

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 – 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

Simulation #1.bkp - Aspen Plus V9 - aspenONE

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Properties

All Items

- Setup
- Components
 - Specifications
 - Molecular Structure
 - Assay/Blend
 - Light End Properties
 - Petro Characterization
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
 - UNIFAC Groups
 - Polymers
- Methods
 - Chemistry
- Property Sets
 - Data
- Estimation
 - Analysis
- Customize
- Results

Components - Specifications

Selection Petroleum Nonconventional Enterprise Database Comments

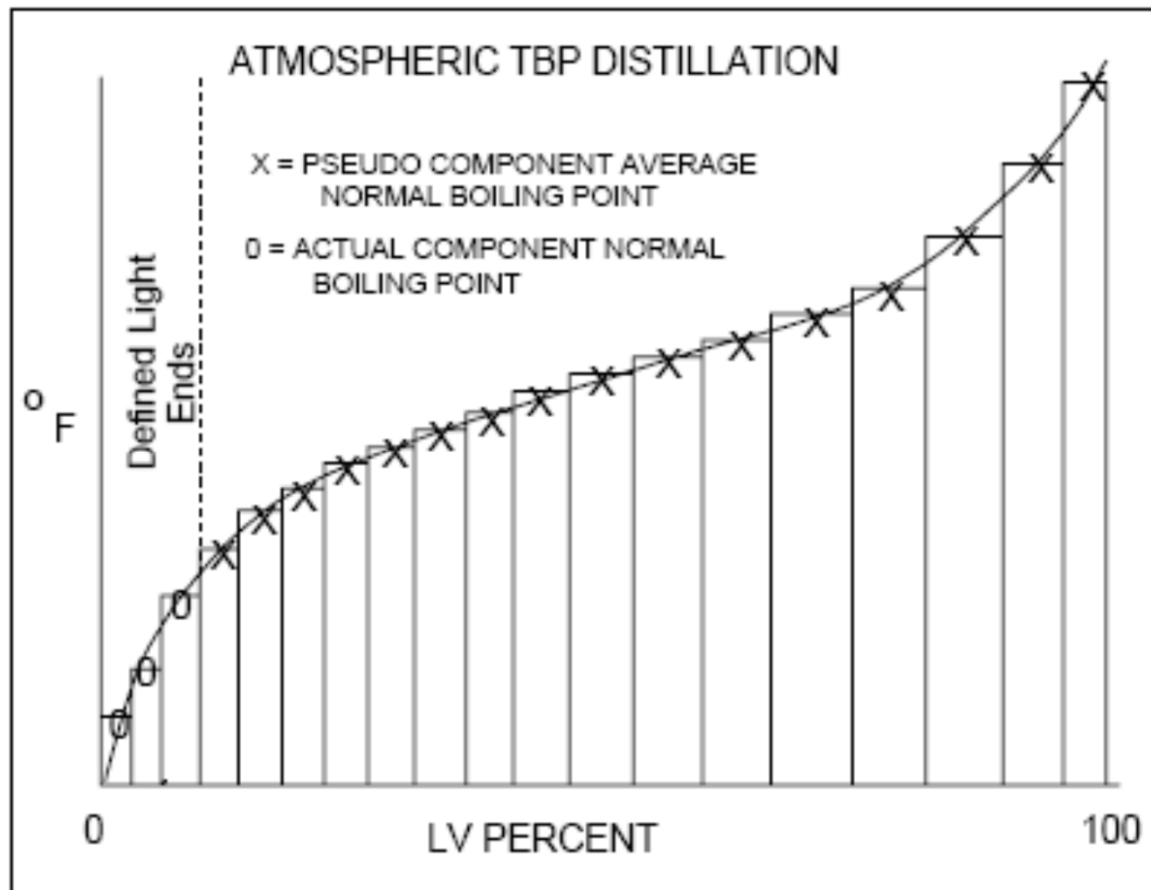
Select components

| Component ID | Type | Component name | Alias |
|--------------|--------------|-----------------|---------|
| WATER | Conventional | WATER | H2O |
| C1 | Conventional | METHANE | CH4 |
| C2 | Conventional | ETHANE | C2H6 |
| C3 | Conventional | PROPANE | C3H8 |
| IC4 | Conventional | ISOBUTANE | C4H10-2 |
| NC4 | Conventional | N-BUTANE | C4H10-1 |
| IC5 | Conventional | 2-METHYL-BUTANE | C5H12-2 |
| NC5 | Conventional | N-PENTANE | C5H12-1 |
| OIL1 | Assay | | |
| OIL2 | Assay | | |
| MIXOIL | Blend | | |

