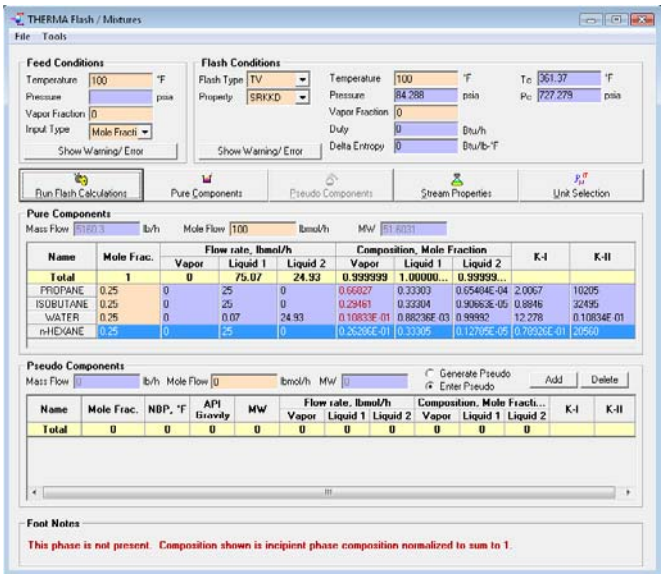
Flash-Mixture Calculations

Introduction

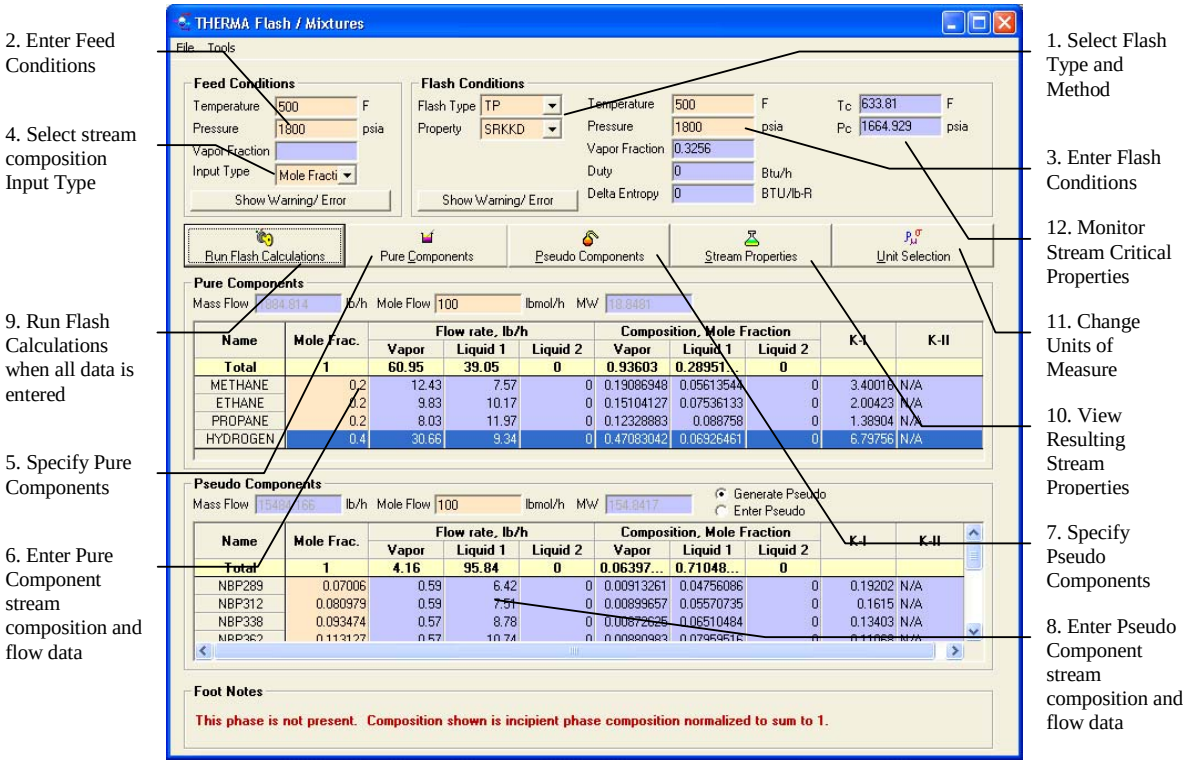
EPCON International's THERMA™ Flash/Mixture Calculations screen allows the user to estimate vapor-liquid equilibria (VLE) or vapor-liquid-liquid equilibria (VLLE) and associated phase properties, for mixtures of pure and/or pseudo-components. Properties of pure or pseudo-components and their mixtures are computed with the DIPPR® or API database and associated correlations (the DIPPR® database is used for pure components only). The three-phase flash (VLLE) engine enables the user to predict phase splits involving a vapor and two liquid phases, wherein the second liquid phase (if present) is an aqueous phase. The three-phase flash is able to determine up-front if a second liquid phase if water is present, and reduces to a two-phase flash if there is no aqueous/water phase.



