Process Engineering Simulation with Aspen Plus

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

Aspen Plus as Process Engineering Tool

Owned & marketed by Aspen Tech

- Developed as DOE-funded project at MIT in late 1970s
- Aspen Tech formed to market program
- Aspen Tech grown over years through development & acquisitions
  - HYSYS purchased from Hyprotech.

Core calculations for steady state mass & energy balances

- Dynamic capabilities as add-on package

Historical orientation towards chemical & synthetic fuels industry. Capabilities added for the oil & gas industry

- Components
  - Extensive pure component database of hydrocarbons & other compounds
  - 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

Composition

Pure component database

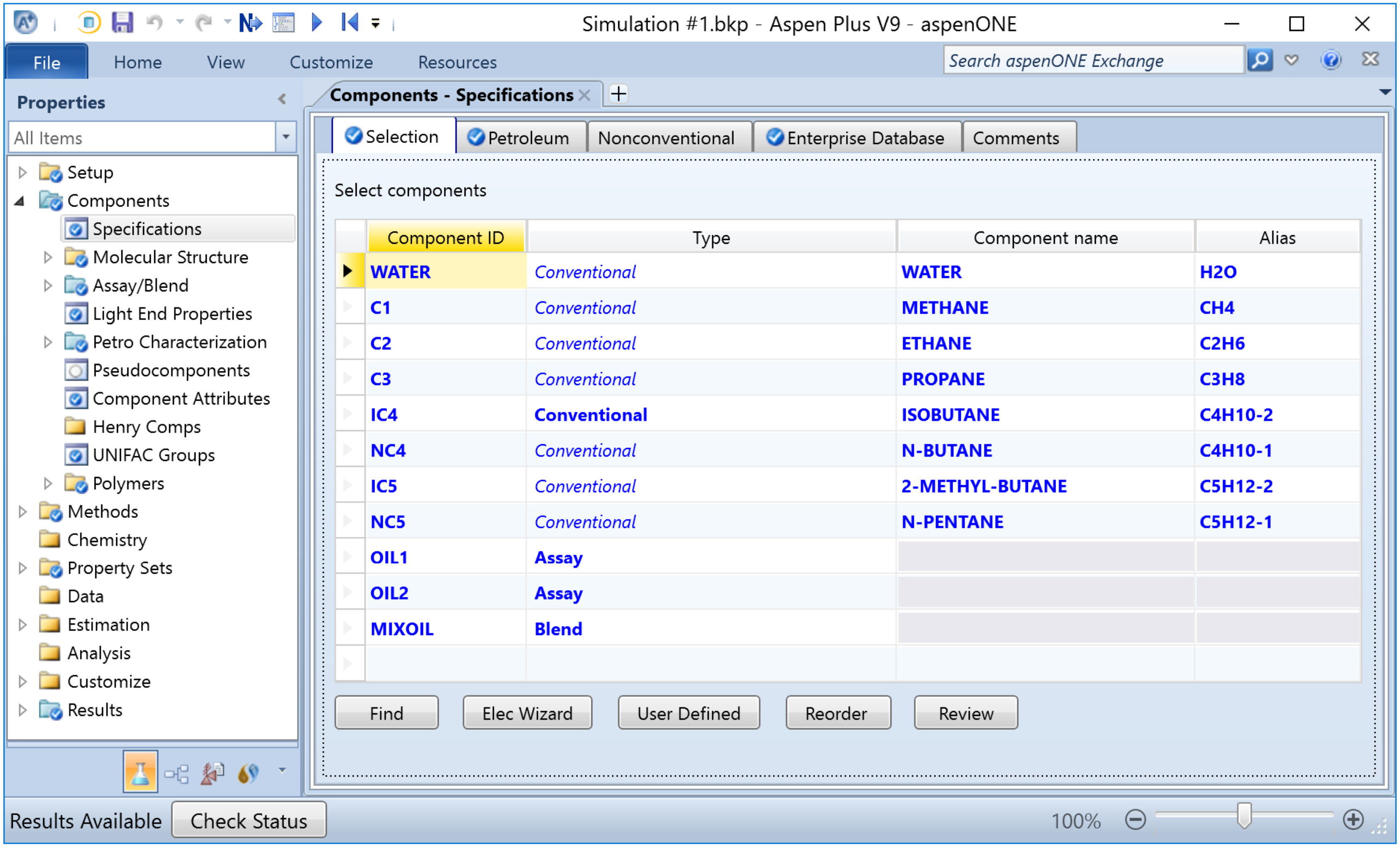
- Typically use a small number of light hydrocarbons (C_1 – nC_5), CO_2, H_2S, & H_2O

Pseudo/hypothetical components

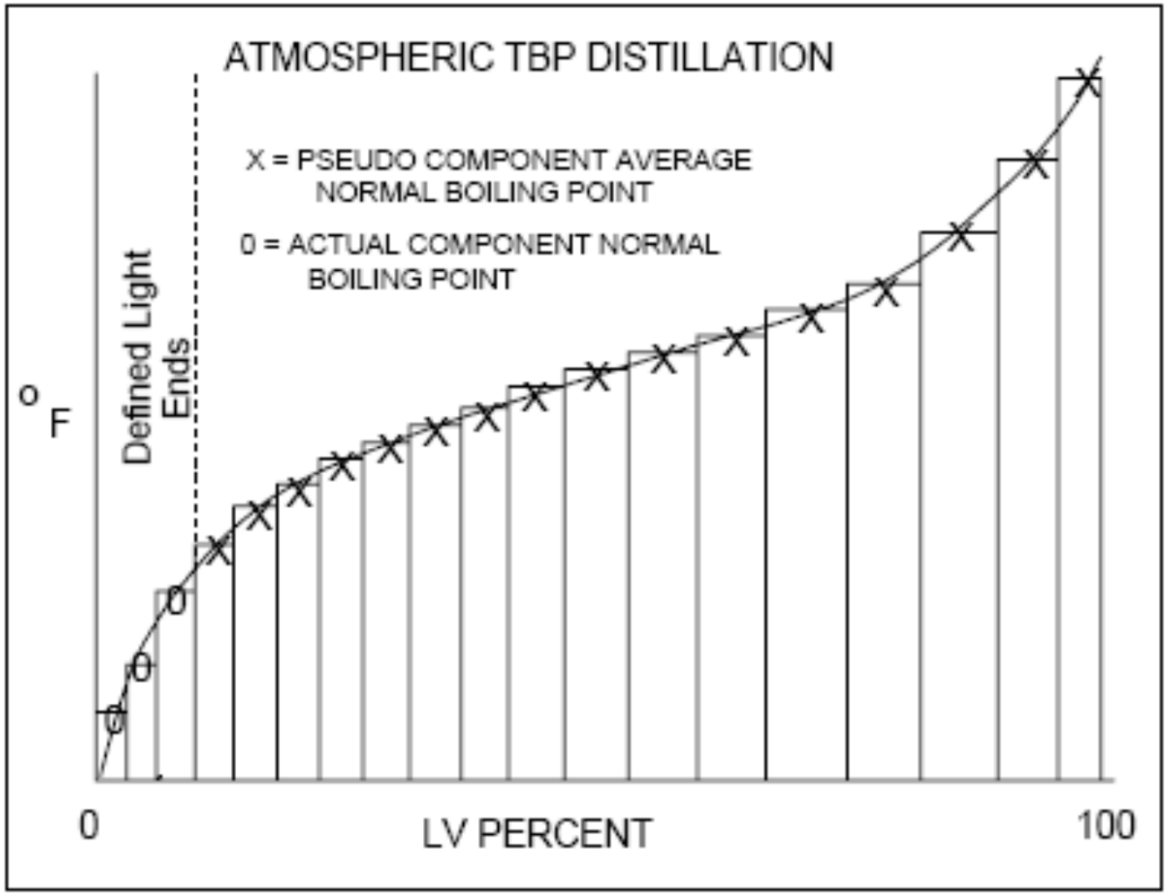
- Narrow boiling point fractions from distillation analysis
- Assumption that all components in range will have the same split between vapor & liquid
  - Not a good assumption if chemical structure plays a big part in separation or reaction
- Correlations to generate "average" properties for the fraction
  - 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



