# **Flash-Mixture Calculations**

# Introduction

EPCON International's THERMA<sup>™</sup> 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

100 0 Mole Fracti	₽ Pma	Flash 1 Proper	Type TV ty SRKX	• 0 •	Temperature Pressure	100 84 288	F	Te 361.3	17 'F
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siculations	Pure	Compon	ents	Etéudo (	Components	Stream	Properties	U.	nit Selection
nents									
80.3	b/h M	tole Flow	100	Rmol/1	h MW 盾	1.6831			
-		Flow	rate lbm	al/h	Compo	sition Mole F	raction		1
Mole Fra	IC. Va	por	Liquid 1	Liquid 2	Vapor	Liquid 1	Liquid 2	K-1	K-II
1		0	75.07	24.93	0.999999	1.00000	0.99999		
0.25	0	4	5	0	0.66827	0.33303	0.65484E-04	2.0067	10205
0.25	0	4	5	0	0.29461	0.33304	0.906638-05	0.8846	32495
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1	lb/h Mole	Flow U	1	Ibmol/h M	w u	( En	ter Pseudo	Add	Delete
		API		Flow	rate, Ibmol/h	Compo	sition. Mole	Fracti	
Mole Frac.	NBP, T	Gravil	y MW	Vapor	Liquid 1 Liqu	uid 2 Vapor	Liquid 1	liquid 2	K-I K-II
	Mole Fra	Kularions     Purrents       initial     Burn     N       Mole Frac.     Va       0,25     0       0,25     0       0,25     0       0,25     0       0,25     0       0,25     0       0,25     0       0,25     0       0,25     0       Mole Frac.     NDP, "f	Multiplications     Flow       Inclusions     Price Components       Mole Frac.     Vapor       1     0       0,25     0	Lif     Lif       exteriors     Pure Components       int     Mole Flaw     100       1     0     75.07       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0,25     0     25       0     0     7       Mole Frac.     NBP. T< API     MV	Li     Pre-Components     Pre-Model       03     Brh     Mole Flaw     100     Bund/h       Mole Frac.     Flow rate, Ibmol/h     100     Bund/h       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0       0.25     0     25     0	W     Pure Components     Pure Components       tents     Pure Components     Pure Components       03     tu/h     Mole Flaw     100     Ismot/h     WW       Mole Frac.     Flow rate, Ibmot/h     Compo     0     0.000/h     0.0000/h       1     0     7.5.0     0.0000/h     0.0000/h     0.0000/h     0.0000/h       0.25     0     2.5     0     0.0000/h     0.0000/h     0.0000/h       0.25     0     0.00000/h     7.5     0     0.00000/h     0.00000/h <th>M     Preve Components     Preve Components     Stream       ictuations     Preve Components     Preve Components     Stream       ictuations     Extra Mode Flows     100     Ismoth     Mode Flows     Ismoth     Ismoth     Ismoth     Mode Flows     Ismoth     Ismoth&lt;</th> <th>Million     Flow     Components     Previde Components     Stream Properties       tents     Previde Components     Stream Properties     Stream Properties       03     tenh     Mole Flaw     100     tamoth     MV FileR031       04     Flow rate, Ibmol/h     Composition, Mole Fraction     Liquid 2     Vapor     Liquid 1     Liquid 2       0.25     0     25     0     0.059939     1.00000L     0.999939       0.25     0     25     0     0.23458     0.333041     0.99958.45       0.25     0     25     0     0.23458     0.333041     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     0.255562.01     0.33304     0.99958.45     0.19878.45       0.25     0     0.255562.01     0.33305</th> <th>Multiplications     Terms Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Components     K-4       Initial State     Flow table, Ibaaci/h     Components     Components     K-4       Initial State     Initial State     Components     Components     Components     K-4       Initial State     Initial State     Initial State     Components     Components     Components     Components       Initial Flow     Initial State     Flow table, Ibaaci/h     Mole Flow     Components     Add       Initial Flow     Initial State     Flow table, Ibaaci/h     Components     Add</th>	M     Preve Components     Preve Components     Stream       ictuations     Preve Components     Preve Components     Stream       ictuations     Extra Mode Flows     100     Ismoth     Mode Flows     Ismoth     Ismoth     Ismoth     Mode Flows     Ismoth     Ismoth<	Million     Flow     Components     Previde Components     Stream Properties       tents     Previde Components     Stream Properties     Stream Properties       03     tenh     Mole Flaw     100     tamoth     MV FileR031       04     Flow rate, Ibmol/h     Composition, Mole Fraction     Liquid 2     Vapor     Liquid 1     Liquid 2       0.25     0     25     0     0.059939     1.00000L     0.999939       0.25     0     25     0     0.23458     0.333041     0.99958.45       0.25     0     25     0     0.23458     0.333041     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     25     0     0.254562.01     0.33304     0.99958.45       0.25     0     0.255562.01     0.33304     0.99958.45     0.19878.45       0.25     0     0.255562.01     0.33305	Multiplications     Terms Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Stream Properties     U       Initial State     Flow table, Ibaaci/h     Components     Components     K-4       Initial State     Flow table, Ibaaci/h     Components     Components     K-4       Initial State     Initial State     Components     Components     Components     K-4       Initial State     Initial State     Initial State     Components     Components     Components     Components       Initial Flow     Initial State     Flow table, Ibaaci/h     Mole Flow     Components     Add       Initial Flow     Initial State     Flow table, Ibaaci/h     Components     Add