Find Elec Wizard User Defined Reorder Review

Results Available Check Status 100%

Pseudo Components from Assay



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

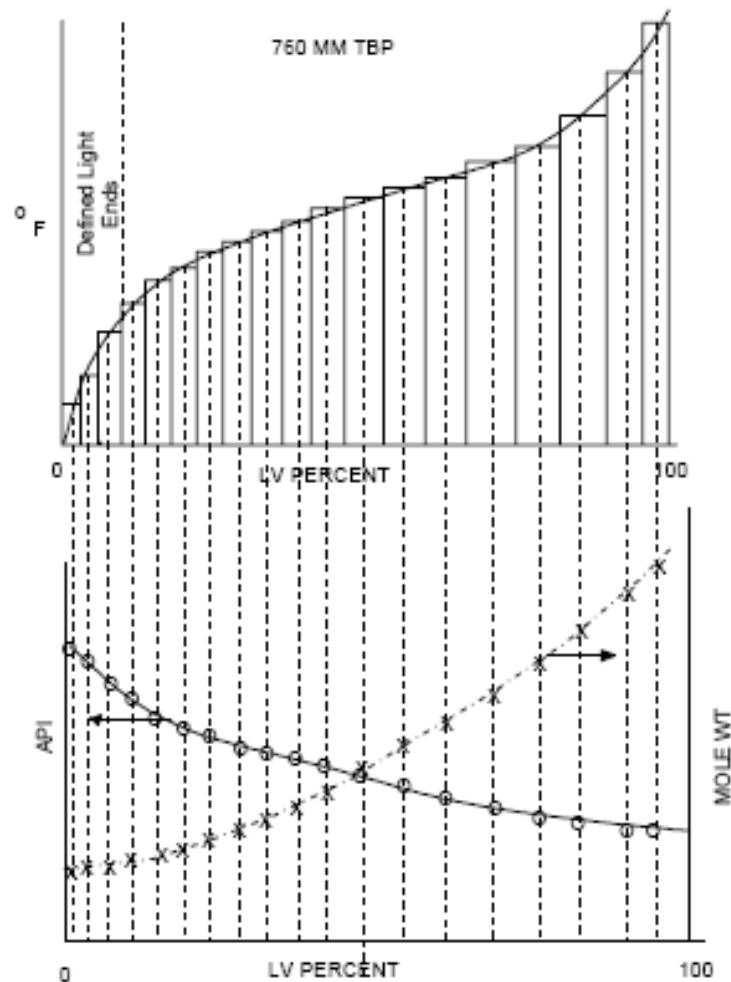
Pseudo Components from Assay

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



Pseudo Components from Assay

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Properties

All Items

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 - Assay/Blend
 - MIXOIL
 - OIL1
 - Basic Data**
 - Property Curves
 - Results
 - OIL2
 - Light End Properties
 - Petro Characterization
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
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 - Polymers
 - Methods
 - Chemistry

OIL1 - Basic Data

☒ Dist Curve ☒ Light-Ends ☒ Gravity/UOPK Molecular Wt Options Comments

Distillation curve

Distillation curve type
True boiling point (liquid volume basis)

Pressure 0.193335 psia

Bulk gravity value

☐ Specific gravity

☒ API gravity 31.4

| Percent distilled | Temperature F |
|-------------------|------------------|
| 6.8 | 130 |
| 10 | 180 |
| 30 | 418 |
| 50 | 650 |
| 62 | 800 |
| 70 | 903 |
| 76 | 1000 |
| 90 | 1255 |

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Pseudo Components from Assay

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Properties

All Items

- Setup
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 - Methods
 - Chemistry

OIL1 - Basic Data

Dist Curve Light-Ends Gravity/UOPK Molecular Wt Options Comments

Light-ends fraction

Light-ends analysis

| Component | Fraction <i>Stdvol</i> | Gravity | Molecular weight |
|-----------|---------------------------|---------|------------------|
| C1 | 0.001 | | |
| C2 | 0.0015 | | |
| C3 | 0.009 | | |
| IC4 | 0.004 | | |
| NC4 | 0.016 | | |
| IC5 | 0.012 | | |
| NC5 | 0.017 | | |

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Pseudo Components from Assay

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Properties

All Items

- Setup
- Components
 - Specifications
 - Molecular Structure
 - Assay/Blend
 - MIXOIL
 - OIL1
 - Basic Data
 - Property Curves
 - Results
 - OIL2
 - Light End Properties
 - Petro Characterization
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
 - UNIFAC Groups
 - Polymers
 - Methods
 - Chemistry
 - Property Sets
 - Data

