

## GET THE MOST FROM THE CRUDE OIL DATA YOU HAVE

Aurelio Ferrucci PROMETHEUS  
Executive V.P. Piazza Borgo Pila 40, 16129 Genova Italy  
Tel: +39010542011 Fax: +39010581451  
Email [aurelio.ferrucci@prometh.it](mailto:aurelio.ferrucci@prometh.it)

### **Abstract**

Inaccurate crude oil characterisation affects the results of planning and scheduling applications leading to uneconomical decisions: it may arise from analytical errors, lack of data or unavailability of updated crude assays reflecting the actual quality fed to the Refinery.

The author describes an innovative method permitting to highlight analytical errors and/or inconsistencies in crude assay and in field data and to build a consistent characterisation database available both for planning/scheduling applications and for process simulators.

Pseudo component breakdown and quality calculation is managed through a multidimensional regression that finds the best agreement between quality balances and distribution curve shape. The method works well also with poorly characterised oils and/or starting from plant data and permits to evaluate a crude oil even with few data available.

The typical issues to be faced within the elaboration of a crude assay are discussed through real examples as well as the available systems to realign characterisation data to actual crude oil quality (crude oil blending and recalculation).

After being elaborated, each Crude Oil can be easily re-cut to the format required by client application, also accounting for the real fractionation occurring in complex (multi column) distillation systems.

## **Introduction**

There are many factors influencing crude oil quality (production region, type of reservoir, field age) and its characterisation is essential to evaluate both its value (from producer side) and its profitability (from refiner side).

Generally speaking, excluding market fluctuations due to demand and offer the crude oil intrinsic value depends on the amount of high value products (gasoline and mid distillates) that the refinery can obtain processing it.

In this evaluation the contribution of conversion plants transforming heavy into lighter fractions should also be considered (as a matter of fact the market value of a crude oil is usually higher of the combined value of the resulting Straight Run fractions).

Thus the price is not the sole factor influencing the effective crude oil profitability: the refinery supply service also accounts for:

- Finished products market demand.
- Impact on refinery facilities (capacity and operative constraints due to feed quality).
- Refinery conversion capability.
- Possible advantages resulting from the combined processing with other crude oils.

All these tasks can be analysed only disposing of reliable and detailed crude oil characterisation data providing with all the information needed to predict the yields and the key properties of crude oil fractions.

This information is contained in the “Crude Assay”, the document reporting the results of the laboratory test data made to characterise a Crude Oil: regardless of the specific detail (number of fractions characterised and of laboratory tests reported) a Crude Assay is expected to contain at least the following information:

- Crude Oil:
  - Distillation curve (usually ASTM D2892 or “TBP” Distillation)
  - Light ends content (C5 minus yields)
  - Physical and Chemical property values useful to characterise the Crude (for example Specific Gravity, API Gravity, Sulphur, Neutralisation Factor, Viscosity, Characterisation Factor, Metals, etc.)
- Fractions (a meaningful number of fractions, covering the entire crude oil boiling range ought to be provided):
  - Yield on crude
  - Initial and Final Boiling Point (referred to Crude Oil TBP)
  - Physical and Chemical property values useful to characterise the Fraction: there are tests that are meaningful for any fraction (for example Specific Gravity, Sulphur,

Viscosity, Characterisation Factor, Distillation, etc.) and others that are executed depending on the specific fractions' Boiling Range.

The detail of a crude assay depends on the number of fractions that are characterised and on the number of tests that are executed on each fraction: at least one fraction ought to be tested in the boiling ranges reported in Table 1.

Description	Initial Boiling Point Range [Deg. C]	Final Boiling Point Range [Deg. C]	Average Fraction's Boiling Range [Deg. C]
Light Naphtha	C5	60-80	50
Heavy Naphtha	60-80	140-180	90
Kerosene	140-180	220-260	80
Light Gasoil	220-260	320-360	100
Heavy Gasoil	320-360	360-400	40
Vacuum Gasoil	360-400	500-580	160
Atmospheric Residue	360-400	Final Boiling Point	400 <sup>1</sup>
Vacuum residue	500-580	Final Boiling Point	250 <sup>1</sup>

Table 1 – Petroleum Fractions Average Boiling Ranges

Crude Assay data are input to many software applications developed to deploy various important tasks in the Oil Industry: some typical applications are:

- Upstream Planning: to determine the economic viability of new fields / discoveries.
- Supply Organisations: to assign crude value for individual grades.
- Refinery Operations: to schedule processed crude slate and calculate resulting product yields and quality.
- Downstream planning: to optimise refining and distribution assets.
- Process Engineering: equipment design and process planning.

In most cases results are deeply affected by input data reliability and – considering the growing amount of work that nowadays is being commissioned to this kind of applications – the availability of reliable Crude Oil characterisation data is getting more and more critical.

### **Crude Assay Data Handling**

Some problems may arise when using Crude Assay data to build a database useful for software applications:

- Crude Assay not in desired format. Some applications require a fixed (or uniform) pattern for Fractions' Cut Temperatures. This means that initial and final TBP boiling temperatures of the fractions must coincide for every crude oil contained in the database. If the boiling temperatures of the Crude Assay's fractions differ from those required by the database it is necessary to estimate the fractions' properties at different TBP cut temperatures, and this "re-cutting" exercise requires time and experience.

<sup>1</sup> The average boiling range of residual fractions is calculated assuming a Crude Oil final boiling point equal to 800°C

- Inconsistent Crude Assay data. Sometimes there are inconsistencies in Crude Assay data (as result of analysis or reporting errors) that, due to the high number of values involved, are very difficult to highlight. If not identified these are transmitted to the database affecting the results of the applications fed with it. A couple of macroscopic real examples is showed in Figure 1
- Actual quality differs from Crude Assay characterisation. It is well known that Crude Oil grades are not steady: the quality of each well's product evolves over time as well as the composition of the crude oil blend Marketed. The result is that the available Crude Assay does not reflect the actual Crude Oil quality and should be updated. If it is not possible to update the Crude Assay (a reliable crude inspection study takes time and is resource expensive) it is necessary to estimate new yields and quality data basing on the old Assay, and this job might lead to inconsistencies.

Tab. 1b: ASTM D2892			Tab. 4: GASOILS				
TBP CUT POINT	DISTILLATE % ON CRUDE	CU %	TBP RANGE	°C	230-320	320-370	370-400
°C	m/m	%	YIELD % ON CRUDE	% m/m	21.63	9.21	4.66
Gas+Gpl	0.4			% v/v	21.41	8.66	4.29
80	3.5		DENSITY @ 15°C	Kg/l	0.8397	0.8843	0.9024
100	3.6		SPECIFIC GRAVITY @ 60/60°F		0.8401	0.8848	0.9029
120	3.9		API GRAVITY @ 60/60°F		36.9	28.4	25.2
140	4.0		✓ SULPHUR (Total)	%m/m	0.04	0.18	0.21
160	2.4		✓ NITROGEN (Total)	ppm			970
160	2.1		✓ BASIC NITROGEN	ppm			384
180	4.4		✓ ACIDITY (Total)	mg KOH/g	0.04	0.18	0.30
210	5.2		✓ WAX	%m/m			7.29
230	4.5		✓ CLOUD POINT	°C	-24	+3	+21
250	4.1		✓ POUR POINT	°C	-24	+3	+18
270	4.2		✓ CETANE INDEX by four var. equations		53.6	55.6	58.4
290	3.8		✓ ANILINE POINT	°C	77.0	81.6	84.4
320	5.3		✓ AROMATICS				
350	5.7		Monocyclic	%v/v	16.6	19.3	20.3
370	4.2		Bicyclic	%v/v	5.3	10.0	11.3
400	4.5		Tri + Tetracyclic	%v/v	0.1	0.4	0.5
400+	34.2		Total	%v/v	21.9	29.6	32.1
			✓ REFRACTIVITY INDEX @70°C		1.4464	1.4700	1.4809
			✓ CARBON RESIDUE (Conradson)	%m/m			
			✓ KINEMATIC VISCOSITY @ 40 °C	mm <sup>2</sup> /s	4.383		
			✓ " " " 50 °C	mm <sup>2</sup> /s	3.966	3.97	15.78
			✓ " " " 50 °C	VBN	16.60	16.60	25.98
			✓ " " " 60 °C	mm <sup>2</sup> /s		3.560	11.320

Figure 1 – Examples of Crude Assay Inconsistencies

### Pseudo-Component Representation

Crude Oil is complex mixture of organic compounds, hydrocarbons (mainly Paraffines, Naphtenes and Aromatics but also Asphaltenes and Resins) and heteroatomic organic compounds (sulphur, oxygen, nitrogen and organometallic compounds) with a number of carbon atoms ranging from one to sixty and boiling temperatures up and beyond 800 °C.