Pseudo Components from Assay



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

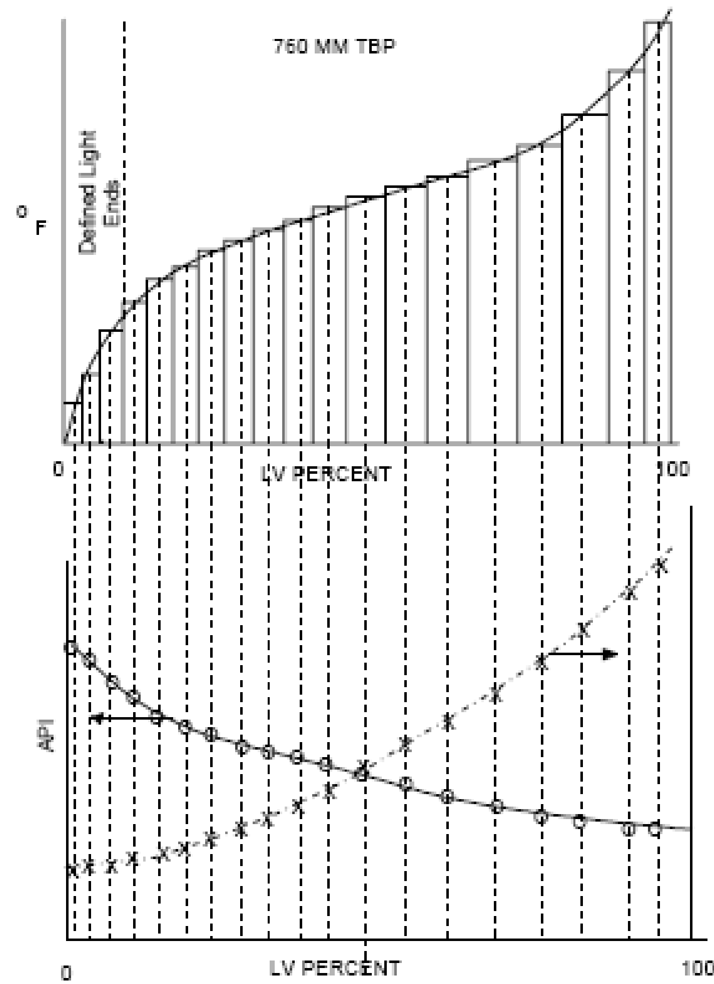
Pseudo Components from Assay

Split the yield curve into boiling point ranges

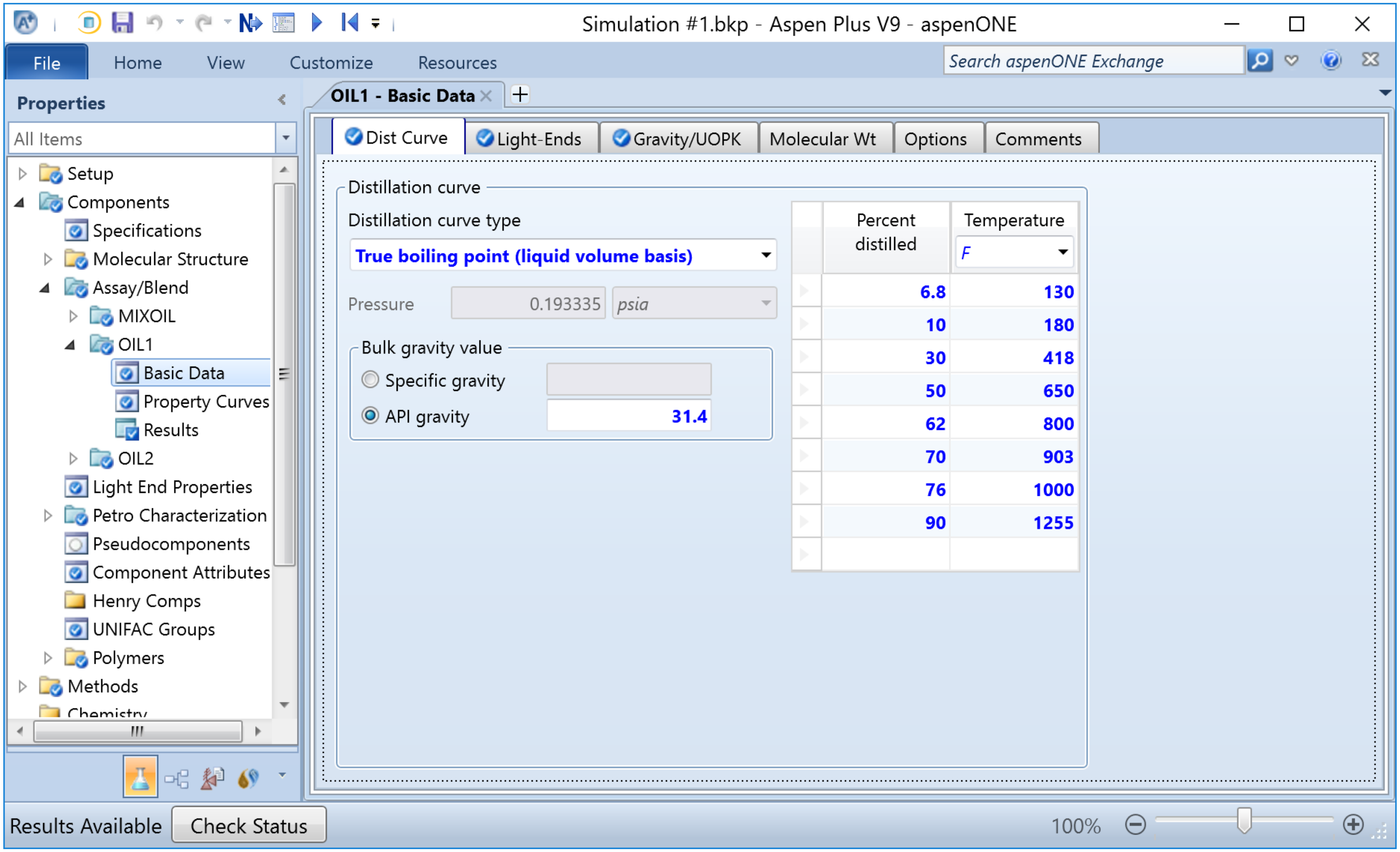
Use the property curves to generate consistent with measured data