OIL1 - Basic Data

Dist Curve Light-Ends Gravity/UOPK Molecular Wt Options Comments

Data type

☐ Specific gravity ☒ API gravity ☐ UOPK

API gravity curve data

Bulk value 31.4

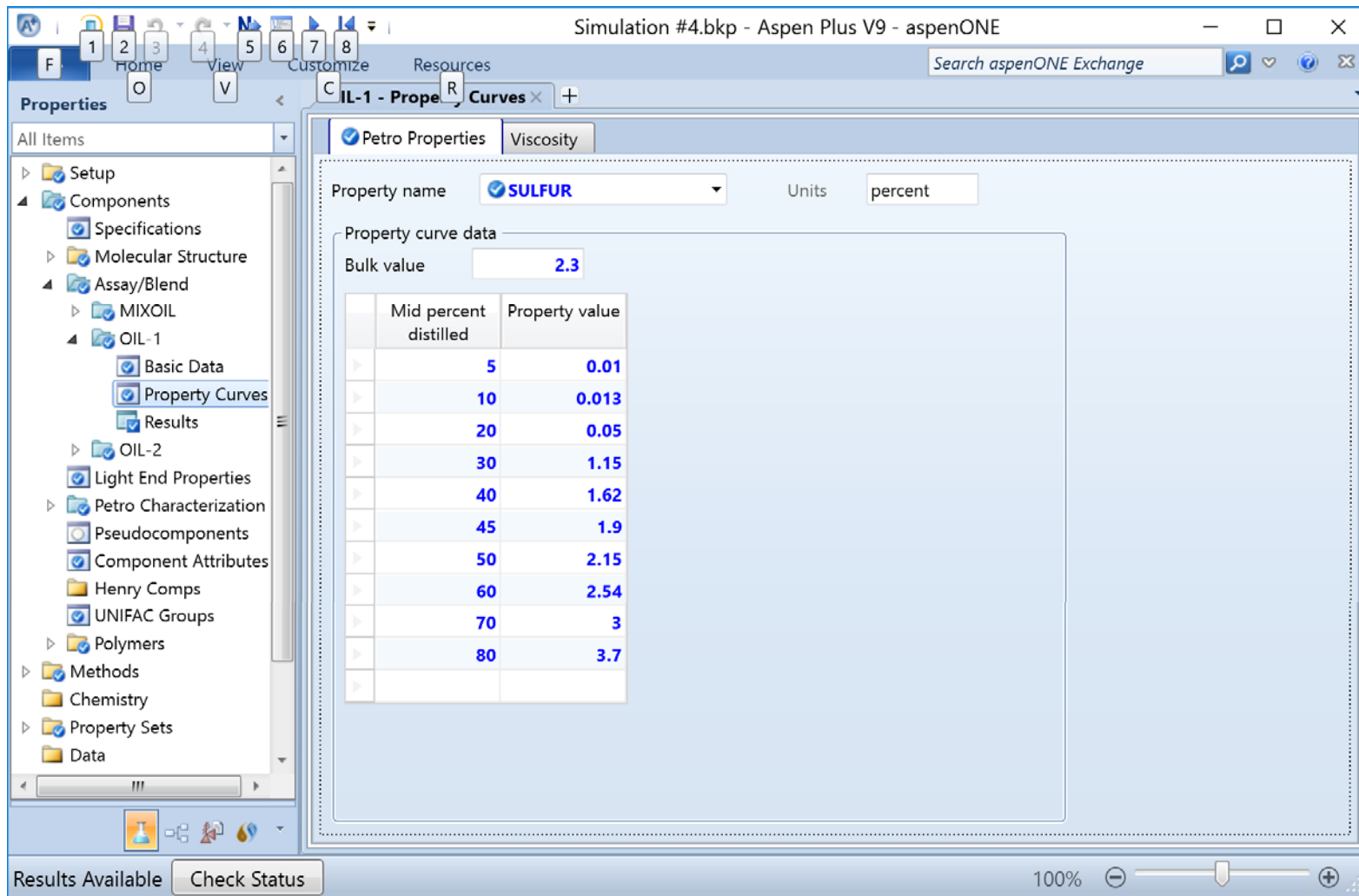
| | Mid percent distilled | API gravity |
|--|-----------------------|-------------|
| | 2 | 0 |
| | 5 | 90 |
| | 10 | 68 |
| | 15 | 59.7 |
| | 20 | 52 |
| | 30 | 42 |
| | 40 | 35 |
| | 45 | 32 |
| | 50 | 28.5 |
| | 60 | 23 |
| | 70 | 18 |
| | 80 | 13.5 |

