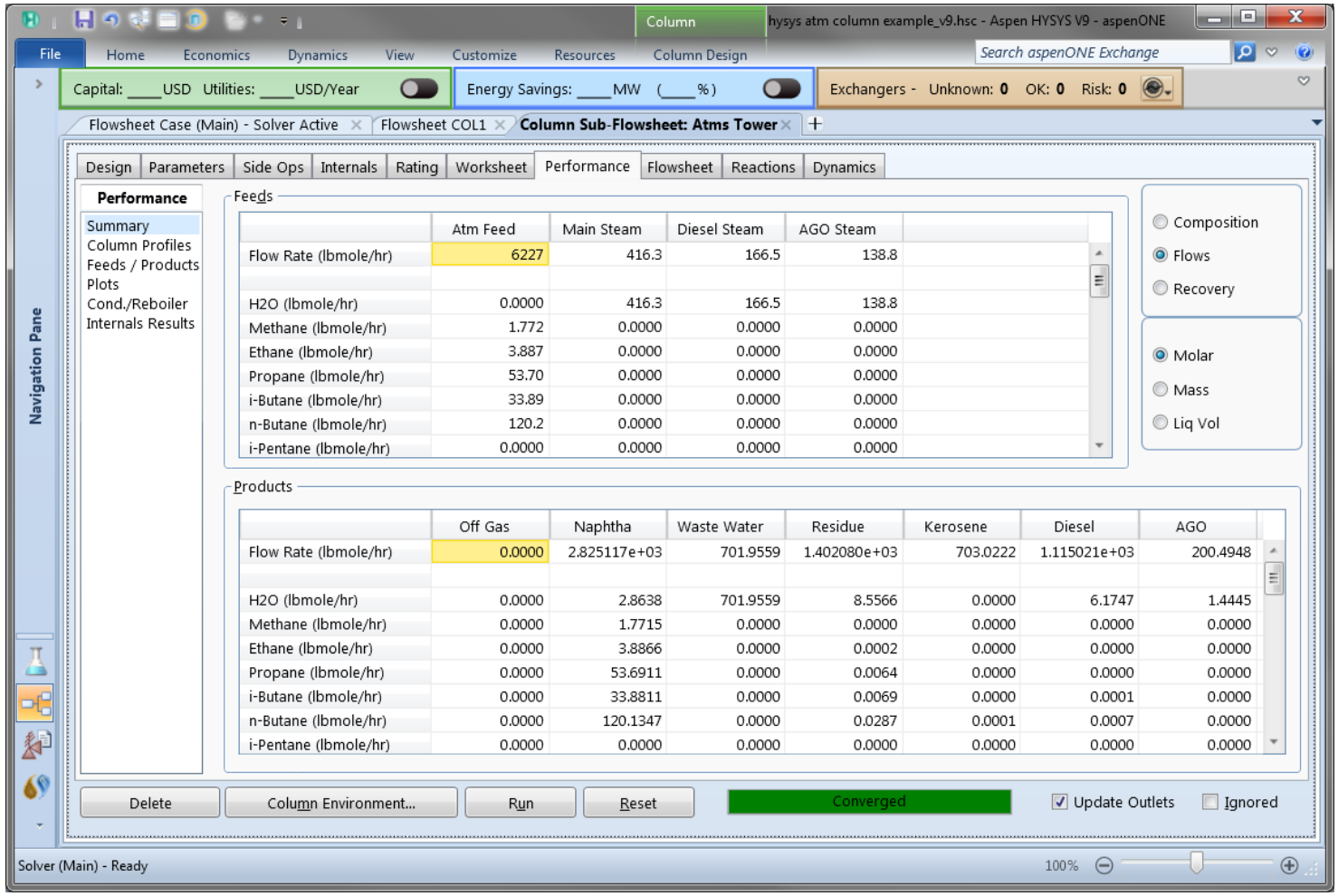
Rules of Thumb for Chemical Engineers, 4th ed.
Carl Branan, Gulf Professional Publishing, 2005