The THERMA Flash/Mixture screen consists of two tables where pure component and pseudo components may be entered. The toolbar at the top allows for the selection of components, access to other screens, performing the calculations and for viewing tabulated results over a range of temperatures and corresponding graphs. A databank of quality SRK and NRTL parameters are included that are automatically selected for component pairs -providing 3-phase flash results as shown below as good as or better than any major simulator.

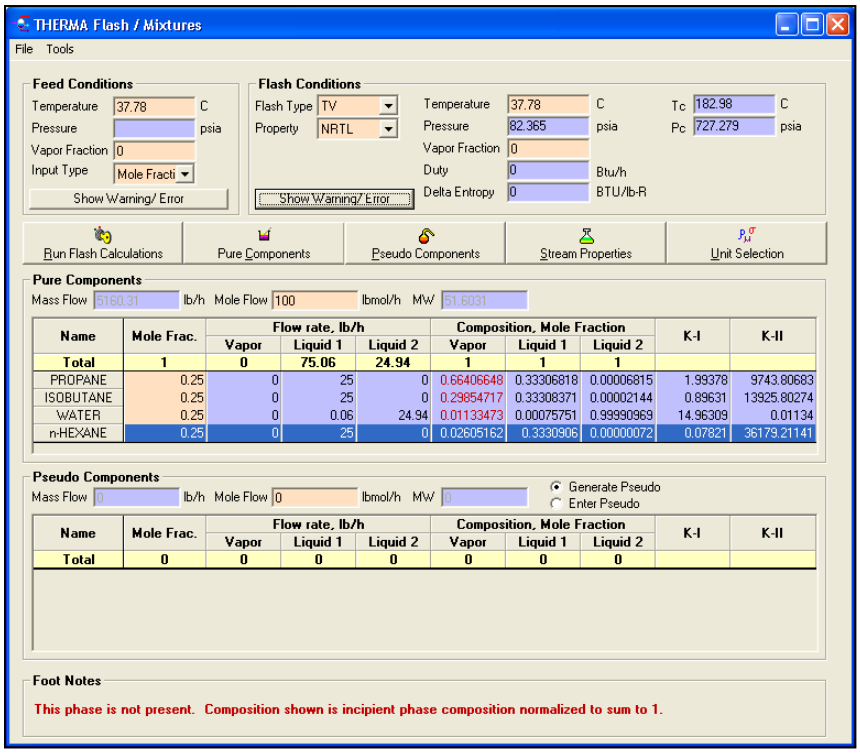
Using the Program

Click on the Flash/Mixture Calculations button to load the flash program.



Follow the above steps to enter data and view results as detailed below.

Shown is a 3-Phase Flash calculation of pure components using the NRTL method and build-in parameters to accurately determine two liquid phases for a Temperature, Vapor Fraction (TV) flash type – do not use NRTL with Psuedo Components.



Select Flash Type & Method (Step 1)

Select a Flash Type from the drop down list of options shown as follows:

1. **TP** - Temperature and Pressure known
2. **PV** - Pressure and Vapor Fraction known
3. **TV** - Temperature and Vapor Fraction known
4. **PH** - Pressure and Enthalpy known
5. **PS** - Pressure and Entropy Change known

Select a Method Type from the drop down list of options shown as follows:

1. **SRKKD** - API Soave Redlick Kwong equation of state with the Kabbadi-Danner correlation for water phase interactions.
2. **NRTL** - Non-Randon, Two Liquid phase interaction parameter method

From these selections, the available interaction parameters will be automatically loaded and the required inputs defined. The SRKKD method is recommended for use with hydrocarbon systems and water while the NRTL method is recommended for chemical systems with pure components only.