Use correlations to estimate unmeasured & unmeasurable properties

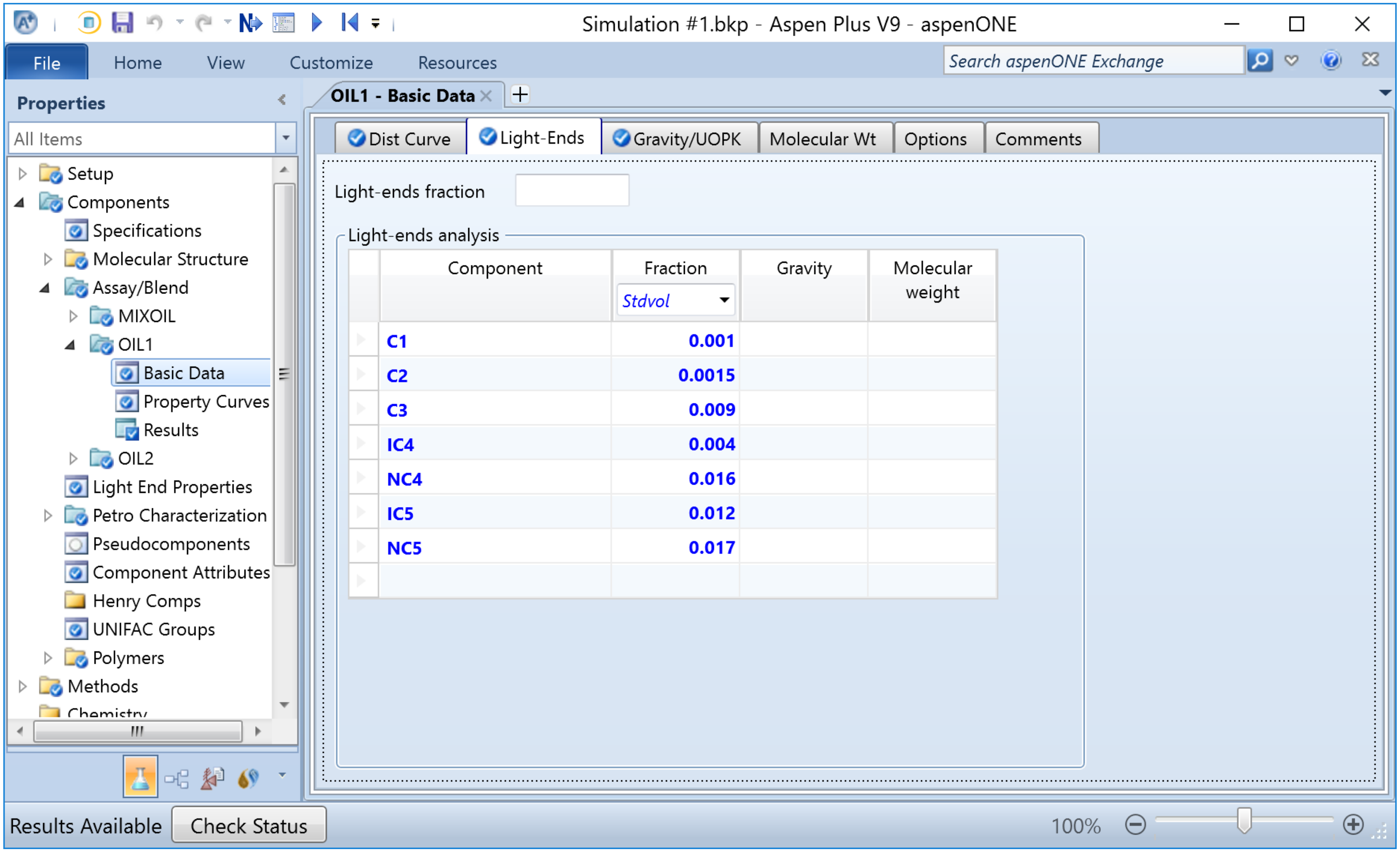
- Critical properties
- Accentric factor
- Binary interaction coefficients