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



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Unit Operations Results

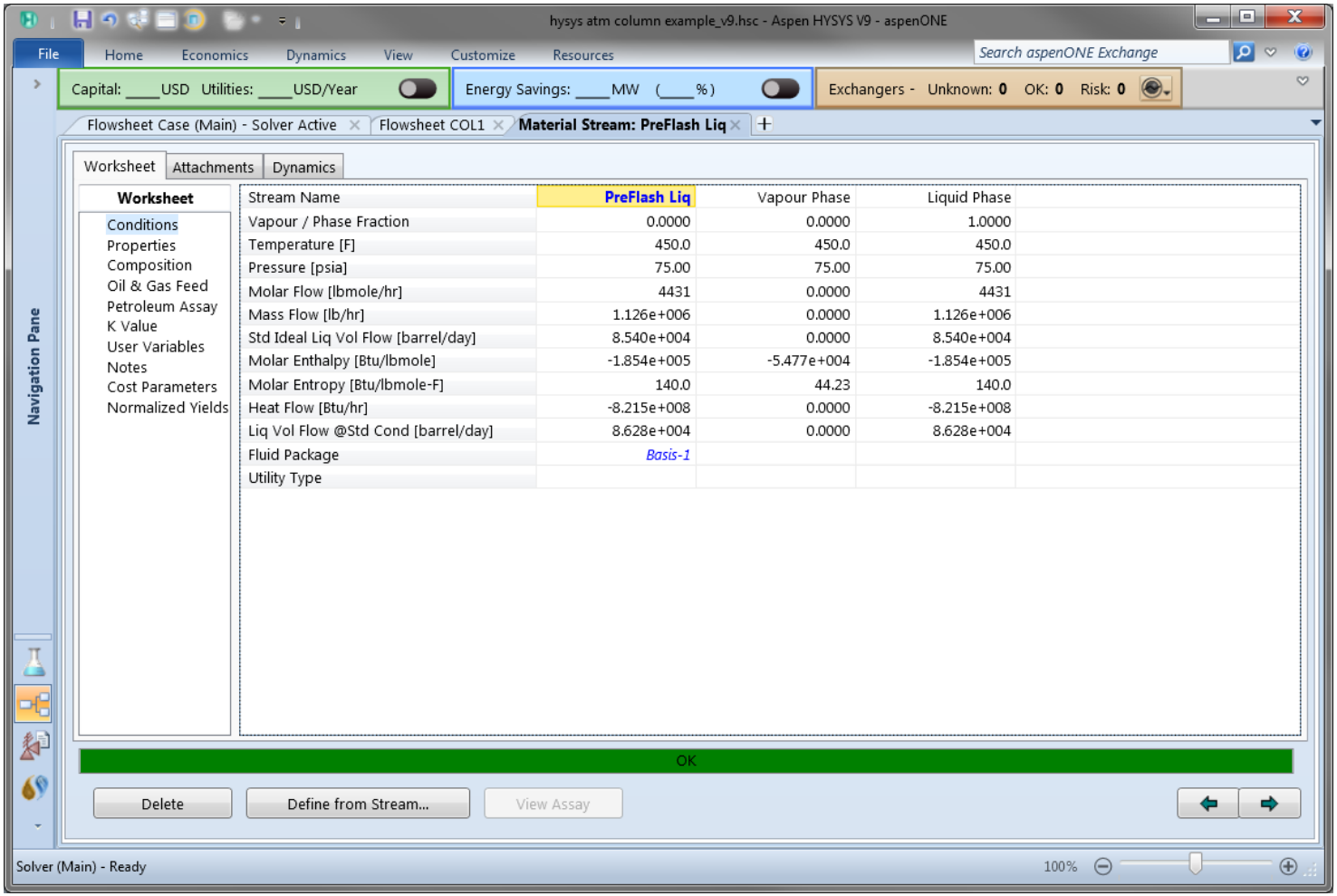


	Atm Feed	Main Steam	Diesel Steam	AGO Steam
Flow Rate (lbmole/hr)	6227	416.3	166.5	138.8
H2O (lbmole/hr)	0.0000	416.3	166.5	138.8
Methane (lbmole/hr)	1.772	0.0000	0.0000	0.0000
Ethane (lbmole/hr)	3.887	0.0000	0.0000	0.0000
Propane (lbmole/hr)	53.70	0.0000	0.0000	0.0000
i-Butane (lbmole/hr)	33.89	0.0000	0.0000	0.0000
n-Butane (lbmole/hr)	120.2	0.0000	0.0000	0.0000
i-Pentane (lbmole/hr)	0.0000	0.0000	0.0000	0.0000