Enter Feed Conditions (Step 2)

Enter the known values as specified in the Flash Type for the feed conditions shown with a light red background (unknown values become de-activated with a light blue background).

Enter Flash Conditions (Step 3)

Enter the known values as specified in the Flash Type for the flash conditions shown with a light red background (unknown values become de-activated with a light blue background).

Select Stream Composition Input Type (Step 4)

Select a stream composition Input Type as follows:

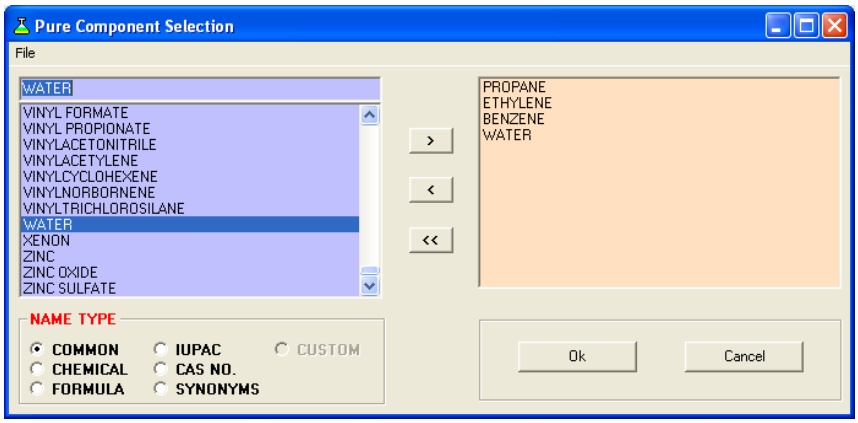
1. Mole Fraction
2. Mole Percentage
3. Mole Flow
4. Mass Flow
5. Volume Flow

The inputs for entry of pure and pseudo component data will be adjusted accordingly.

Specify Pure Components (Step 5)

Select the Pure Components button to display the selection screen for pure components. A list of the AIChE DIPPR 801 Database is displayed that include the majority of API component data for selection. The list may be viewed in a number of different ways as follows:

1. Common Name - AIChE DIPPR common naming convention
2. Chemical Name - ACS common naming convention
3. Formula - The chemical formula specification (potential duplicates may appear - insure the desired component is selected)
4. IUPAC - International Union of Physical and Applied Chemistry
5. CAS No. - Chemical Abstracts Number
6. Synonyms - Multiple choices of common industry synonym names



Select the component by typing the first letter of the component in the text entry box until the desired component is visible in the list. Then select the component from the list by clicking once and selecting the right-arrowed button or double-clicking to move the component to the selection list on the right side of the screen. Components can be selected with varying Name Types. If a component needs to be removed, select that component in the right selection list and select the left-arrowed button to remove it from the selection list. When completed, select the OK button to place the components into the pure component table of the Flash/Mixture Calculations program.

***Note**: You can not directly type in the name of the component in the pure component grid. The component must be selected from the list.*