Consequently, since it is not possible to characterise a Crude Oil defining its composition, this approach is not applied except then in case of light fractions (usually up to light naphtha boiling range rarely up to full range naphtha boiling range).

Usually the level of characterisation of a Crude Assay (where average boiling range of the fractions is around 100°C) is not enough detailed for applications requiring a different “re-cutting” of Crude Oil: in those cases the elaboration of Crude Assay Data is advisable.

A pseudo-component (or hypothetical component) is a small slice of a petroleum fraction, having a boiling range of 3 to 30°C and represents a mixture of close boiling components for which the chemical structure is unknown and the characterising properties must be estimated<sup>2</sup>.

The pseudo-component representation has been originally introduced to simplify the Crude Oil characterisation problem (reducing the number of components needed to simulate its behaviour) in order to perform Vapour Liquid Equilibria (VLE) calculations<sup>2</sup>. This representation must be applied to perform thermodynamic calculations on complex hydrocarbon systems because it is not possible to predict correctly mixture’s thermo-physical behaviour just using bulk values.

Besides permitting Thermodynamic calculations, pseudo-component representation eases jobs like Crude Oil Re-cutting (estimation of yield and quality of fractions with boiling ranges different from those available in the Crude Assay) and Crude Oil Blending (prediction of the quality of a mixture of Crude Oils), frequently needed by various applications.

This approach is currently widely applied by “state to art” process simulators and foresees:

- breaking down the oil fraction into a number of pseudo-components,
- calculation (through integration methods) of each pseudo-component’s Normal Boiling Point (NBP) and Specific Gravity (SG),
- estimation of other basic thermodynamic variables (Molecular Weight, Critical Variables, Acentric Factor) and other Chemical-Physical Properties applying various correlations fed by NBP and SG; many correlations have been developed for these purposes<sup>3</sup>.

Later on Riazi<sup>4</sup> developed a two-parameter distribution model NBP, Molecular Weight, Density and Refractive Index aimed to distribute mixture bulk properties over pseudo components.

This well established approach works fine for the properties involved with VLE calculations, but results not exhaustive for certain Chemical-Physical properties (like

---

<sup>2</sup> Wayne C. Edmister – Applied Hydrocarbon Thermodynamics – Volume 2 – Computer simulation techniques for thermodynamic properties and processes of discrete and pseudo components – Gulf Publishing Company

<sup>3</sup> API Technical Data Book – Petroleum Refining – Chapters 2,4

<sup>4</sup> Riazi, M., "Distribution Model for Properties of Hydrocarbon-Plus Fractions," Ind. Eng. Chem. Res., Vol. 28 (1989), pp. 1831-35.

Viscosity, Cold Properties, Antiknock, RVP) less important in case of process calculations but fundamental for planning applications. This depends on the lack of universal correlations reliably estimating these properties as function of basic thermodynamic variables.

The “Multidimensional Regressive” approach can be considered complementary to the traditional approach: in this case pseudo-component properties are not correlated to basic thermodynamic variables but are directly derived from the values contained in the Crude Assay.

Property distribution curves (each point representing a pseudo-component property value) result from the regression of the property values of the fractions characterised in the crude assay: this approach is not based on “universal” assumptions and establishes a direct link between Crude Assay data and pseudo-component quality.

A property distribution is “acceptable” if it permits to re-calculate the initial property value of each fraction by re-mixing the pseudo-components boiling in the same range.

To provide reliable results also in case of Crude Oil re-cutting it is important to account not only for Crude Assay Data but also for the “shape” of the distribution that should reflect the slow natural process which lead to Crude Oil generation.

### **Multi-dimensional Regression for Pseudo-Component Quality Calculation**

The data contained in a Crude Assay are not independent among each other and it is possible to identify equations putting in relation some of them.

The multi-dimensional regression method makes use of the relations that can be defined between Crude Oil, Oil Fractions and Pseudo-components to calculate reliable distribution property curves (Property versus Boiling Temperature).

Traditional regressive methods calculate – assumed a given mathematical function form (polynomial, logarithmic, exponential, etc) – the set of function’s coefficients permitting to fit at best the regressed data. Nevertheless this case presents particularities: defining property distribution means to find a “discrete” number of results, precisely one value for each pseudo-component boiling within the property’s existence domain: this permits to handle the problem applying operational research techniques rather than a traditional regression approach.

Handling the problem with operational research techniques permits to reach a higher degree of flexibility since the set of values constituting the result is not necessarily represented by a continuous mathematical function.

#### *Blending Methods*

An important issue to be considered when defining Crude Oil inner relations is the prediction of hydrocarbon mixtures’ properties: in some cases for a reliable prediction of

mixture's quality, property values must be converted into indexes before being linearly blended on weight or volume basis.

The calculation of properties with linear behaviour is represented by Equation 1, being  $P_i$  and  $Q_i$  the property value and the quantity (weight or volume) respectively of each blending component and  $P_M$  and  $Q_M$  the property value and the quantity of the mixture:

$$P_M \cdot Q_M = \sum_i (P_i \cdot Q_i)$$

*Equation 1 – Linear behaviour*

If linearisation indexes are needed, the formula becomes Equation 2 being  $Id( )$  the linearisation function applied to the property value:

$$Id(P_M) \cdot Q_M = \sum_i [Id(P_i) \cdot Q_i]$$

*Equation 2 – Linearisation indexes*

Table 2 lists the blending algorithms that are useful to predict the behaviour of main hydrocarbon properties in the corresponding boiling range domains.

PROPERTY	UNIT	Blending Rule	Boiling Range
Weight TBP Yield	% weight	Linear weight	Whole Crude
Volume TBP Yield	% volume	Linear volume	Whole Crude
Density@15°C	kg/dm <sup>3</sup>	Linear volume	Whole Crude
Sulphur Content	% weight	Linear weight	Whole Crude
Mercaptan Sulphur Content	% weight	Linear weight	Whole Crude
Kinematic Viscosity @50°C	cst	Index weight	Whole Crude
Kinematic Viscosity @100°C	cst	Index weight	Whole Crude
Acidity	mg KOH/gr	Linear weight	Whole Crude
Aromatics Content [FIA]	% volume	Linear volume	Gasoline
Naphthenes Content [FIA]	% volume	Linear volume	Gasoline
Paraffins Content [FIA]	% volume	Linear volume	Gasoline
Aromatics Content [Gas chromatography]	% weight	Linear weight	Gasoline
Naphthenes Content [Gas chromatography]	% weight	Linear weight	Gasoline
Paraffins Content [Gas chromatography]	% weight	Linear weight	Gasoline
Octane Number Motor Method (MON)		Linear volume	Gasoline
Octane Number Research Method (RON)		Index volume	Gasoline
RON + Tetra Ethyl Lead 0.5		Index volume	Gasoline
RON + Tetra Methyl Lead 0.5		Index volume	Gasoline
Reid Vapour Pressure	PSIA	Index volume	Gasoline
Cyclopentane Content	% weight	Linear weight	Gasoline
Cyclohexane Content	% weight	Linear weight	Gasoline
i-Hexanes Content	% weight	Linear weight	Gasoline
n-Hexane Content	% weight	Linear weight	Gasoline
Benzene Content	% weight	Linear weight	Gasoline
Methylcyclopentane Content	% weight	Linear weight	Gasoline
CC5 Content	% weight	Linear weight	Gasoline
Freezing Point	°C	Index volume	Mid Distillates
Cloud Point	°C	Index volume	Mid Distillates
Pour Point	°C	Index volume	Mid Distillates
Aniline Point	°C	Linear weight	Mid Distillates
Total Nitrogen Content	ppm weight	Linear weight	Mid Distillates and Residua
Basic Nitrogen Content	ppm weight	Linear weight	Mid Distillates and Residua
Ash Content	ppm weight	Linear weight	Mid Distillates and Residua
Asphaltenes Content	% weight	Linear weight	Mid Distillates and Residua
Conradson Carbon Residue	% weight	Linear weight	Mid Distillates and Residua
Nickel Content	ppm weight	Linear weight	Mid Distillates and Residua
Vanadium Content	ppm weight	Linear weight	Mid Distillates and Residua
Wax Content	% weight	Linear weight	Mid Distillates and Residua

Table 2 – Crude Oil Properties Blending Method

### Quality balances

Let's now consider the relation between the bulk Crude Oil property value and the property values of Crude Oil fractions: the bulk Crude Oil is the mixture of Crude Oil fractions thus, once identified a reliable Blending Method, it is possible to define a property balance formalising the relation.