	Off Gas	Naphtha	Waste Water	Residue	Kerosene	Diesel	AGO
Flow Rate (lbmole/hr)	0.0000	2.825117e+03	701.9559	1.402080e+03	703.0222	1.115021e+03	200.4948
H2O (lbmole/hr)	0.0000	2.8638	701.9559	8.5566	0.0000	6.1747	1.4445
Methane (lbmole/hr)	0.0000	1.7715	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane (lbmole/hr)	0.0000	3.8866	0.0000	0.0002	0.0000	0.0000	0.0000
Propane (lbmole/hr)	0.0000	53.6911	0.0000	0.0064	0.0000	0.0000	0.0000
i-Butane (lbmole/hr)	0.0000	33.8811	0.0000	0.0069	0.0000	0.0001	0.0000
n-Butane (lbmole/hr)	0.0000	120.1347	0.0000	0.0287	0.0001	0.0007	0.0000
i-Pentane (lbmole/hr)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

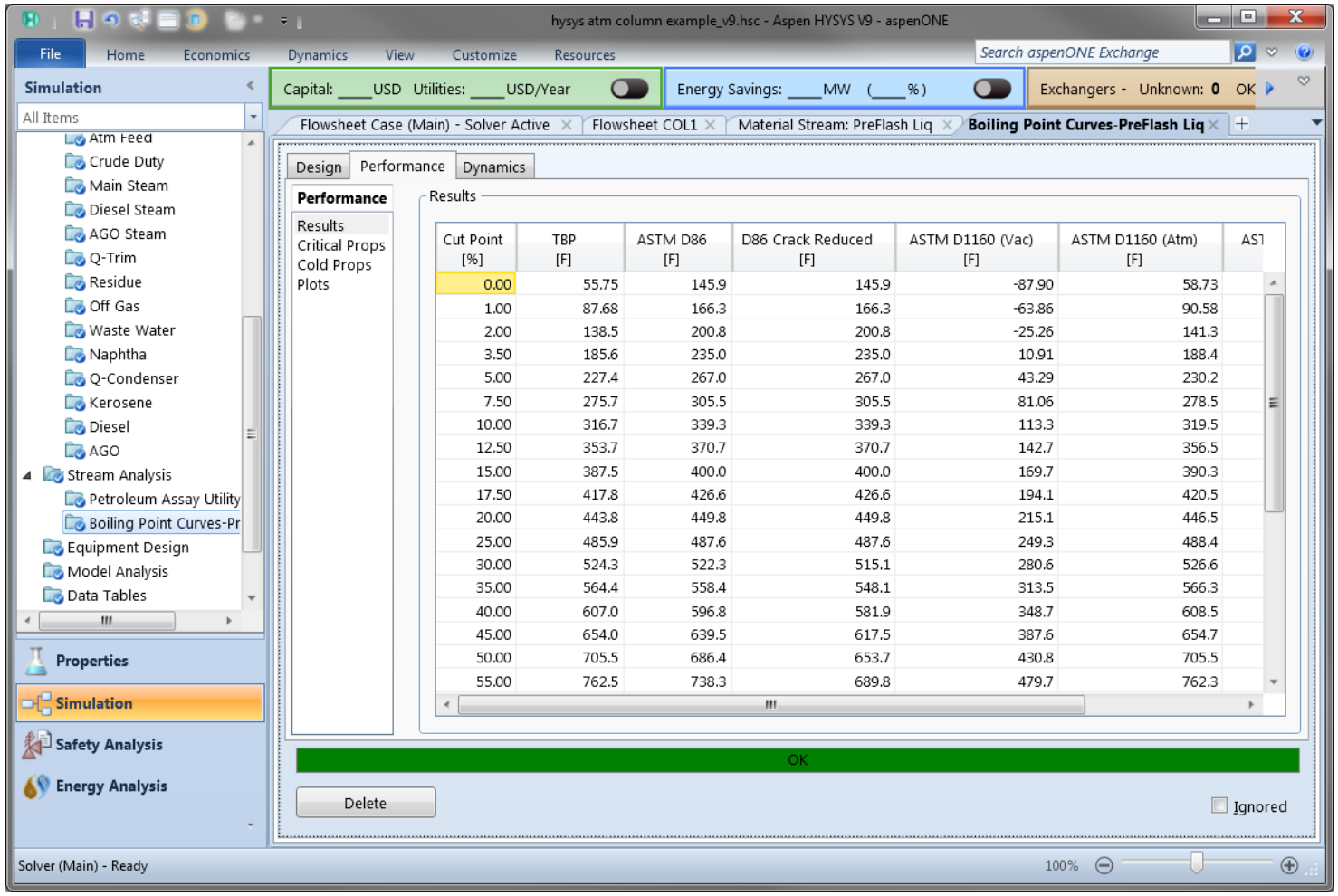
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Stream Results