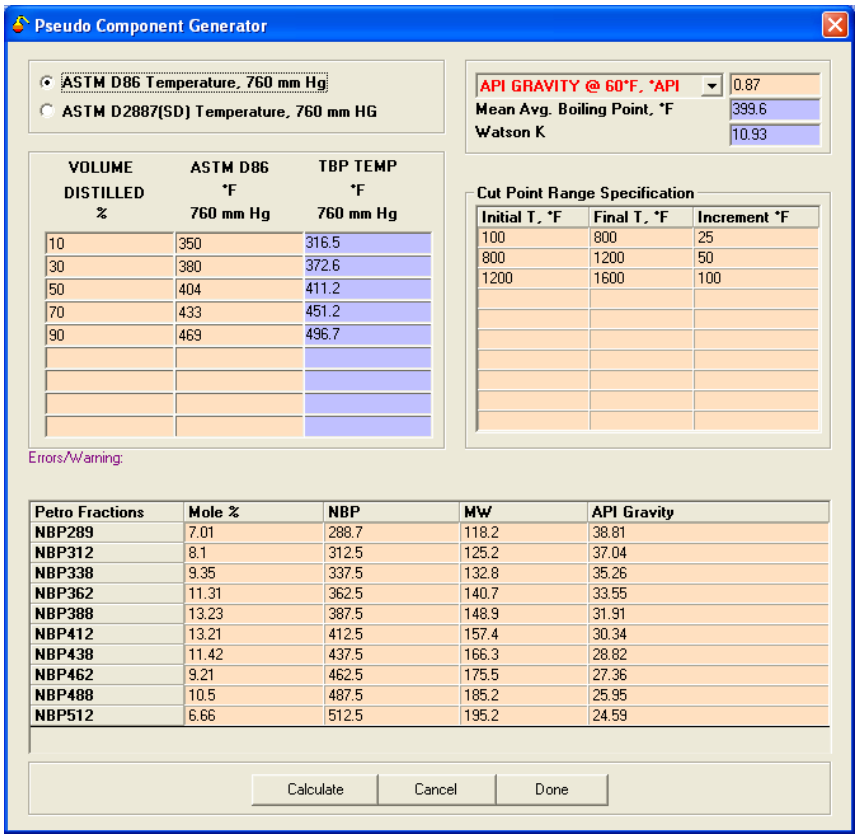
Enter Pure Component Data (Step 6)

Enter the composition data for each component and the flow data as applicable based on the selection in Step 4, selection of stream composition input type. The same grid is used to display output results for predicted phase splits and K-I and K-II equilibrium constants for the liquid 1 and liquid 2 phases respectively.

Name	Mole Frac.	Flow rate, lb/h			Composition, Mole Fraction			K-I	K-II
		Vapor	Liquid 1	Liquid 2	Vapor	Liquid 1	Liquid 2		
Total	1	60.95	39.05	0	0.93603	0.28951...	0		
METHANE	0.2	12.43	7.57	0	0.19086948	0.05613544	0	3.40016	N/A
ETHANE	0.2	9.83	10.17	0	0.15104127	0.07536133	0	2.00423	N/A
PROPANE	0.2	8.03	11.97	0	0.12328883	0.088758	0	1.38904	N/A
HYDROGEN	0.4	30.66	9.34	0	0.47083042	0.06926461	0	6.79756	N/A

Specify Pseudo Components (Step 7)

Select either the Generate Pseudo or Enter Pseudo radio button to indicate the entry mode of pseudo components.

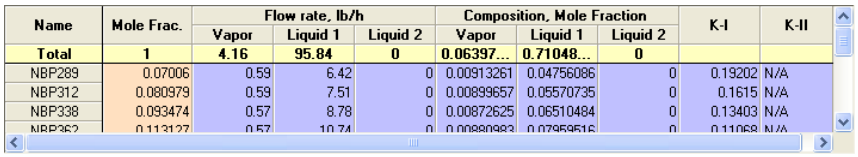


The same program module is used from the Flash/Mixture Calculations program for generation of Pseudo components. Detailed instructions for generating pseudo components is found in the previous section on Pseudo Component Generator. Assay data for either D86 or D2887 is required along with either an API Gravity or Specific Gravity. Select Done in the Pseudo Component Generator to transfer the pseudo component data into the Flash/Mixture Calculations Pseudo Components table. The data in the Pseudo Component Generator will remain in memory for re-display when selecting the Pseudo Component button.

Enter Pseudo Component Data (Step 8)

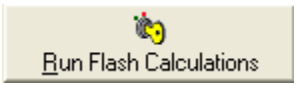
When generating pseudo components, no further entry is required since the composition of each petro fraction is determined as apart of the pseudo

component generation calculations. When selecting the Enter Pseudo radio button, the pseudo component data is manually entered. The Name field is user defined; the midpoint Normal Boiling Point (NBP) is used as the Name when using the Pseudo Component Generator.