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Pseudo Components from Assay



Simulation #4.bkp - Aspen Plus V9 - aspenONE

Search aspenONE Exchange

Properties

All Items

- Setup
- Components
 - Specifications
 - Molecular Structure
 - Assay/Blend
 - MIXOIL
 - OIL-1
 - Basic Data
 - Property Curves
 - Results
 - OIL-2
 - Light End Properties
- Petro Characterization
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
 - UNIFAC Groups
- Polymers
- Methods
- Chemistry
- Property Sets
- Data

IL-1 - Properties

Petro Properties Viscosity

Property name: SULFUR Units: percent

Property curve data

Bulk value: 2.3

| Mid percent distilled | Property value |
|-----------------------|----------------|
| 5 | 0.01 |
| 10 | 0.013 |
| 20 | 0.05 |
| 30 | 1.15 |
| 40 | 1.62 |
| 45 | 1.9 |
| 50 | 2.15 |
| 60 | 2.54 |
| 70 | 3 |
| 80 | 3.7 |

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Pseudo Components from Assay

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Properties

All Items

- Setup
 - Components
 - Specifications
 - Molecular Structure
 - Assay/Blend
 - MIXOIL
 - Mixture
 - Results
 - OIL-1
 - OIL-2
 - Light End Properties
 - Petro Characterization
 - Generation
 - Analysis Options
 - Selected Methods
 - Results
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
 - UNIFAC Groups
 - Polymers
 - Methods

MIXOIL - Results

Light Ends Analysis Component Breakdown Distillation Curves Blend Composition Status

| 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

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Properties

All Items

- Setup
 - Components
 - Specifications
 - Molecular Structure
 - Assay/Blend
 - MIXOIL
 - OIL - 1
 - OIL - 2
 - Light End Properties
 - Petro Characterization
 - Generation
 - Analysis Options
 - Selected Methods
 - Results
 - Pseudocomponents
 - Component Attributes
 - Henry Comps
 - UNIFAC Groups
 - Polymers
 - Methods
 - Chemistry
 - Property Sets

Petro Characterization - Results

Summary Petro Properties Viscosity Status

| Pseudocomponent | Average NBP F | API gravity | Specific gravity | UOPK | Molecular weight | Critical temperature F | psi |
|-----------------|------------------|-------------|------------------|---------|------------------|---------------------------|-----|
| 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 | |