Being formalised according to specific Blending Methods, these equations include both property values and mixing component's yields: thus the regression of pseudo-component's property values (Property versus Boiling Temperature) cannot abstract from component's yields and is multidimensional.

Similar relations can be defined between pure/pseudo components and Oil fractions and between pure/pseudo components and Crude Oil.



*Natura non facit saltum (Nature does nothing in jumps)*

The well-known Latin adage “*Natura non facit saltum*” has been frequently applied to synthesise that nature systems move gradually.

Crude Oil is the result of a natural process lasting millions of years, hence it is reasonable to affirm that, (except than in some particular cases) property distribution curves ought to have a harmonic shape, without jumps or discontinuities.

To model this natural behaviour specific equations are considered by the multidimensional regression method avoiding distribution jumps and discontinuities.

*Weights and Reliability Factors*

As previously mentioned, inconsistent data may be present in the Crude Assay causing quality equations unbalances, or the respect of quality balance would lead to disharmonic distribution curves.

In these cases it is necessary to highlight data inconsistencies or to be able to find the best compromise between input data and curve shape.

For this purposes the method foresees *Reliability Factors* (changing the acceptable range of values of Oil Fractions and Crude Oil quality equations) and *Weights* permitting to influence regression results privileging either the distribution shape or the quality balances.

Thanks to these tools it is possible to define punctual or global priorities to be considered by regression algorithm in order to exclude the contribution of inconsistent data.

### Sulphur Distribution Example

As an example we will to define the Sulphur pseudo-component distribution curve of a Crude Oil starting from the data reported in Table 3:

Oil Fraction	Boiling Range [°C]	Yield [%Wt]	Sulphur [%Wt]
Whole Crude	C2 – 850	100	1.85
FR Naphtha	C5 – 160	15.6	0.08
Kerosene	160 – 240	12.3	0.29
Gasoil	240 – 360	20.7	1.37
Atmospheric Residue	360 – plus	50.0	3.05

Table 3 – Sulphur Distribution Assay Data

Problem input is summarised by Figure 2; typical pseudo-components boiling ranges are 10°C below 450°C, 30°C from 450 to 690°C and one final pseudo-component up to Crude EP. Thus in this case the crude will be represented by 50 pseudo components (41+ 8 + 1).

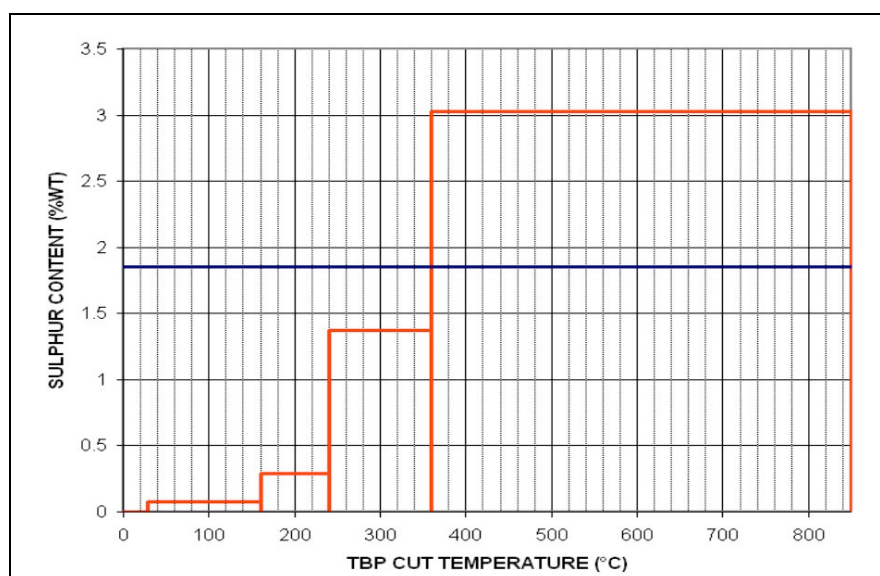


Figure 2 – Problem Graphical Representation

Let's call:

$S_i$  = Sulphur content of pseudo component "i" (result of regression)

$Y_i$  = Yield of pseudo component "i" (calculated by TBP data regression)

$f_{iF}$  = Fraction of pseudo component "i" boiling within the range of fraction "F"

$S_F$  = Sulphur content of TBP fraction

$S_C$  = Sulphur content of Crude Oil

$Y_F$  = Yield of TBP fraction

Sulphur content is blended linearly in weight (see Equation 1), thus the following balances should be considered:

For each pseudo component boiling in given fraction's range:

$$\sum_i (S_i \cdot Y_i \cdot f_{iF}) = S_F \cdot Y_F$$

Equation 3 – Sulphur Example – Fraction Balance

In this specific case:

$\sum_i (S_i \cdot Y_i \cdot f_{iF}) = 0.08 \cdot 15.6$	<i>(with <math>f_{iF} = 1</math> below 160°C)</i>
$\sum_i (S_i \cdot Y_i \cdot f_{iF}) = 0.29 \cdot 12.3$	<i>(with <math>f_{iF} = 1</math> in the range 160-240°C)</i>
$\sum_i (S_i \cdot Y_i \cdot f_{iF}) = 1.37 \cdot 20.7$	<i>(with <math>f_{iF} = 1</math> in the range 240-360°C)</i>
$\sum_i (S_i \cdot Y_i \cdot f_{iF}) = 3.03 \cdot 50.0$	<i>(with <math>f_{iF} = 1</math> beyond 360°C)</i>

Moreover for each pseudo component:

$$\sum_i (S_i \cdot Y_i) = S_C \cdot 100$$

Equation 4 – Sulphur Example – Crude Oil Balance

In this specific case:

$\sum_i (S_i \cdot Y_i) = 1.85 \cdot 100.0$
---

No reliability factors have been associated to input data since all the fractions of this example are contiguous and there is no risk of inconsistent input due to oil fraction's cut points overlapping.

Additional equations have been considered to control the distribution shape and to specify input data reliability (permitting to manage input inconsistencies).

All these equations are fed to the Algorithm that finds the distribution best matching Assay Data and Distribution Shape.

The results of Multidimensional Regression (Blue Line) and the Broken Line obtained joining Fraction's Sulphur Values (Red Line) are shown in Figure 3. Corresponding values are reported in Table 4:

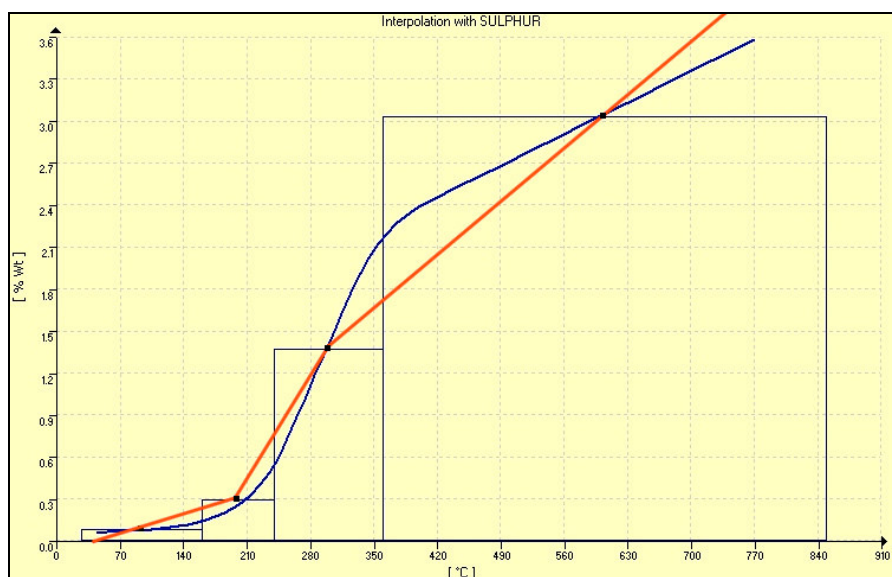


Figure 3 – Sulphur Example – Regression Results

PSC Name	Initial BP [°C]	Final BP [°C]	Yield [% Wt.]	Multidim. Regression	Broken Line	PSC Name	Initial BP [°C]	Final BP [°C]	Yield [% Wt.]	Multidim. Regression	Broken Line
A45	40	50	1.297	0.057	0.000	C95	290	300	1.790	1.327	1.316
A55	50	60	1.297	0.061	0.004	D05	300	310	1.790	1.476	1.397
A65	60	70	1.297	0.065	0.024	D15	310	320	1.738	1.624	1.452
A75	70	80	1.297	0.068	0.044	D25	320	330	1.688	1.772	1.506
A85	80	90	1.297	0.072	0.063	D35	330	340	1.638	1.910	1.560
A95	90	100	1.297	0.076	0.083	D45	340	350	1.591	2.025	1.615
B05	100	110	1.297	0.081	0.103	D55	350	360	1.544	2.121	1.669
B15	110	120	1.297	0.087	0.122	D65	360	370	1.263	2.201	1.724
B25	120	130	1.297	0.094	0.142	D75	370	380	1.226	2.268	1.778
B35	130	140	1.297	0.103	0.162	D85	380	390	1.190	2.323	1.833
B45	140	150	1.297	0.115	0.182	D95	390	400	1.156	2.369	1.887
B55	150	160	1.337	0.130	0.201	E05	400	410	1.122	2.408	1.941
B65	160	170	1.379	0.148	0.221	E15	410	420	1.089	2.440	1.996
B75	170	180	1.421	0.171	0.241	E25	420	430	1.057	2.472	2.050
B85	180	190	1.465	0.199	0.260	E35	430	440	1.027	2.504	2.105
B95	190	200	1.511	0.234	0.280	E45	440	450	0.997	2.536	2.159
C05	200	210	1.557	0.279	0.344	E65	450	480	2.991	2.601	2.268
C15	210	220	1.605	0.334	0.452	E95	480	510	2.991	2.697	2.431
C25	220	230	1.655	0.403	0.560	F25	510	540	2.991	2.793	2.595
C35	230	240	1.706	0.490	0.668	F55	540	570	2.991	2.889	2.758
C45	240	250	1.759	0.598	0.776	F85	570	600	2.991	2.986	2.921
C55	250	260	1.790	0.734	0.884	G15	600	630	2.991	3.082	3.084
C65	260	270	1.790	0.882	0.992	G45	630	660	2.991	3.178	3.248
C75	270	280	1.790	1.030	1.100	G75	660	690	2.991	3.275	3.411
C85	280	290	1.790	1.179	1.208	H70	690	850	15.949	3.579	3.928

Table 4 – Sulphur Example – Regression and Broken Line Results

Back – calculating Oil Fractions' Sulphur content from the pseudo-component values obtained through multidimensional regression and broken line it is possible to quantify the percentile error involved by property distribution process.

The error is negligible (mainly due to numerical rounding) in case of multidimensional regression while ranges from –6.6% up to 34.1% in case of “Broken Line” distribution. Back-calculation results are reported in Table 5.

Oil Fraction	Initial BP [°C]	Final BP [°C]	Mid BP [°C]	% S Assay	Multidim. Regression		Broken Line	
					Calculated	ERR %	Calculated	ERR %
FR Naphtha	27	160	93.5	0.08	0.080	-0.2%	0.090	12.2%
Kerosene	160	240	200	0.29	0.290	-0.1%	0.389	34.1%
Gasoil	240	360	300	1.37	1.370	0.0%	1.279	-6.6%
Atmospheric Residue	360	850	605	3.03	3.030	0.0%	3.003	-0.9%

Table 5 – Sulphur Example – Assay data back calculation

Once property distribution to pseudo-component is available it is possible to estimate the Sulphur content of oil fractions not characterised in the Crude Assay.

Table 6 shows the results of the calculation performed with the two distributions: the reported percentile error is, in this last case, referred to the value estimated using multidimensional regression property distribution.

Initial BP [°C]	Final BP [°C]	Mid BP [°C]	% S Assay	Multidim. Regression		Broken Line	
				Calculated	ERR%	Calculated	ERR%
140	220	180	-	0.206	-	0.278	34.96%
380	400	390	-	2.346	-	1.859	-20.74%
400	510	455	-	2.565	-	2.208	-13.93%
510	850	680	-	3.291	-	3.438	4.49%

Table 6 – Sulphur Example – Different Cuts property estimation

The percentile error calculated in this last example gives an idea of the level of uncertainty involved with the indirect estimation of oil fractions not characterised in the Crude Assay. Since it takes in consideration quality balances, the multidimensional regression approach provides the “intrinsic” validation of distribution results reducing the potential error associated to these operations.

The example described above is particularly simple, Property Distribution Problems may be much more complicated for the higher number of fractions involved, fractions overlapping and inconsistent input data: Figure 4 summarises a typical regression example.

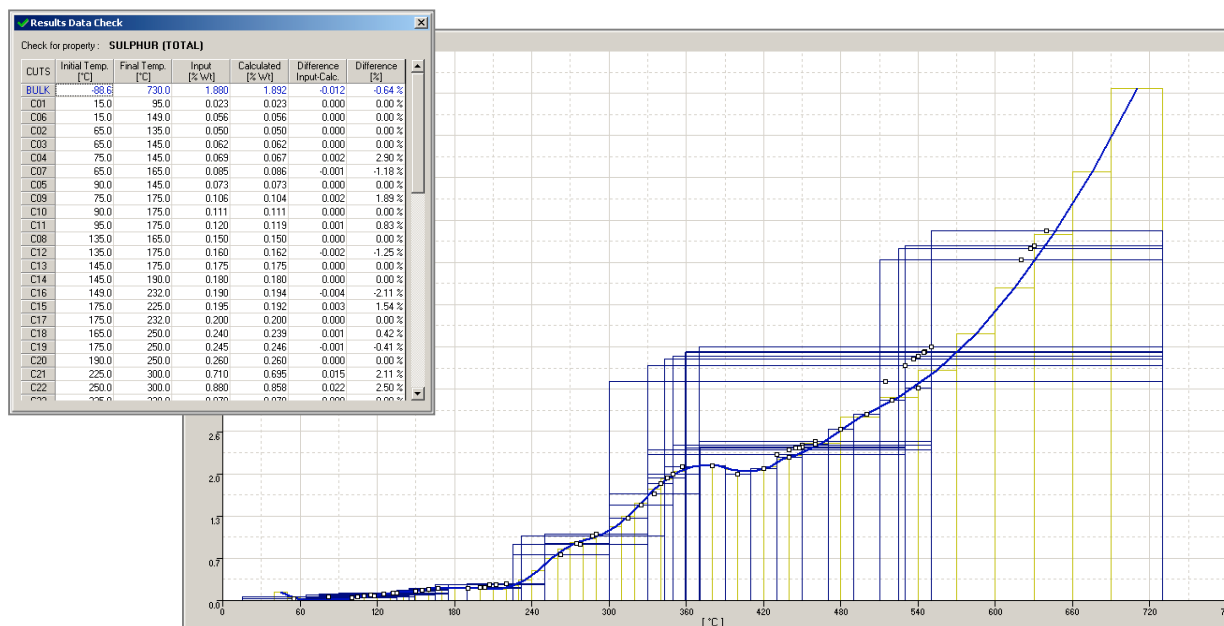


Figure 4 – Sulphur Property Distribution – Real Case

### Crude Oil Re-cutting and Blending

A similar approach can be applied to distribute over pseudo-component any crude assay property whose blending method is known; this distribution process will characterise the pseudo-components providing them with the information contained in the Crude Assay.

Crude Oil's behaviour can now be modelled using the pseudo-component list, with a higher flexibility in crude oil data handling processes: problematic jobs like crude oil re-cutting and blending are simply solved just performing pseudo-component blending calculations.

Crude Oil Re-cutting can be executed by blending together the pseudo-components boiling within each oil fraction's range. Pseudo-component's yields will determine the blending recipes necessary for calculations.

Crude Oil mixtures can be calculated by "one to one" blending of the crude oils' pseudo-components boiling in the same range: blending recipes will depend on respective pseudo-component's yields and on Crude blend composition.

Figure 5 shows the density curve characterising the blend of two Crude Oils (Es Sider 45% – Kirkuk 55% in this example): each point of the Blend Curve (Blue Curve) is calculated blending the corresponding oil pseudo-components of the mixed crude oils (Red and Green Curves).