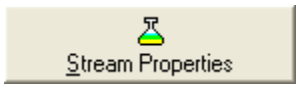
Name	Mole Frac.	Flow rate, lb/h			Composition, Mole Fraction			K-I	K-II
		Vapor	Liquid 1	Liquid 2	Vapor	Liquid 1	Liquid 2		
Total	1	4.16	95.84	0	0.06397...	0.71048...	0		
NBP289	0.07006	0.59	6.42	0	0.00913261	0.04756086	0	0.19202	N/A
NBP312	0.080979	0.59	7.51	0	0.00899657	0.05570735	0	0.1615	N/A
NBP338	0.093474	0.57	8.78	0	0.00872625	0.06510484	0	0.13403	N/A
NBP362	0.113127	0.57	10.74	0	0.00880983	0.07959516	0	0.11068	N/A

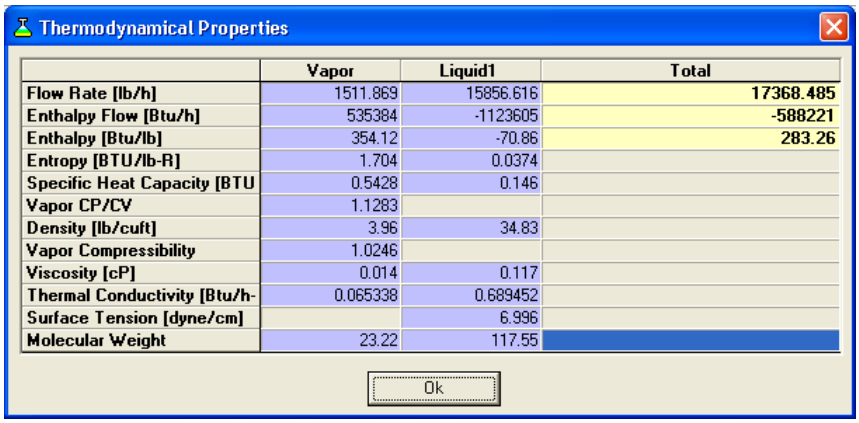
Run Flash Calculations (Step 9)



Select the Run Flash Calculations button when all of the data has been entered to determine phase splits and stream properties. The phase splits will be displayed in the Pure and Pseudo data tables which represent the stream compositions for the Pures and Pseudos considered as independent streams.

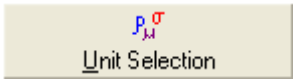
View Stream Properties (Step 10)





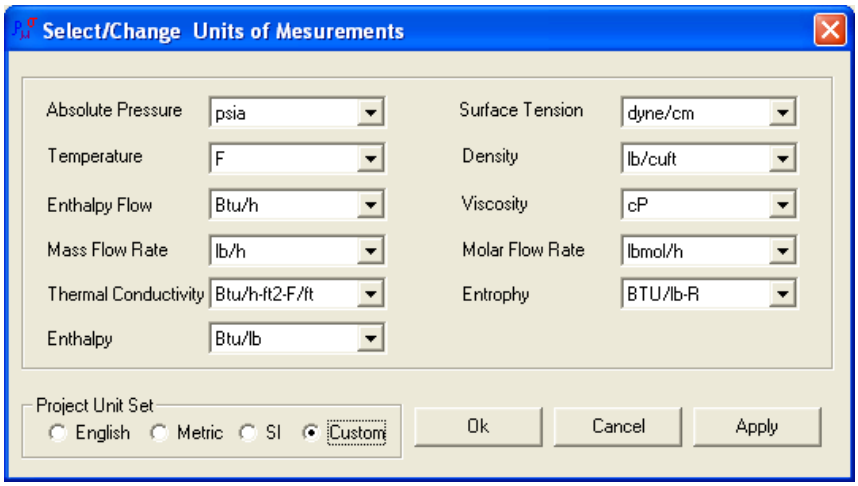
The stream properties for the combined stream is shown by selecting the Stream Properties button. This combines these two streams according to the flowrates specified for each and determined total stream properties for a number of important physical properties required in engineering and design calculations.