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Property Models & Methods

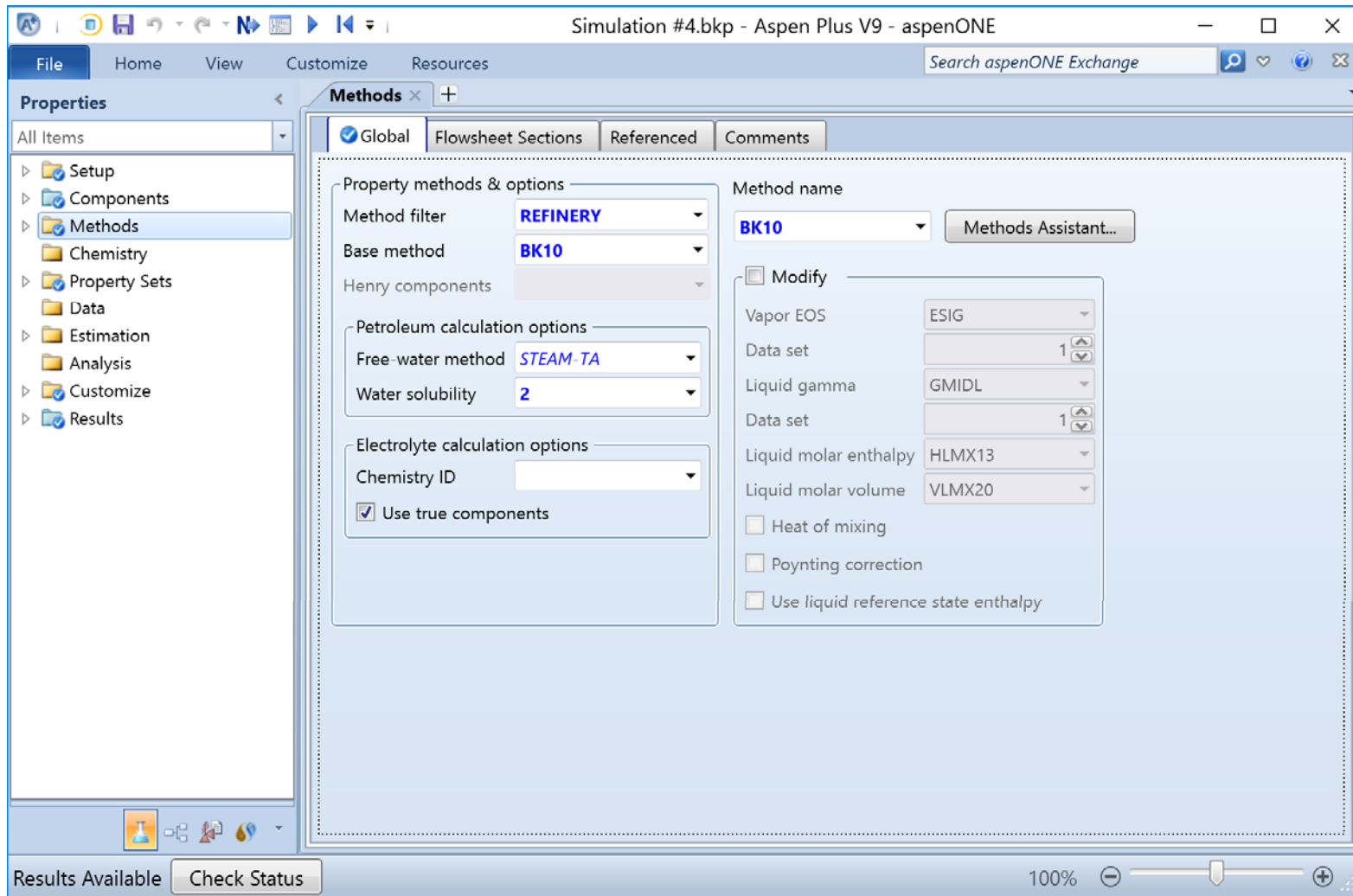
Typically use an equation of state (EOS) for properties

- 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

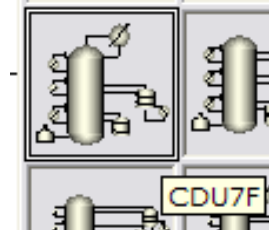
“Typical” unit operation models

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

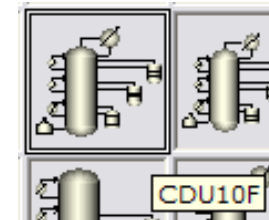
Towers – multiple configurations & solution techniques

- DSTWU
- RADFRAC
- PETROFRAC

- CDU7F



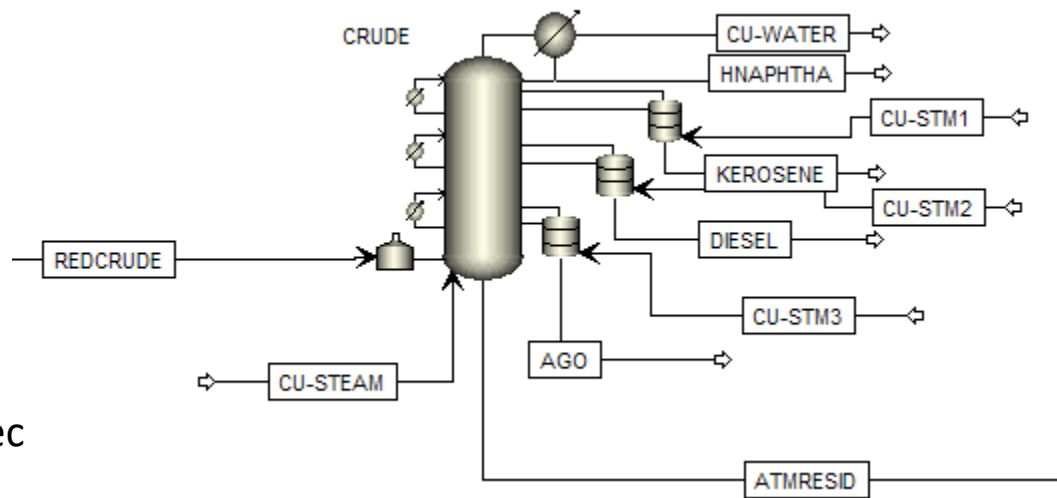
- CDU10F



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 – 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