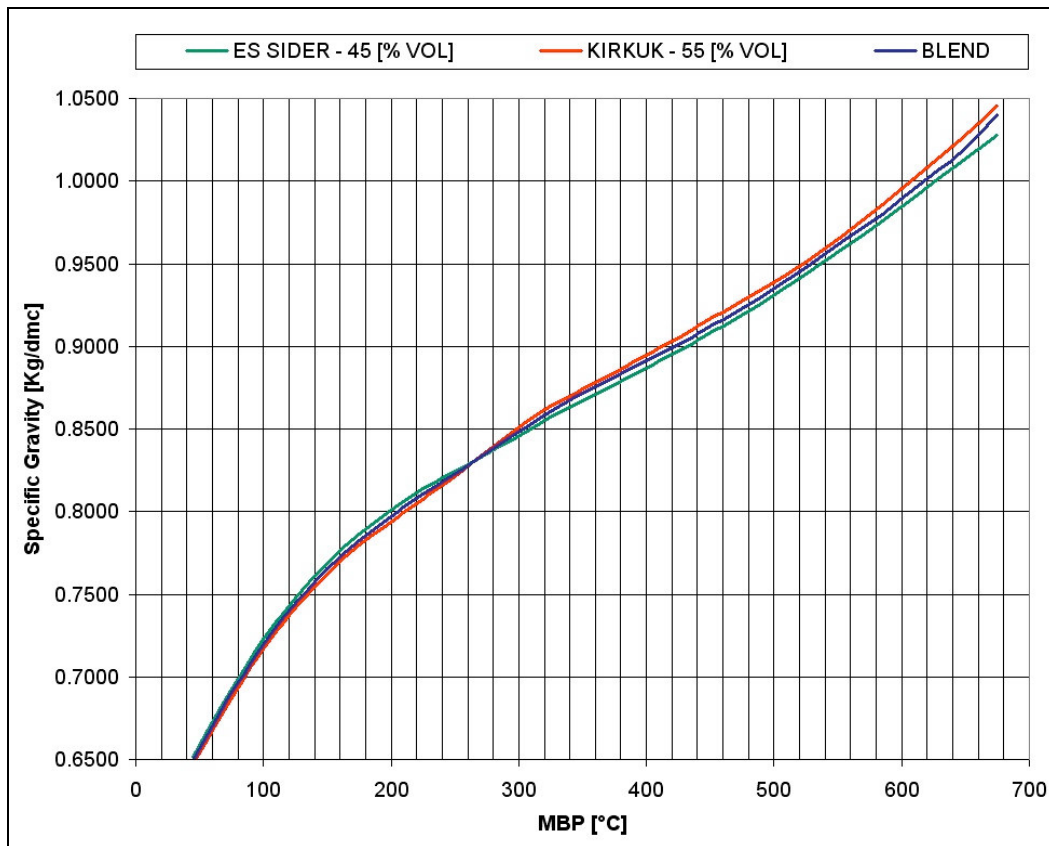


Figure 5 – Crude Oil Blend Density Distribution Curve

## **Implementing the Method: CUTS**

### *CUTS Generalities*

The multidimensional regression method is implemented by CUTS, the “Prometheus DSS” application dedicated to the elaboration and management of crude oil data.

CUTS characterises every Crude Oil as a mix of pure components (C5 minus) and “pseudo-components” (C6 plus), which overall cover the entire crude boiling range. Each pseudo component envelops pure components boiling in a narrow range of 10/30 °C.

This level of characterisation is quite “unusual” for planning and scheduling commercial applications, but permits to embed shortcut plant simulators into the models.

Applying the Multidimensional regression, CUTS’ elaborates crude assay data, finding a harmonic and consistent distribution of property values to pseudo-components. Once the pseudo-components property values are available, it is possible to estimate the properties of any fraction of the crude oil, keeping the results consistent with crude assay data.

The algorithm is designed to calculate consistent values for contiguous pseudo components, while special operating parameters are available to harmonise the shape of the resulting curve, if necessary.

Moreover the system provides proper user calibration and takes care of reliability of input data: if the original assay is consistent, fraction and global balances will be always satisfied, otherwise inconsistent input data will be highlighted. The curves are always validated by comparison with original input values.

The pseudo-component characterisation eases the calculation of the properties of fractions resulting from crude oils mixtures: the crude oil mix is characterised by a list of pseudo-components whose properties are calculated blending the pseudo-components of the original crude oils with the same boiling range.

### *Example 1: Simulating the Distillation Process*

Pseudo-component characterisation is the starting point of further calculations: one example is the prediction of Distillation effluents’ yields and properties.

The main issue to cope with when calculating a Distillation consists in the definition of the obtainable fractionation degree: the fractionation obtained with ASTM D2892 method (TBP Distillation) – that is intimately connected to pseudo-component definition – is higher than the one usually observed in industrial plant.

Assuming TBP as the higher fractionation degree theoretically obtainable, we can think to simulate a poorer fractionation assuming a different distribution of pseudo-components over distillation products.

When performing re-cutting calculations it is possible to consider either a straight distribution (each cut contains only the pseudo-components within its Boiling Range, Figure

7) or a complex distribution (each cut contains also the pseudo-components boiling outside its boiling range, Figure 8).

In the first case we reproduce the results of a laboratory characterisation since the fractionation efficiency assumed in the calculation is the same of the TBP distillation (ASTM D2982).

In the second case we reproduce the results obtainable by an industrial distillation characterised by lower fractionation efficiency. In this case, besides the fractionating structure (both single and multi column systems are managed), for each Oil fraction the following parameters must be provided:

- **Distillation Cut Point Temperature:** referred to feed TBP, defines the yield that can be obtained for a given cut depending on the feed distillation curve.
- **Fractionation Index:** defines the quality of fractionation obtainable between two consecutive fractions: low values mean good fractionation, high values mean poor fractionation.

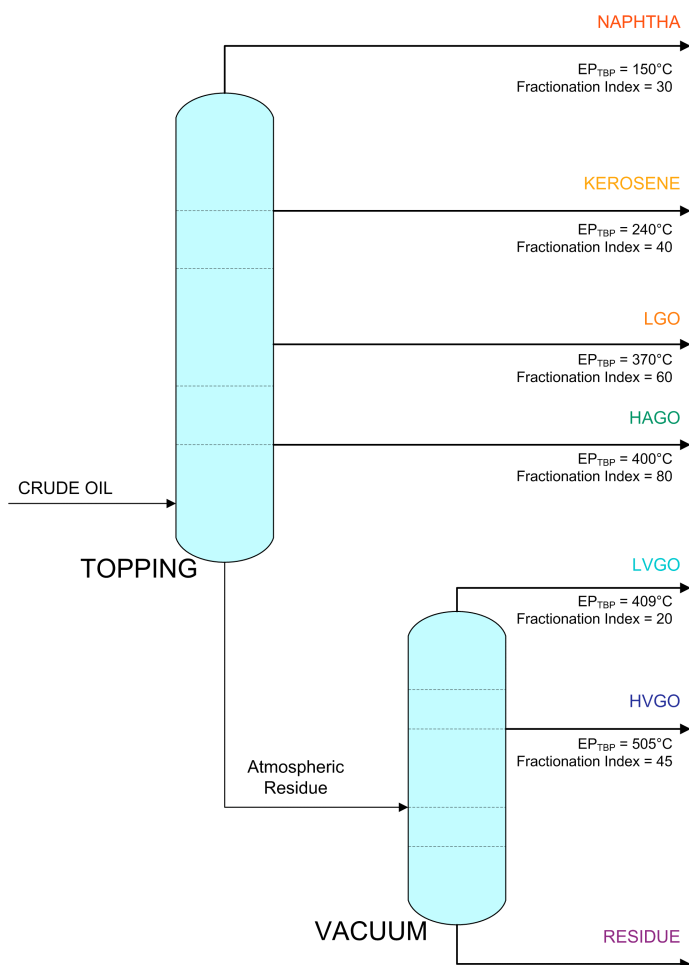


Figure 6 – Distillation example

Using these values, the algorithm calculates the distribution of feed pseudo-components to actual distillation effluents.

Let's consider the example showed in Figure 6: we want to estimate the quality of the products of a Topping Vacuum distillation unit given the quality of the feedstock and the TBP cut temperatures (related to feedstock curve). In particular we want to quantify the impact of fractionation on products quality: then we will compare the results from a "TBP Like" fractionation with those from a "Real" one, applying the typical indexes reported in figure.



Figure 7 shows what would be the distribution of feed pseudo-components to distillation fractions having the maximum fractionation efficiency (like in TBP laboratory tests): each pseudo-component of the feed boiling within a given range will totally remain in the same range after the distillation.