Change Units of Measure (Step 11)



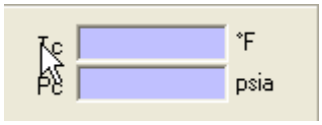
Flexible selection of units of measure is provided in the Flash/Mixture Calculations program. Select either a standard set (English, Metric, SI) or choose Custom to select modifications to a standard set that was previously

selected. Once selected, the units of measure chosen will become the default when the program is next loaded.



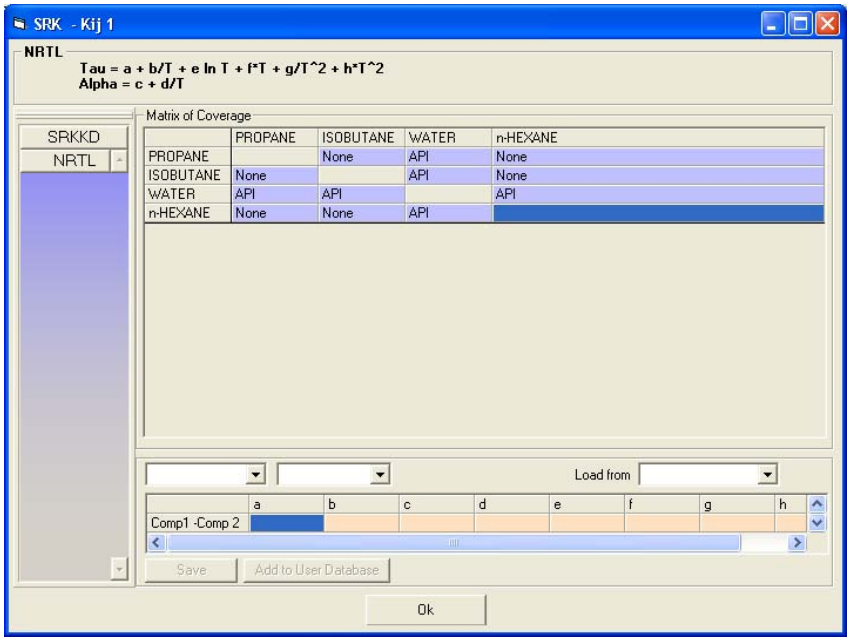
Monitor Stream Critical Properties (Step 12)

It is recommended to monitor the calculated critical properties shown. If the stream properties exceed the critical properties, potential erroneous results can be obtained. Also monitoring of any errors reported at the bottom of the screen is advisable to avoid an erroneous result.



Binary Interaction Parameter Coverage

Coverage provided for binary interaction parameters can be reviewed by selecting this option in the Tools menu. For binary pairs that binary parameters are provided and utilized, 'API' will be displayed in the grid. Additional parameters and user entry of parameters are available separately from EPCON International. If there are questions for a particular flash calculation, e-mail a saved THERMA file to EPCON International for review at techsupport@epcon.com.


SRK - Kij 1
NRTL
Tau = a + b/T + e ln T + f*T + g/T^2 + h*T^2
Alpha = c + d/T
SRKKD
NRTL
Matrix of Coverage
PROPANE
ISOBUTANE
WATER
n-HEXANE
Load from
a
b
c
d
e
f
g
h
Comp1 -Comp 2
Save
Add to User Database
Ok

Psuedo Component Generator

The Pseudo Component Generator screen allows the user to overlay a set of cut point temperatures on a True Boiling Point (TBP) distillation curve and produce a component set that models the TBP Curve. The properties of these pseudo components can be used to predict liquid and gas properties. The pseudo components can also be used in flash calculations. As part of the calculation, mole fraction, normal boiling point, molecular weight and API gravity are generated for each of the pseudo components.

The normal boiling point, specific gravity, and molecular weight of a pseudo component is computed as follows. First the TBP curve is fitted to a cubic spline equation. Volume percents are then computed at the beginning and end temperature of each cut point interval to determine the amount of material in each cut. The normal boiling point for each cut is also computed from the interval beginning and end temperatures. The specific gravity of each cut is computed from the normal boiling point and the Watson K (assumed constant). For each cut, the molecular weight is computed from a correlation using normal boiling point and specific gravity. The API gravity is computed directly from specific gravity.