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Specialized Stream Reports



Updated: July 5, 2017

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

User Interface

Graphically build the flowsheet by dragging & dropping unit models

Calculations performed automatically as information is entered

Copy & paste capabilities

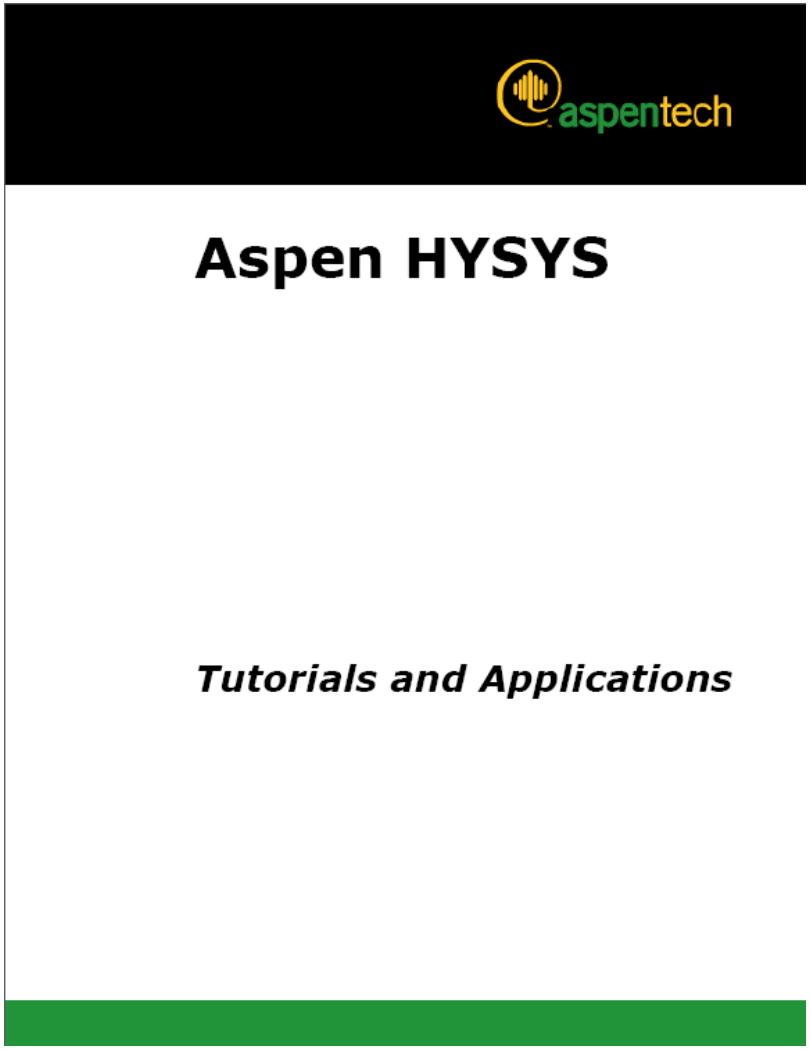
- Pasting in from other locations limited

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.



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

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

Updated: July 5, 2017