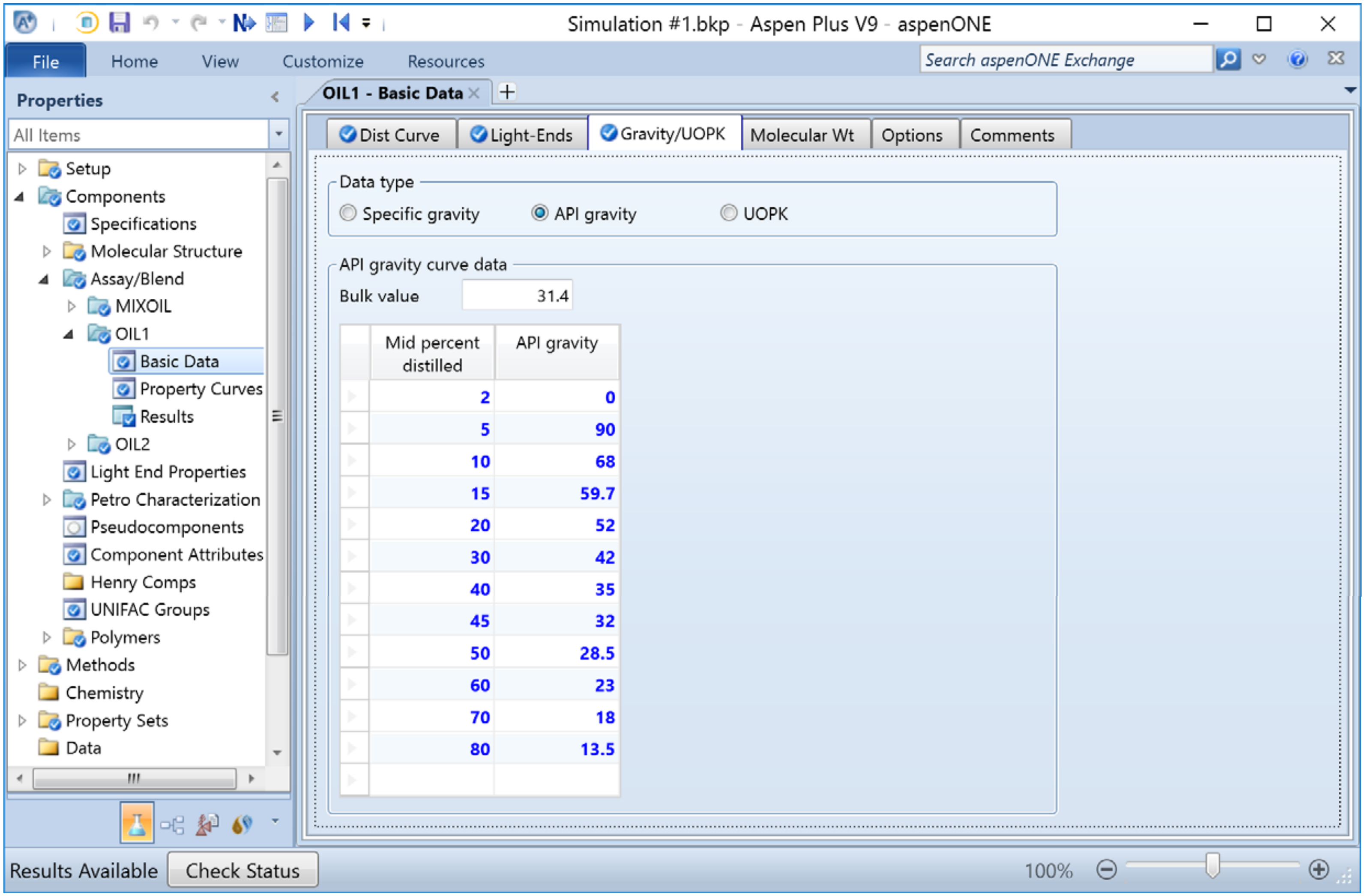
Pseudo Components from Assay



Pseudo Components from Assay



Pseudo Components from Assay



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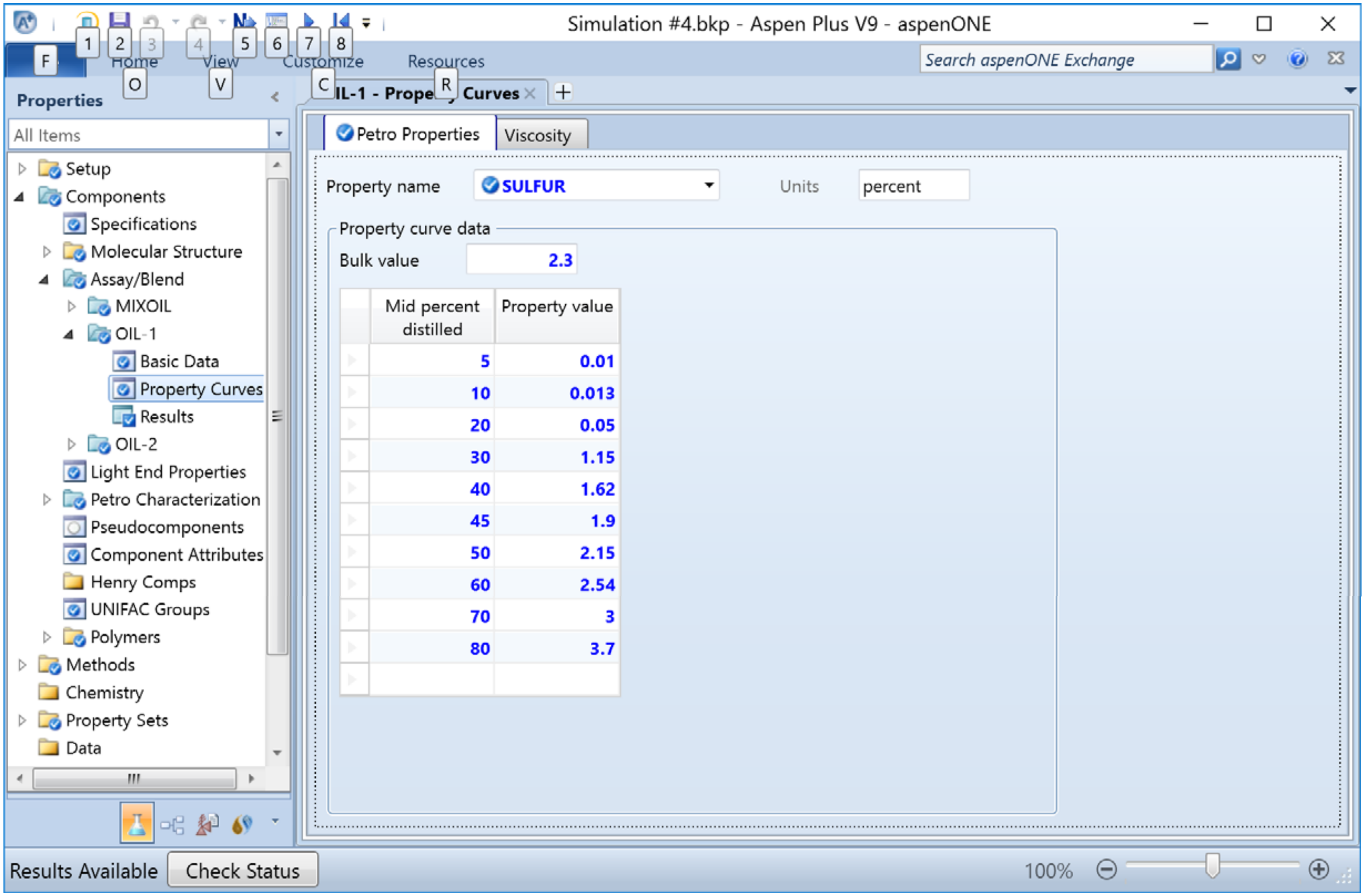
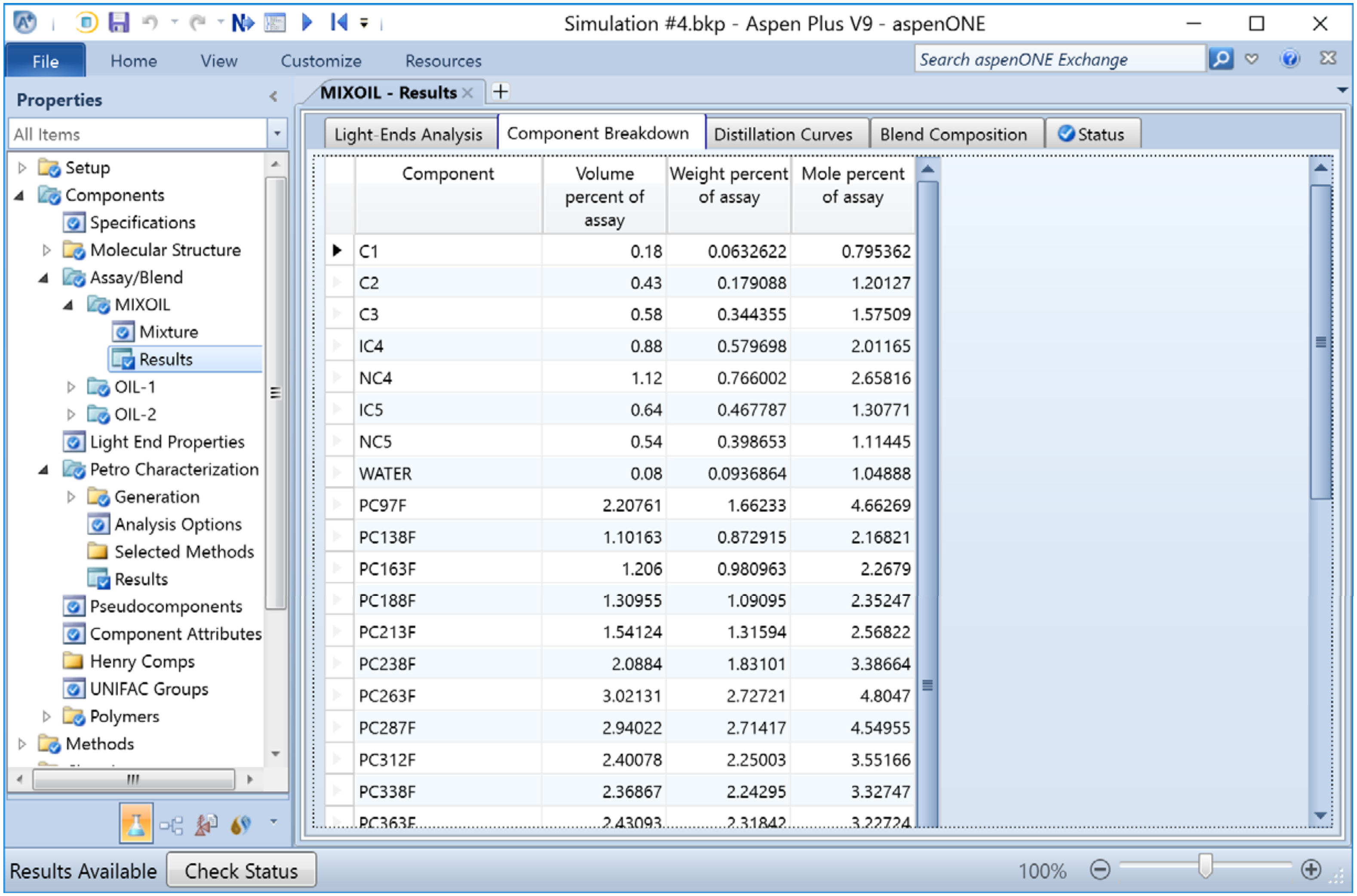
Pseudo Components from Assay