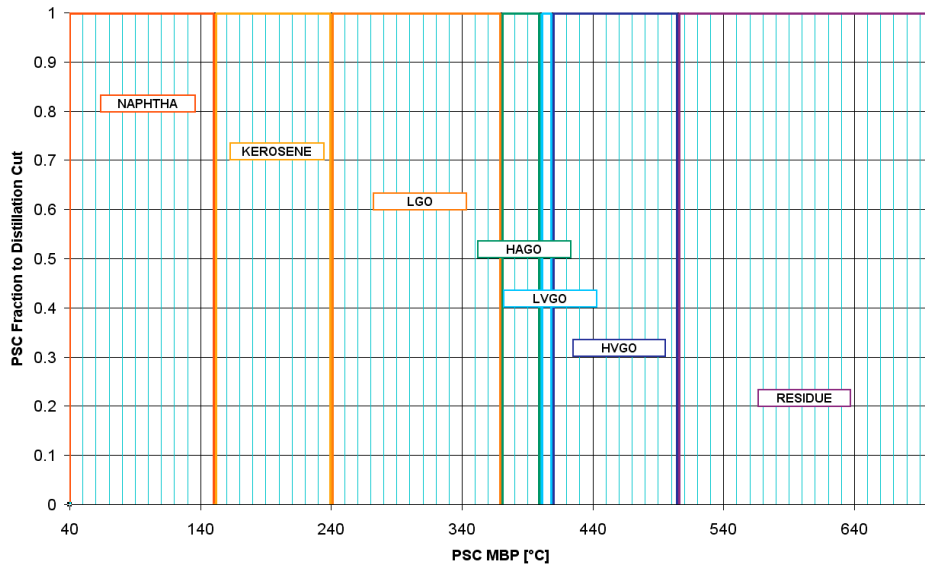


Figure 7 – Pseudo-component fraction to distillation products for TBP fractionation

Figure 8 shows the pseudo-component distribution functions calculated using Fractionation Indexes: in this case the same pseudo-component can be distributed to more products and effluents' initial and final boiling points do not coincide anymore with TBP cut points.

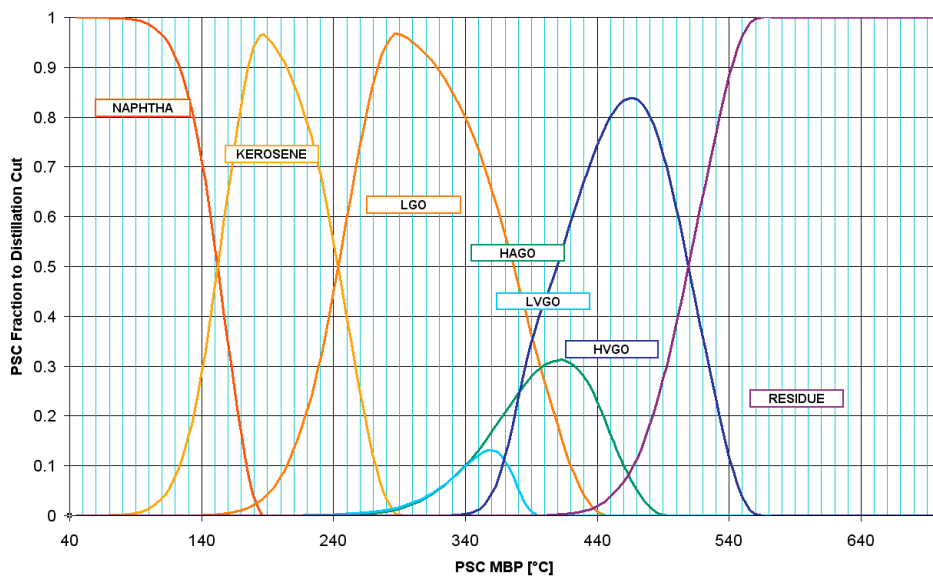


Figure 8 – Pseudo-component fraction to distillation products for real fractionation

The different pseudo-component distribution due to real fractionation affects both products' distillation curves and effluent's property values (the distillation tails resulting from pseudo-component distribution of Figure 8 as well as the comparison of the main qualities are showed in Figure 9).

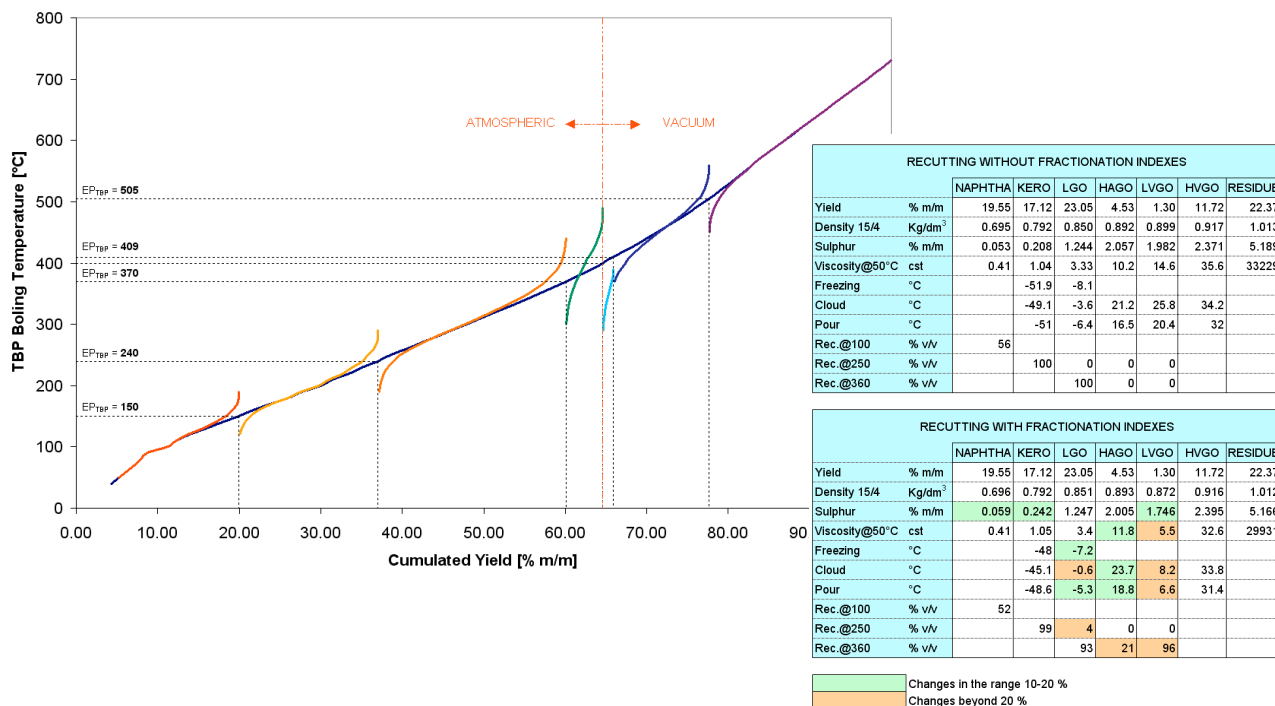


Figure 9 – Distillation curves and main quality calculated for real fractionation

Besides the important quality variations of atmospheric mid distillates (mainly in case of cold properties) it impresses the quality change of LVGO whose TBP curve is completely below the crude oil TBP in the correspondent boiling range. This is possible thanks to the vacuum column that – with its higher fractionation efficiency – permits to recover the lighter fractions lost in the atmospheric column for the poor fractionation of the HAGO cut.

Fractionation indexes' values are empirically calculated by “trial and error” starting from field data. Once identified a reliable set of data, it can be applied for any different feed.

*Example 2 – Characterising a reconstituted – Crude Oil*

An inland refinery is placed nearby an oil well and serves the local market. Since there are no dedicated pipelines available to transfer the products not consumed locally (80% of the Light Naphtha and 60% of the Fuel Oil) these ones are blended back into the crude oil that is sent by pipeline to a coast refinery.

We want to characterise the feedstock of the coast refinery; the problem is summarised by Figure 10.