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.

💈 THERMA Flash / Mixtures Tool Shown is a 3-Flash Conditions Feed Condition: Phase Flash Temperature С Tc 182.98 Temperature 37.78 с Flash Type TV 37.78 С Pressure 82.365 Pc 727.279 psia calculation of Property NRTL psia Pressure psia • Vapor Fraction 🚺 Vapor Fraction pure Duty Input Type Mole Fracti 💌 Btu/h Delta Entropy 🚺 BTU/Ib-R components Show Warning/Error Show Warning/ Error using the 10 ъŕ  $P_{\mu}^{\sigma}$ Run Flash Calculations Unit Selection Pure Components Pseudo Components Stream Properties NRTL method Pure Components and build-in Mass Flow 5160.3 b/h Mole Flow 100 Ibmol/h MW 51.60 Flow rate, Ib/h Liquid 1 Mole Fraction Co parameters to Name Mole Frac K-I K-II Vapor .iquis 75.06 25 Liquid 2 Vapor Liquid 1 Liquid 2 Total 0 24.94 accurately PROPANE 0.66406648 0.33306818 0.00006815 1.99378 9743,80683 0.25 0.25 0.25 determine two **ISOBUTANE** 25 Π 0.29854717 0.33308371 0.00002144 0.89631 13925.80274 WATER 0.01133473 0.00075751 0.99990969 24.94 14.96309 0.01134 0.06 n-HEXANE liquid phases for a Pseudo Components Generate Pseudo
C Enter Pseudo Mass Flow 🥫 lb/h Mole Flow 🚺 lbmol/h MW 🔟 Temperature, Flow rate, Ib/h Com sition. Mole Fraction K-II Name Mole Frac. K-I Vapor Liquid 1 Liquid 2 Vapor Liquid 1 Liquid 2 Vapor Total Π Π 0 0 0 Fraction (TV) flash type – do not use NRTL with Psuedo Foot Note Components. This phase is not present. Composition shown is incipient phase composition normalized to sum to 1.