Pseudo Components from Assay



Component	Volume percent of assay	Weight percent of assay	Mole percent of assay
C1	0.18	0.0632622	0.795362
C2	0.43	0.179088	1.20127
C3	0.58	0.344355	1.57509
IC4	0.88	0.579698	2.01165
NC4	1.12	0.766002	2.65816
IC5	0.64	0.467787	1.30771
NC5	0.54	0.398653	1.11445
WATER	0.08	0.0936864	1.04888
PC97F	2.20761	1.66233	4.66269
PC138F	1.10163	0.872915	2.16821
PC163F	1.206	0.980963	2.2679
PC188F	1.30955	1.09095	2.35247
PC213F	1.54124	1.31594	2.56822
PC238F	2.0884	1.83101	3.38664
PC263F	3.02131	2.72721	4.8047
PC287F	2.94022	2.71417	4.54955
PC312F	2.40078	2.25003	3.55166
PC338F	2.36867	2.24295	3.32747
PC363F	2.43093	2.31842	3.22724

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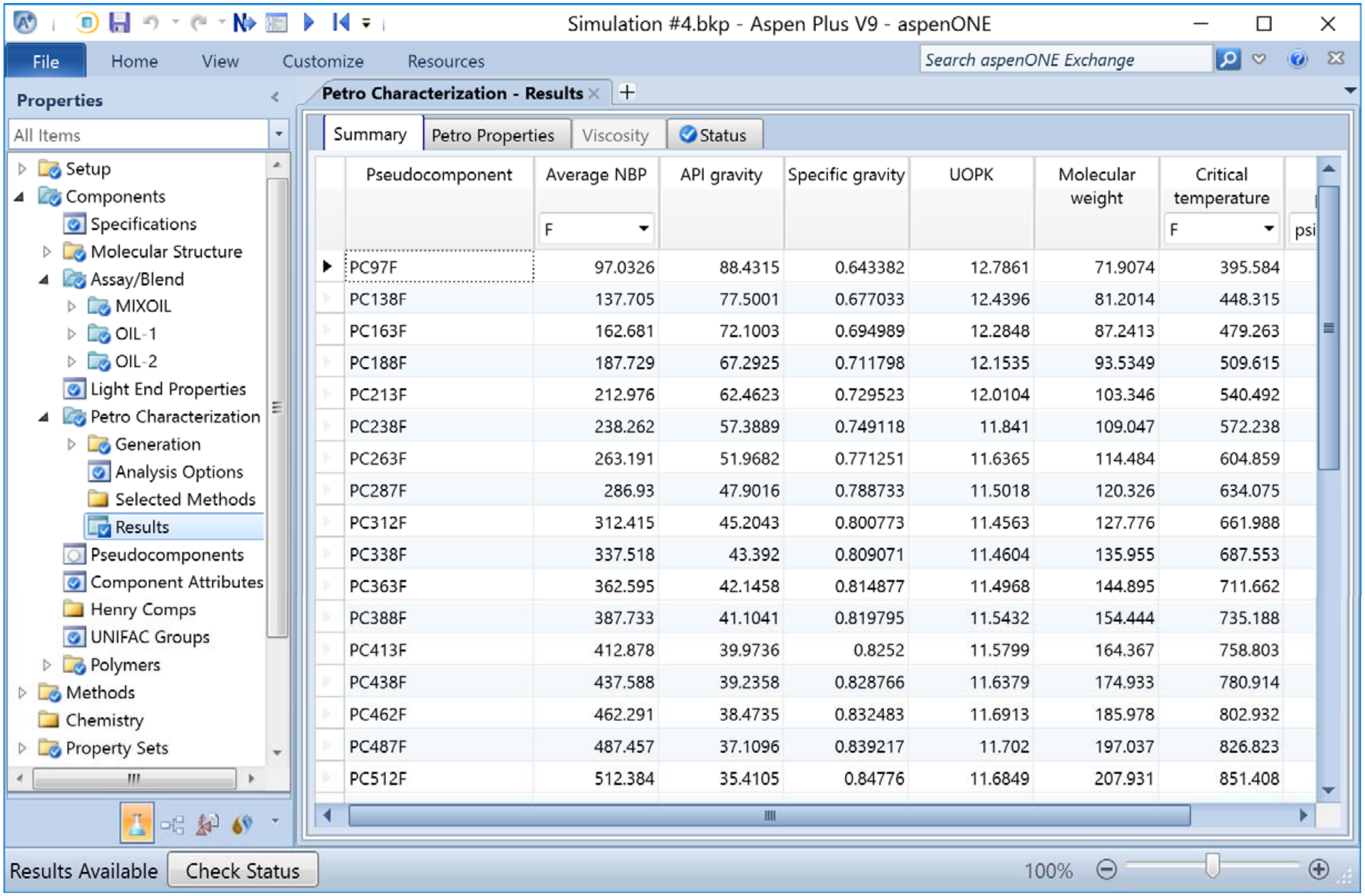
Pseudo Components from Assay



Pseudocomponent	Average NBP (F)	API gravity	Specific gravity	UOPK	Molecular weight	Critical temperature (F)
PC97F	97.0326	88.4315	0.643382	12.7861	71.9074	395.584
PC138F	137.705	77.5001	0.677033	12.4396	81.2014	448.315
PC163F	162.681	72.1003	0.694989	12.2848	87.2413	479.263
PC188F	187.729	67.2925	0.711798	12.1535	93.5349	509.615
PC213F	212.976	62.4623	0.729523	12.0104	103.346	540.492
PC238F	238.262	57.3889	0.749118	11.841	109.047	572.238
PC263F	263.191	51.9682	0.771251	11.6365	114.484	604.859
PC287F	286.93	47.9016	0.788733	11.5018	120.326	634.075
PC312F	312.415	45.2043	0.800773	11.4563	127.776	661.988
PC338F	337.518	43.392	0.809071	11.4604	135.955	687.553
PC363F	362.595	42.1458	0.814877	11.4968	144.895	711.662
PC388F	387.733	41.1041	0.819795	11.5432	154.444	735.188
PC413F	412.878	39.9736	0.8252	11.5799	164.367	758.803
PC438F	437.588	39.2358	0.828766	11.6379	174.933	780.914
PC462F	462.291	38.4735	0.832483	11.6913	185.978	802.932
PC487F	487.457	37.1096	0.839217	11.702	197.037	826.823
PC512F	512.384	35.4105	0.84776	11.6849	207.931	851.408