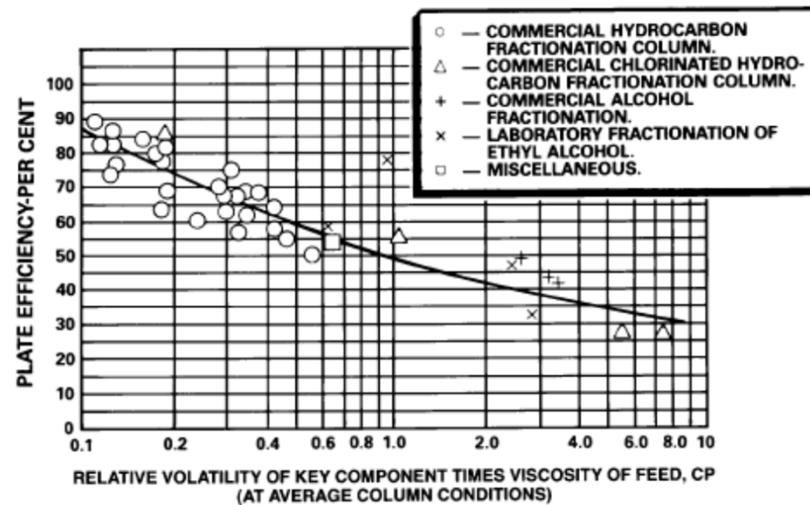
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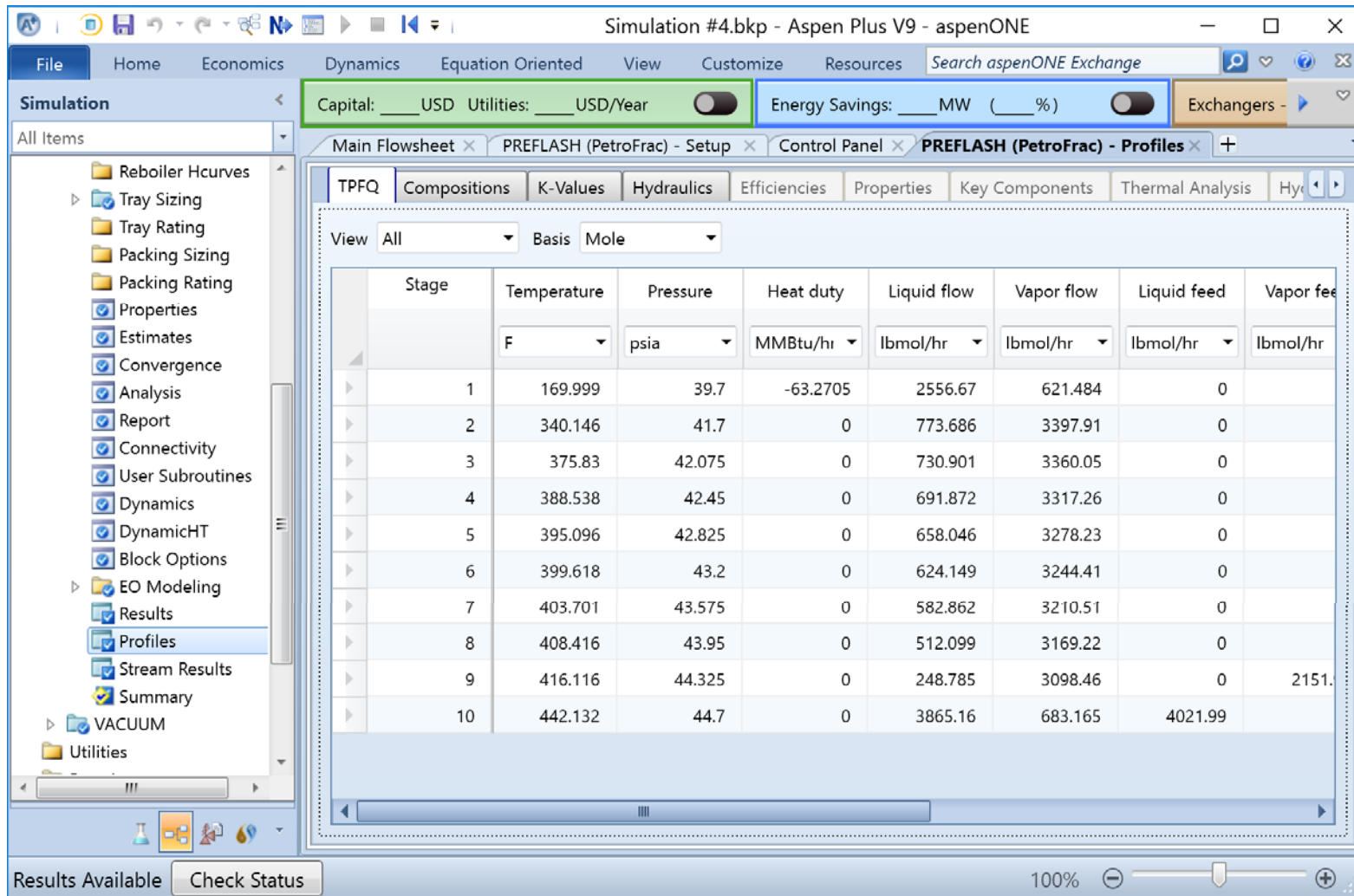
| Viscosity | Maxwell | Drickamer & Bradford in Ludwig |
|-----------|-----------------------------------|--------------------------------|
| cP | Ave Viscosity of liquid on plates | Molal Ave Viscosity of Feed |
| 0.05 | ... | 98 |
| 0.10 | 104 | 79 |
| 0.15 | 86 | 70 |
| 0.20 | 76 | 60 |
| 0.30 | 63 | 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