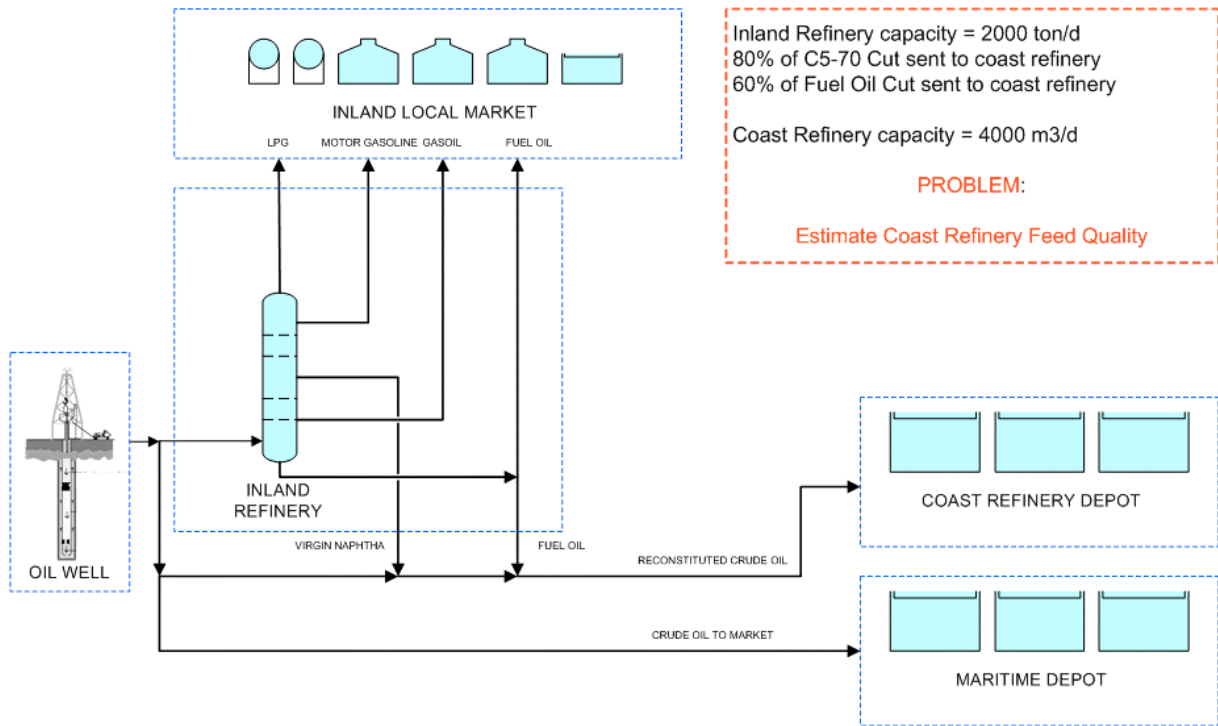


Figure 10 – Reconstituted Crude Oil Problem

This problem has been handled with CUTS oil blending feature: Naphtha and Residue fractions from the inland refinery have been characterised simulating the distillation process and re-blended with the crude to produce the reconstituted oil database.

TBP distillation curves (of blending components and reconstituted oil) and Crude oil bulk qualities are compared in Figure 11.

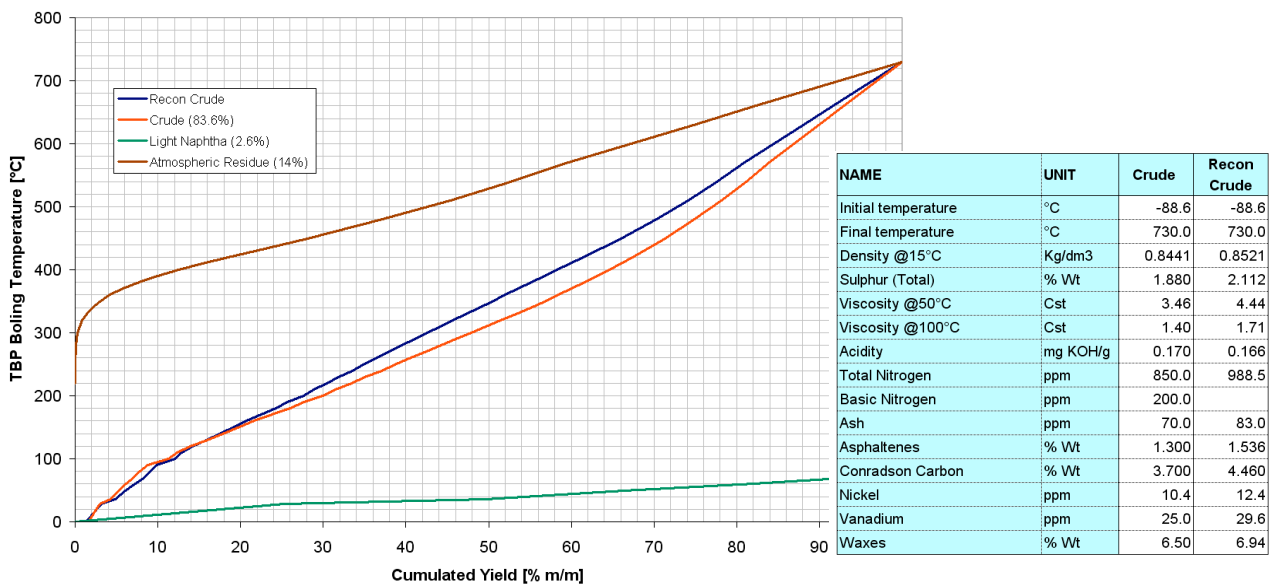


Figure 11 – Reconstituted Crude Oil Quality Change

### Example 3 – Characterising a Crude Oil from Plant data

Sometimes the only data available for crude assay characterisation are those of the distillation unit products; these last are normally influenced by the lower fractionation efficiency and by measurement errors typical of the real plant. Moreover the TBP test method is time consuming and not practical in the ordinary refinery operation and consequently the products distillation curves available are realised with quicker tests like ASTM D86, ASTM D1160 or ASTM D2887: this means that to characterise the unit feedstock we need first to homogenize the distillation data converting them into TBP data with the help of conversion methods. Various methods have been developed and published for these purposes (Edmister, Riazi, Daubert).

A new feature has been recently added to CUTS permitting to characterise a crude oil not only with standard crude assay fractions (fractionated by a TBP column) but also with plant fractions (characterised with different tests) and without disposing of the Crude Oil TBP curve. The procedure homogenises distillation data and elaborates them to produce the feedstock TBP curve. Moreover the detected fractionation efficiency is applied within property curves elaboration process permitting to use plant products property values in the same way of those of standard TBP fractions.

A typical dataset produced by a plant test run is summarised in Figure 12: to characterise the TBP curve of the feedstock we dispose only of Topping products distillations (D86 and D1160), yields and densities.

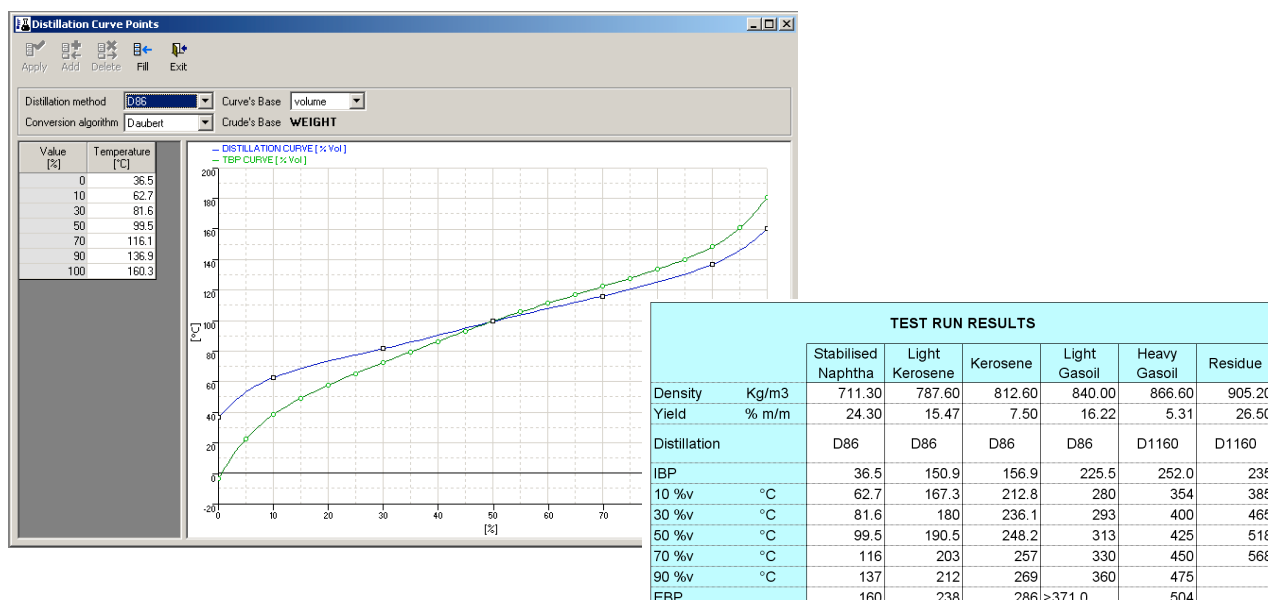


Figure 12 – Plant data elaboration for crude oil characterisation

These data are homogenised to TBP data and elaborated to produce the TBP Weight and Volume distillation curve of the feedstock that are showed in Figure 13; distillation

products TBP curves are showed as well giving an idea of the poor fractionation efficiency of the real unit.