Property Models & Methods

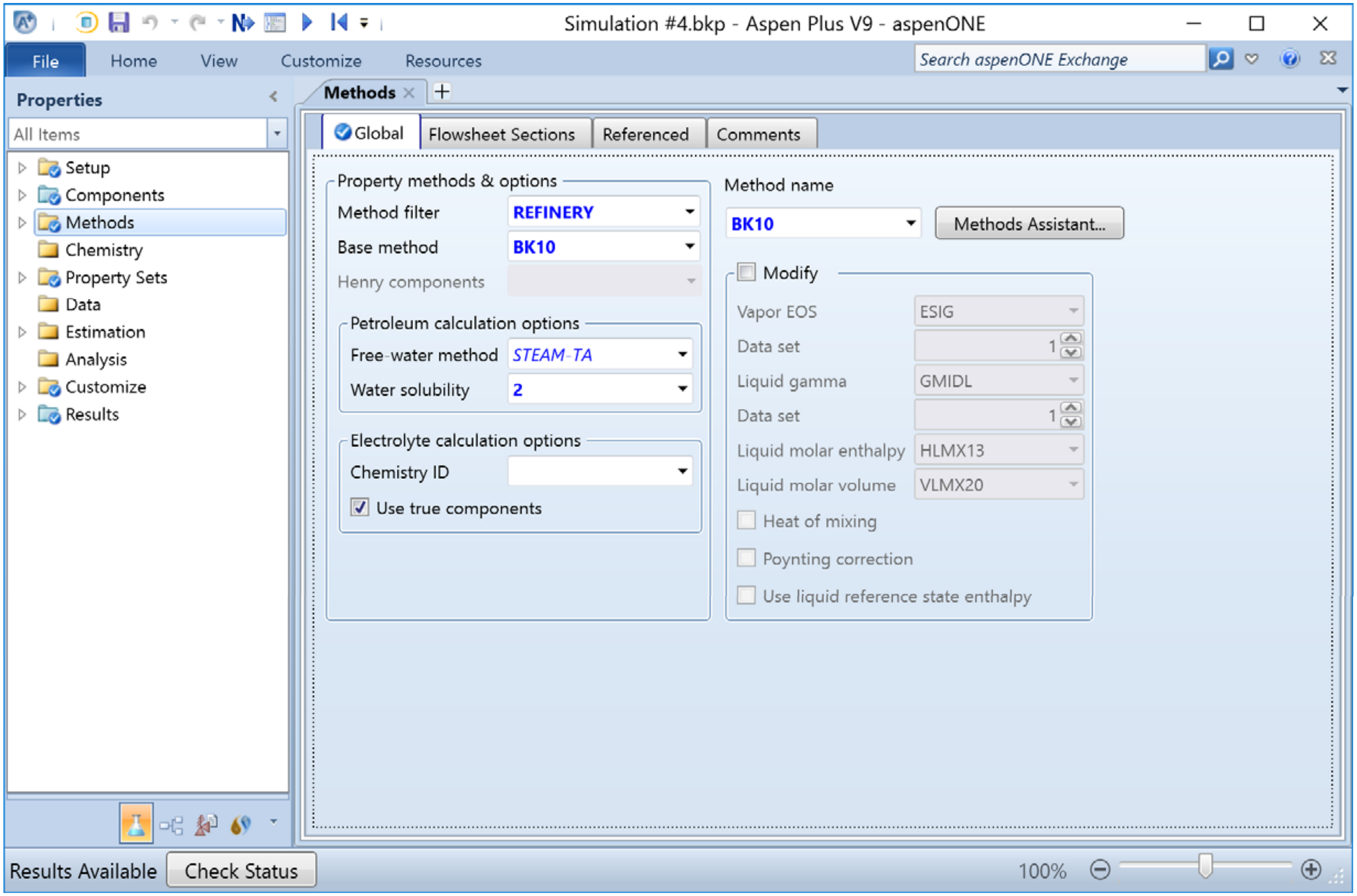
Typically use an equation of state (EOS) for properties

- 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



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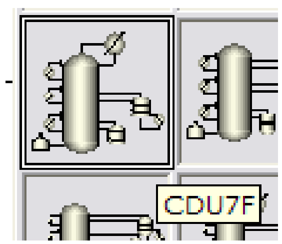
Unit Operation Models

"Typical" unit operation models

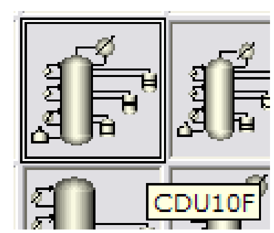
- Valve
- Separators
- Heat exchangers
- Pumps
- Compressors
- Reactors – CSTR & plug flow

Towers – multiple configurations & solution techniques

- DSTWU
- RADFRAC
- PETROFRAC
  - CDU7F



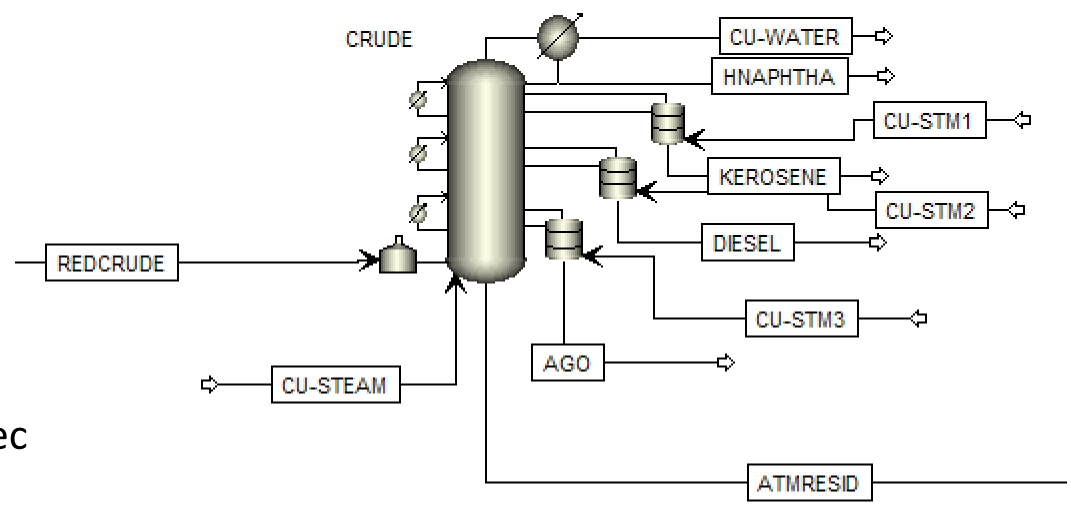
  - CDU10F



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

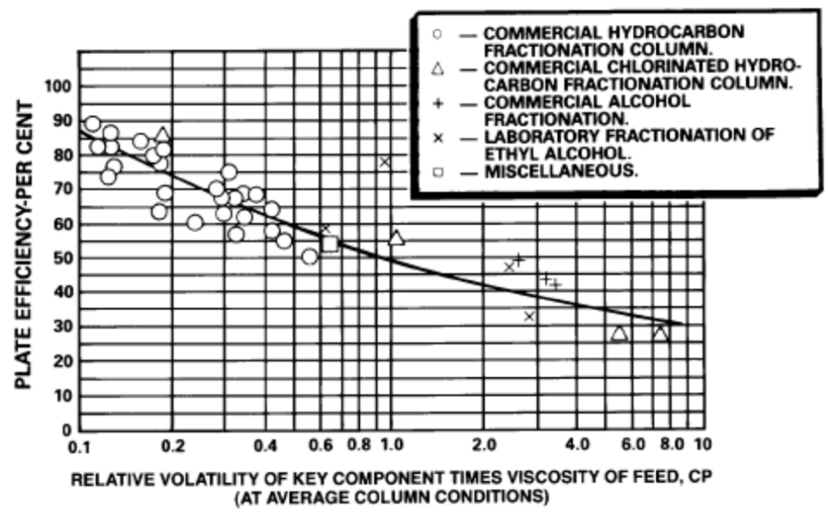
Column Service	Typical No. of Actual Trays	Typical Overall Efficiency	Typical No. of Theoretical Trays
Simple Absorber/Stripper	20 – 30	20 – 30	
Steam Side Stripper	5 – 7		2
Reboiled Side Stripper	7 – 10		3 – 4
Reboiled Absorber	20 – 40	40 – 50	
Deethanizer	25 – 35	65 – 75	
Depropanizer	35 – 40	70 –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