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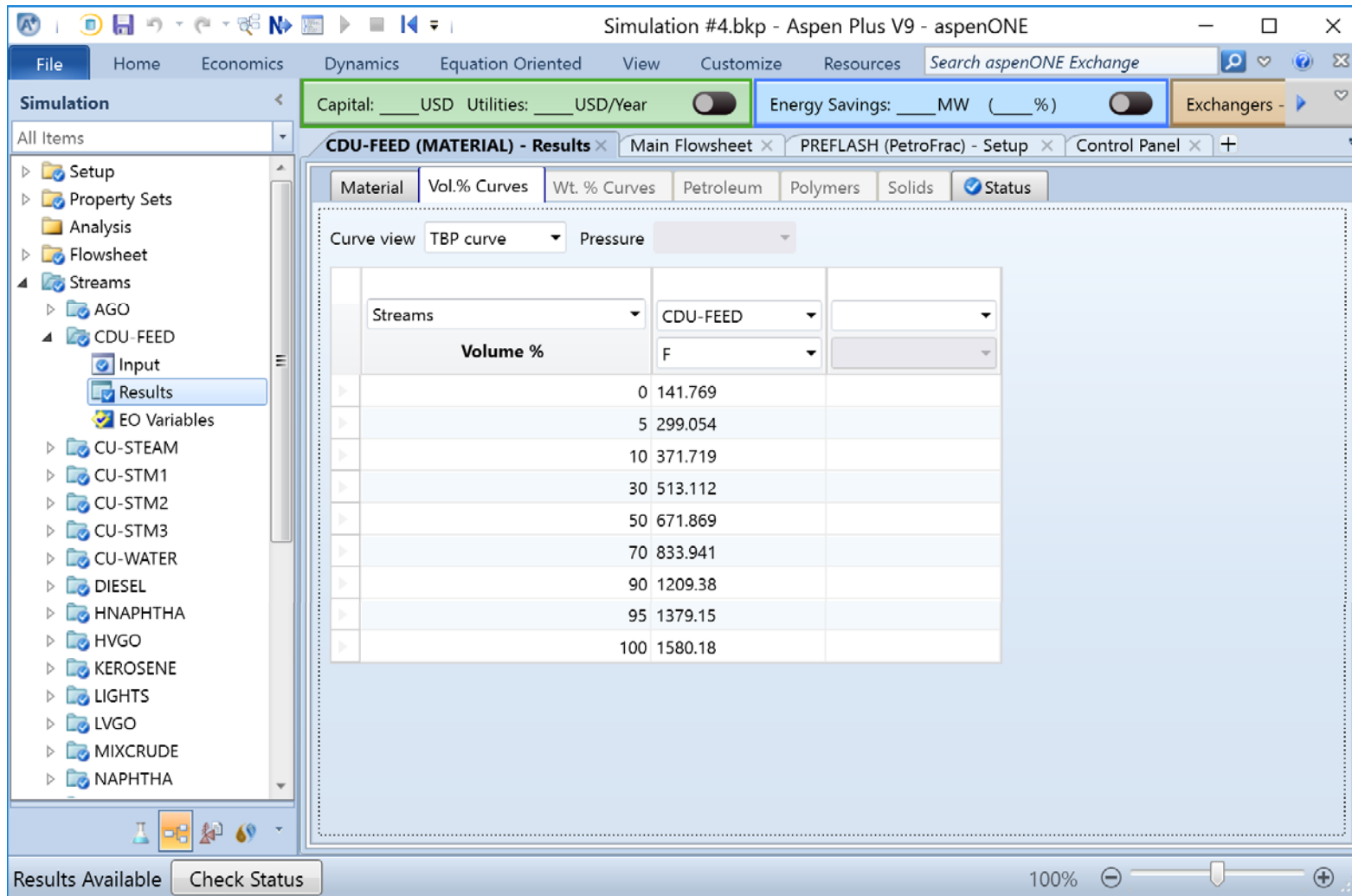
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Stream Results