#### 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)

⊌ Pure <u>C</u>omponents 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

Z Pure Component Selection	
File	
WATER VINYL FORMATE VINYL PROPIONATE VINYLACETONITRILE VINYLACETYLENE VINYLACETYLENE VINYLORBORNENE VINYLTRICHLOROSILANE VINYLTRICHLOROSILANE VATER XENON ZINC ZIN	PROPANE ETHYLENE BENZENE WATER
NAME TYPE COMMON CIUPAC CUSTOM CHEMICAL CAS NO. CFORMULA SYNONYMS	Ok Cancel

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-II and K-II equilibrium constants for the liquid 1 and liquid 2 phases respectively.

Nama	Mala Eraa	F	low rate, Ib/	h	Compos	ition, Mole F	raction	<b>K</b> I	<b>к</b> II
Name	MULE FIAC.	Vapor	Liquid 1	Liquid 2	Vapor	Liquid 1	Liquid 2	N-1	N-11
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.

ASTM D2887	SD) Temperature,	, 760 mm HG	Mean Avg. Bo Watson K	'@ 60°F, 'API iling Point, *F	▼ 0.87 399.6 10.93
VOLUME DISTILLED	ASTM D86 *F	TBP TEMP *F	- Cut Point Ran	ge Specificatio	on
%	760 mm Hg	760 mm Hg	Initial T, *F	Final T, *F	Increment *F
10	350	316.5	100	800	25
30	380	372.6	800	1200	50
50	404	411.2	1200	1600	100
70	433	451.2			
90	469	496.7			
rors/Warning:					
rors/Warning:	Mole %	NBP	MW	API Gravity	
rors/Warning: Petro Fractions IBP289	Mole %	NBP 288.7	<b>MW</b> 118.2	API Gravity 38.81	
rors/Warning: Petro Fractions IBP289 IBP312	Mole % 7.01 8.1	NBP 288.7 312.5	<b>MW</b> 118.2 125.2	API Gravity 38.81 37.04	
rors/Warning: Petro Fractions IBP289 IBP312 IBP338	Mole % 7.01 8.1 9.35	NBP 288.7 312.5 337.5	<b>MW</b> 118.2 125.2 132.8	API Gravity 38.81 37.04 35.26	
Petro Fractions IBP289 IBP312 IBP338 IBP362	Mole <b>%</b> 7.01 8.1 9.35 11.31	NBP 288.7 312.5 337.5 362.5	MW 118.2 125.2 132.8 140.7	API Gravity 38.81 37.04 35.26 33.55	
rors/Warning: Petro Fractions IBP289 IBP312 IBP338 IBP362 IBP388	Mole % 7.01 8.1 9.35 11.31 13.23	NBP 288.7 312.5 337.5 362.5 387.5 362.5	MW 118.2 125.2 132.8 140.7 148.9	API Gravity 38.81 37.04 35.26 33.55 31.91	
rors/Warning: Petro Fractions IBP289 IBP312 IBP338 IBP388 IBP388 IBP412 IBP420	Mole % 7.01 8.1 9.35 11.31 13.23 13.21 13.21	NBP 288.7 312.5 337.5 362.5 387.5 412.5 412.5	MW 118.2 125.2 132.8 140.7 148.9 157.4 157.4	API Gravity 38.81 37.04 35.26 33.55 31.91 30.34 30.34	
rors/Warning: Petro Fractions IBP289 IBP312 IBP312 IBP362 IBP362 IBP362 IBP412 IBP412 IBP422	Mole <b>%</b> 7.01 8.1 9.35 11.31 13.23 13.21 11.42	NBP       288.7       312.5       337.5       362.5       387.5       412.5       437.5       462.5	<b>WW</b> 118.2 125.2 132.8 140.7 148.9 157.4 166.3 157.4	API Gravity 38.81 37.04 35.26 33.55 31.91 30.34 28.82 27.26	
Vetro Fractions IBP289 IBP312 IBP338 IBP362 IBP388 IBP412 IBP438 IBP452 IBP499	Mole <b>%</b> 7.01 8.1 9.35 11.31 13.23 13.21 11.42 9.21 10.5	NBP       288.7       312.5       337.5       362.5       387.5       412.5       437.5       462.5       497.5	MW 118.2 125.2 132.8 140.7 148.9 157.4 166.3 175.5 195.2	API Gravity 38.81 37.04 35.26 33.55 31.91 30.34 28.82 27.36 25.95	
rors/Warning: Petro Fractions IBP289 IBP312 IBP388 IBP362 IBP388 IBP462 IBP488 IBP462 IBP488 IBP512	Mole 2 7.01 8.1 9.35 11.31 13.23 13.21 11.42 9.21 10.5 6.66	NBP       288.7       312.5       337.5       362.5       387.5       412.5       437.5       462.5       487.5       512.5	MW 118.2 125.2 132.8 140.7 148.9 157.4 166.3 175.5 185.2 195.2	API Gravity 38.81 37.04 35.26 33.55 31.51 30.34 28.82 27.36 25.55 24.59	