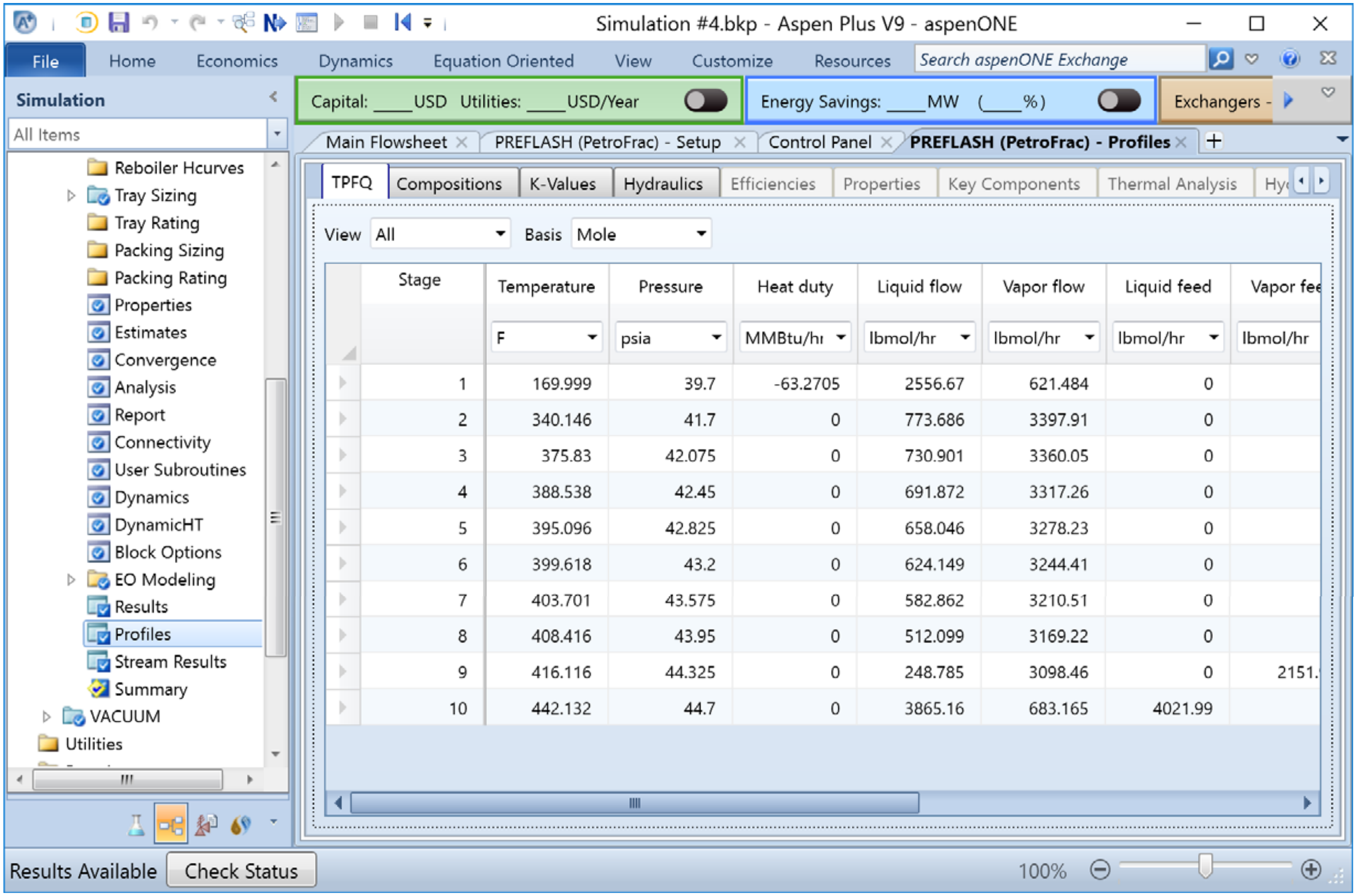
Viscosity	Maxwell	Drickamer & Bradford in Ludwig
cP	Ave Viscosity of liquid on plates	Molal Ave Viscosity of Feed
0.05	…	98
0.10	104	79
0.15	86	70
0.20	76	60
0.30	63	50
0.40	56	42
0.50	50	36
0.60	46	31
0.70	43	27
0.80	40	23
0.90	38	19
1.00	36	17
1.50	30	7
1.70	28	5