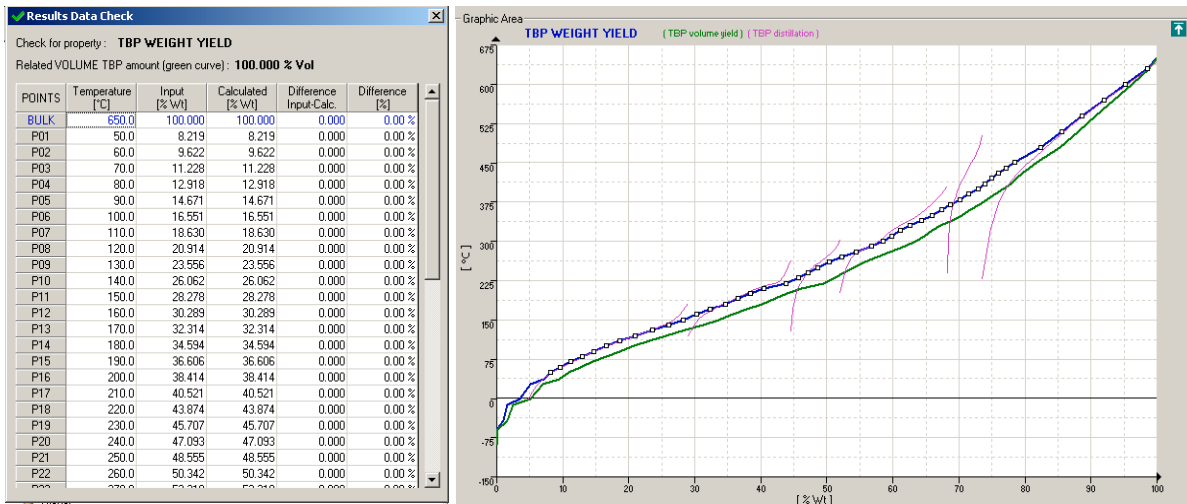


Figure 13 – Plant feed distillation curve rebuilt from product data

Figure 14 shows the pseudo component fraction to distillation products calculated from the input curves: this information is considered not only for feedstock TBP curve definition but also for the elaboration of property distribution curves.

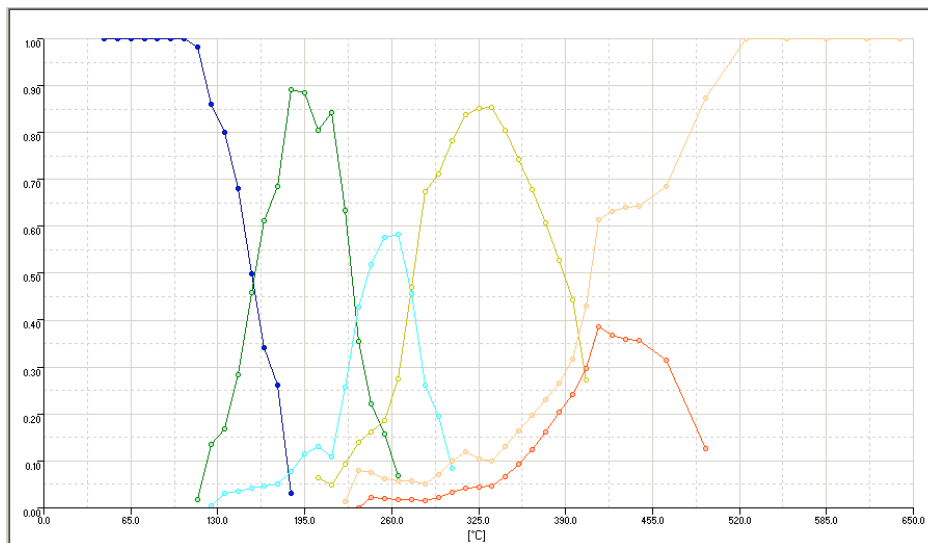


Figure 14 – PSC distribution derived from products distillations

Figure 15 shows the density distribution calculated for this example: even though provided data are from a real plant, this distribution is totally comparable to that obtainable by the elaboration of crude assay data.

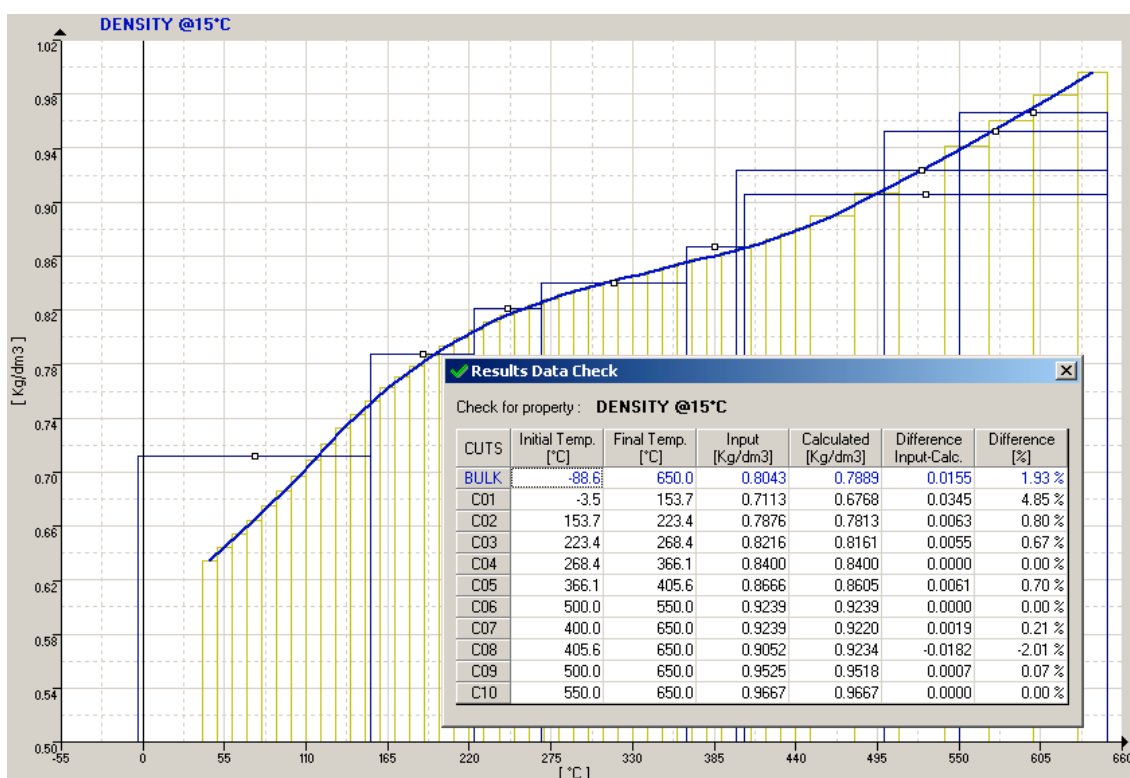


Figure 15 – Calculated distribution for Density

## Conclusions

Crude Oil pseudo-component characterisation permits a higher degree of flexibility while performing calculations both in process engineering and in refinery operation planning disciplines.

The weak point of this approach (especially in case of refinery planning and scheduling applications where the reliable prediction of “difficult properties” is needed) consists in pseudo-component property estimation.

Prometheus has implemented an innovative method (multidimensional regression) permitting to distribute Crude Assay Data over pseudo-components avoiding the errors typically involved by the generation of property distribution curves.

The method, that is implemented by CUTS™, permits to improve the accuracy of calculations like, “crude oil re-cutting”, “crude oil blending” and “crude oil distillation in industrial units” (widely applied by refinery planning applications) and correspondingly the reliability of planning models’ suggestions.