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.

News	Mala Free	F	low rate, Ib/	h	Compos	ition, Mole F	raction	<b>K</b> 1			^
Name	Mole Frac.	Vapor	Liquid 1	Liquid 2	Vapor	Liquid 1	Liquid 2	N-1	N-11		
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		_
NRP362	0 11 31 27	0.57	10.74	0	0.00880983	0.07959516	0	0 11068	NDA		~
<										>	

#### **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)

<u>조</u> Stream Properties			
Z Thermodynamical Proper	ties		
	¥apor	Liquid1	Total
Flow Rate [lb/h]	1511.869	15856.616	17368.485
Enthalpy Flow [Btu/h]	535384	-1123605	-588221
Enthalpy [Btu/lb]	354.12	-70.86	283.26
Entropy [BTU/lb-R]	1.704	0.0374	
Specific Heat Capacity [BTU	0.5428	0.146	
Vapor CP/CV	1.1283		
Density [lb/cuft]	3.96	34.83	
Vapor Compressibility	1.0246		
Viscosity [cP]	0.014	0.117	
Thermal Conductivity [Btu/h-	0.065338	0.689452	
Surface Tension [dyne/cm]		6.996	
Molecular Weight	23.22	117.55	
		Ok	

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)

9<mark>μ</mark>σ <u>U</u>nit Selection

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.

<sup>ງຜູ</sup> ້ Select/Change U	nits of Mesureme	nts			
Absolute Pressure	psia 💌	]	Surface Tension	dyne/cm	•
Temperature	F	]	Density	lb/cuft	•
Enthalpy Flow	Btu/h 💌	]	Viscosity	сP	•
Mass Flow Rate	lb/h 💌	]	Molar Flow Rate	lbmol/h	•
Thermal Conductivity	Btu/h-ft2-F/ft	]	Entrophy	BTU/Ib-R	•
Enthalpy	Btu/lb 💌	]			
Project Unit Set		_			
C English C Met	ric C SI 🖲 Custon	ġ	Ok Car	ncel	Apply

### 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.

M	۴F
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#### **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.

Engineer's Aide Reference Guide

SRA - NIJ I										
IRTL Tau = a 4 Alpha = c	+ b/T + e ln T c + d/T	+ f*T + g/T	^2 + h*T^2							
i	Matrix of Cover	/age								
SRKKD		PROPANE	ISOBUTANE	WATER	n-HEXAN	NE				
NBTL	PROPANE		None	API	None					
The cr c	ISOBUTANE	None		API	None					
	WATER	API	API		API					
1	n-HEXANE	None	None	API						
						Load fro			-	
		•			4	Load fro	n		•	
			b	c	d	Load fro	n  f	9	h	
-	Comp1-Comp	a 2	b	C	d	Load fro	n   f	9	h	
	Comp1-Comp Save	a 2 Add to Us	b er Database	c.	d	Load fro	n   f	9	h	>

# **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.



#### 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	TBP TEMP *F
%	760 mm Hg	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**

Lut Point Range Specification									
Initial I, "F	Final I, "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