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

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



Unit Operations Results



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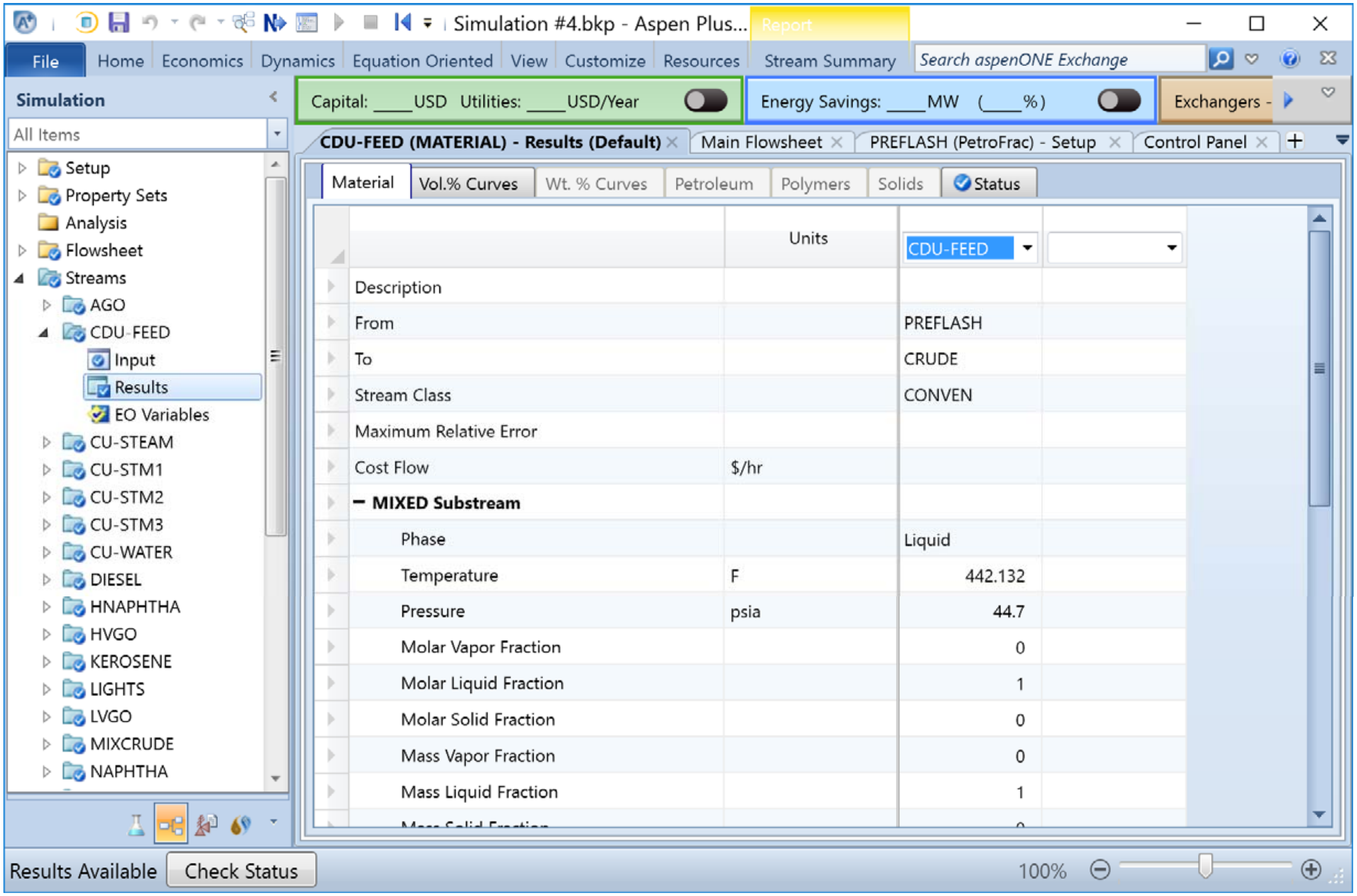
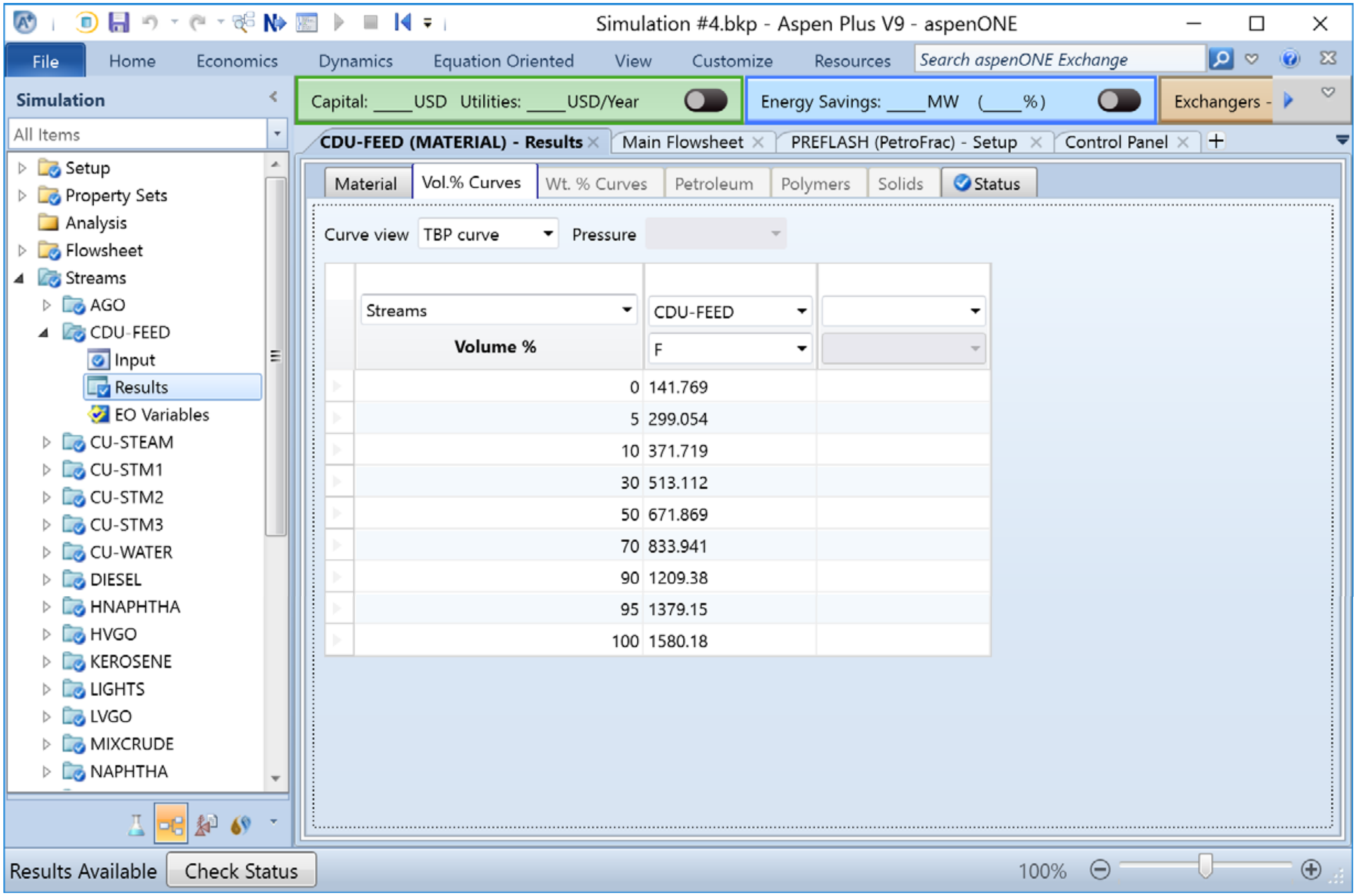
Stream Results



Specialized Stream Reports



User Interface

Graphically build the flowsheet by dragging & dropping unit models

Calculations performed automatically as information is entered

Copy & paste capabilities

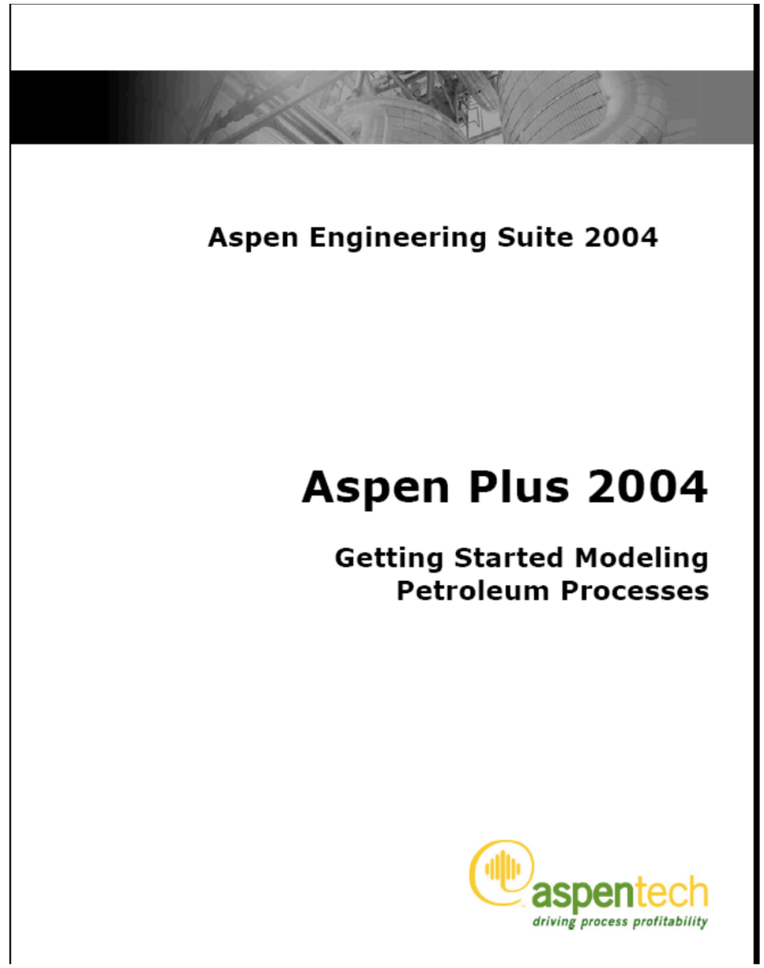
Aspen Simulation Workbook extends capabilities to put custom interface on top of simulation

Aspen Plus crude tower example

From Aspen Tech web site

- Copied to class web site

Additional problem developed specifically for this class.


Aspen Engineering Suite 2004

Aspen Plus 2004

Getting Started Modeling
Petroleum Processes

aspentech
driving process profitability

Summary

Aspen Plus 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 propert 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