The screenshot shows the Aspen Plus interface with the 'CDU-FEED (MATERIAL) - Results (Default)' window open. The window displays a table of stream properties for the 'CDU-FEED' stream. The 'Status' tab is selected, showing properties like Temperature (442.132 F), Pressure (44.7 psia), and Molar/Liquid fractions.

| Material | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids | Status |
|--------------------------|--------------|--------------|-----------|----------|--------|----------|
| Units: CDU-FEED | | | | | | |
| Description | | | | | | |
| From | | | | | | PREFLASH |
| To | | | | | | CRUDE |
| Stream Class | | | | | | CONVEN |
| Maximum Relative Error | | | | | | |
| Cost Flow | | | \$/hr | | | |
| - MIXED Substream | | | | | | |
| Phase | | | | | | Liquid |
| Temperature | | | F | | | 442.132 |
| Pressure | | | psia | | | 44.7 |
| Molar Vapor Fraction | | | | | | 0 |
| Molar Liquid Fraction | | | | | | 1 |
| Molar Solid Fraction | | | | | | 0 |
| Mass Vapor Fraction | | | | | | 0 |
| Mass Liquid Fraction | | | | | | 1 |
| Mass Solid Fraction | | | | | | 0 |

Specialized Stream Reports



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User Interface

Graphically build the flowsheet by dragging & dropping unit models

Calculations performed automatically as information is entered

Copy & paste capabilities

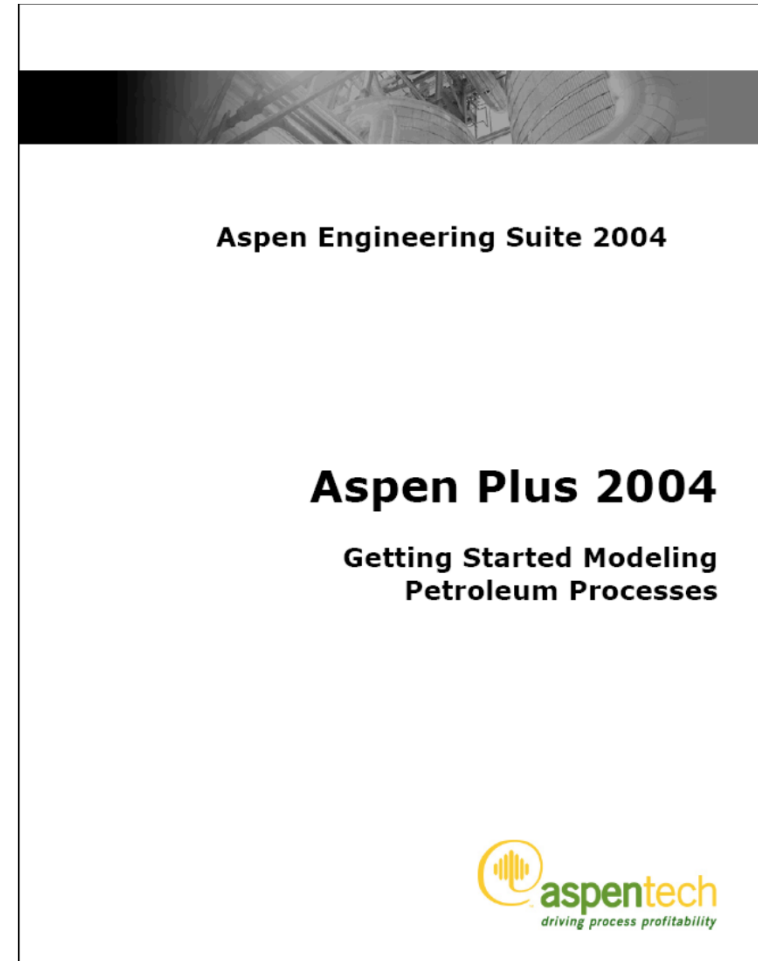
Aspen Simulation Workbook extends capabilities to put custom interface on top of simulation

Aspen Plus crude tower example

From Aspen Tech web site

- Copied to class web site

Additional problem developed specifically for this class.



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