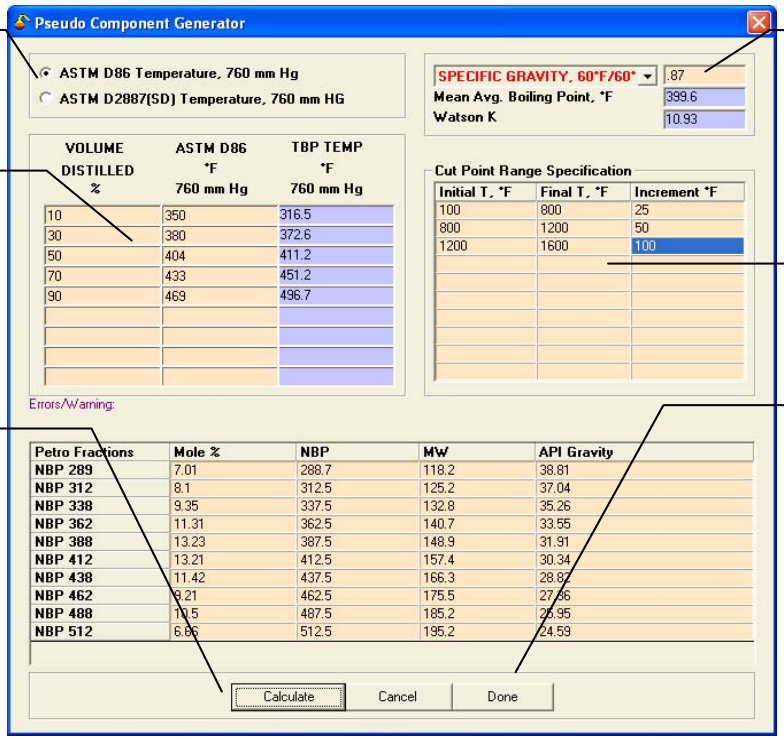
Using the Program

To access the Pseudo Component Generation screen, click on the Pseudo Component Generator icon from the Applications Toolbar. You can alternatively access this directly from the Flash/Mixture Calculations program and the pseudo components results will be placed directly into the pseudo component input fields for immediate use in flash and mixture calculations.

Select either D86 or D2887

Enter TBP stream assay data in this table.

Select Calculate to generate the petro fractions at each Normal Boiling Point midpoint with Mole%, Avg. MW and API Gravity.



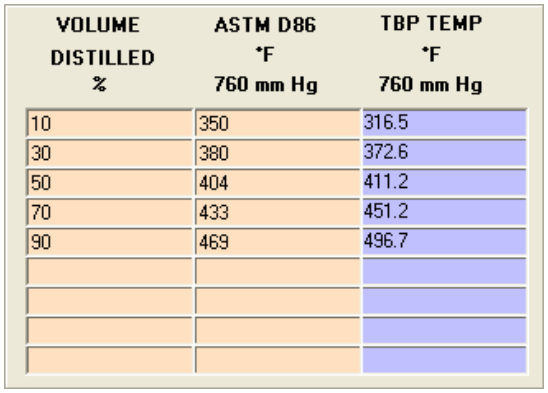
Enter either the API Gravity or Specific Gravity selected from the Drop Down list.

Enter cut point ranges in this table.

Select Done when completed to exit the program and place the pseudo component data in the Flash/Mixture Calculations program if opened from that program.

Specifying Inputs

There are two tables of information that must be completed: the Petroleum Stream Assay Data table (either D86 or D2887 assay data) and the Cut Point Specification table. The Cut Point Range Specification table contains a recommended set of default values. Additionally, either the API Gravity or Specific Gravity of the petroleum stream is required for calculation of the Mean Average Boiling Point and Watson K.

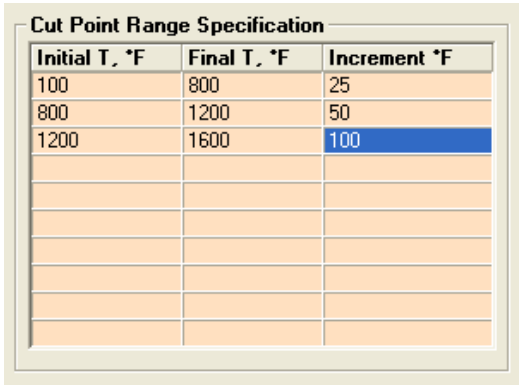


VOLUME DISTILLED %	ASTM D86 °F 760 mm Hg	TBP TEMP °F 760 mm Hg
10	350	316.5
30	380	372.6
50	404	411.2
70	433	451.2
90	469	496.7

Specifying TBP data for the stream

If you already have TBP data for the stream at the specified volume % distilled (D86) or weigh % distilled (D2887), you may enter it directly into the Petroleum Stream Data table. If the distillation data you have is not TBP data, it may be converted in the Petroleum Fraction Distillation Interconversions program. The Distillation Interconversions program allows for saving files with a *.TBP extension. These TBP files can be loaded into the Psuedo Component Generator or the Flash/Mixture Calculations program by selecting the **File ➔ Open TBP Curve** option.

Defining a Cut Point Range



Cut Point Range Specification

Initial T, °F	Final T, °F	Increment °F
100	800	25
800	1200	50
1200	1600	100

At least one cut point range is required and up to 10 cut point ranges may be given. For each cut point range, initial and final temperatures are required. Increments are required and may be specified as either a Delta T or as a number of pseudo components. The defaults are: 25°F increments between 100°F and 800°F. 50°F increments between 800°F and 1200°F and 100°F between 1200°F and 1600°F.

API Tech Data Book Method Implementation

Procedure 4B2.1 - Method for the Critical Pressure of a Mixture of Defined Composition

Procedure 6A3.1 - Densities of Defined Liquid Mixtures at their Bubble Points

Procedure 6B2.2 - Computer Method for the Density of Hydrocarbon and Nonpolar Gas Mixtures

Procedure 7B3.7 - Computer Method for the Enthalpy of Pure Hydrocarbon Liquids and Real Gases

Procedure 7B4.1 - Liquid and Real Gas Enthalpy of Hydrocarbon Mixtures

Procedure 7C1.16 - Computer Method for the Heat of Vaporization of Pure Hydrocarbons

Procedure 7C2.1 - Heat of Vaporization of Mixed Hydrocarbons

Procedure 7D3.6 - Computer Method for the Heat Capacity of Pure Real Gases and Liquids

Procedure 7D4.1 - Isobaric Heat Capacity of Hydrocarbon Gas Mixtures

Procedure 7E2.1 - Heat Capacity Ratio of Hydrocarbon Gas Mixtures

Procedure 7F1.7 - Computer Method for the Entropy of Pure Hydrocarbon Liquids and Real Gases

Procedure 8D1.1 - Computer Method for Hydrocarbon-Hydrocarbon and Hydrocarbon-Nonhydrocarbon Vapor-Liquid Equilibrium K-Values

Procedure 8D1.5 - Computer Method for Flash Calculations and Equilibrium K-Values of Undefined Petroleum Fractions

Procedure 8D1.6 - Computer Method for Flash Calculations and Equilibrium K-Values of Mixtures of Defined and Undefined Components

Procedure 10A2.1 - Surface Tension of Defined Hydrocarbon Mixtures at Low Pressures

Procedure 10A2.2 - Surface Tension of Defined Hydrocarbon Mixtures at High Pressure

Procedure 11A3.1 - Liquid Viscosity of Defined Mixtures at Low Pressures

Procedure 11A4.6 - Liquid Viscosity Blending of Multicomponent Mixtures of Defined and Undefined Compounds

Procedure 11A5.5 - Liquid Viscosity of High Molecular Weight Pure and Mixed Hydrocarbons at High Pressure

Procedure 11B2.1 - Viscosity of Gaseous Mixtures at Low Pressure

Procedure 11B4.1 - Viscosity of Pure Hydrocarbon Gases and their Gaseous Mixtures at High Pressure

Procedure 12A2.1 - Thermal Conductivity of Defined Liquid Hydrocarbons Mixtures

Procedure 12A3.3 - Thermal Conductivity of Liquid Petroleum Fraction Blended with Defined Light Hydrocarbon Liquid Mixtures

Procedure 12B2.1 - Thermal Conductivities of Defined Mixtures of Hydrocarbon Gases