



Monday, June 17, 2013

VMGSim Courses

Hands on Introduction to VMGSim

August 28, 2013 and November 20, 2013.

Calgary, AB, Canada

This one-day course provides process engineers an introduction to VMGSim's features and capabilities using a series of tutorials and demonstrations.

[See full description and topics covered in the course here](#)

To register or for more information, please email us at courses@virtualmaterials.com

Overview of VMGSim

June 12 & 13, 2013

Tulsa, OK, USA

This two-day VMGSim course is a hands-on course where attendees will spend a significant amount of time running VMGSim. You are guided through the creation of a series of typical simulation case examples in VMGSim covering gas processing, petrochemicals, crude oil characterization and fractionation, gas treating with amines and sulfur recovery. The final training problem set will be determined after course signup is complete.

[See full description and topics covered in the course here](#)

To register or for more information, please email us at gerald@virtualmaterials.com

Overview of VMGSim

September 11 & 12, 2013

Houston, TX, USA

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Upcoming Events

Webinars

Oil Characterization in VMGSim, through examples
Thursday, June 20th, 2013

VMGSim Flowsheeting Basics - A Review

Wednesday, July 3rd, 2013

[Register Here](#)

Courses

Hands on Introduction to VMGSim
Calgary
Feb 20

Dynamic Simulation with VMGSim
Houston
March 13 & 14

Overview of VMGSim
Houston
March 27 & 28

[Details...](#)

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recovery. The final training problem set will be determined after course signup is complete.

[See full description and topics covered in the course here](#)

To register or for more information, please email us at gerald@virtualmaterials.com

VMGSim Webinars

These webinar series are designed to help new and seasoned VMGSim users learn about new features and to perform common tasks in a faster and more efficient way. Please feel free to pass this onto colleagues who may be interested.

The schedule and topics for the next two VMGSim Webinars are:

Date	Time (MDT)	Topic
Thursday, June 20, 2013	11:00 AM to 12:00 PM	Oil Characterization in VMGSim - Through Examples
Saturday, July 3, 2013	11:00 AM to 12:00 PM	VMGSim Flowsheeting Basics - A Review

[Register here](#)

What's New

Meet VMG's New Sales Partner in South East Asia



We are pleased to announce our sales partnership with with EDSA Solutions Pte Ltd. for South East Asia, covering Singapore, Malaysia, Indonesia and Thailand.

The new sales reps above finished their VMGSim training and we anticipate great things from them. Welcome aboard!

Contact Info:

Engineering Design Solutions Asia
www.eds-asia.com
EDS Asia Sdn. Bhd.
L1-33, SSTwo Mall,
No. 40, Jalan SS 2/72,
47300 Petaling Jaya, Selangor
Malaysia
Tel: +60 (3) 7956-3399
Ask for Keane Cheng

Warm Welcome to Our New Sales Reps CMSI Korea Inc.

CMSI Korea Inc. is VMG's new South Korean sales representative. Sales Manager David Kim from CMSI Korea Inc. will be our contact in South Korea.

Contact Info:

David Kim

Sales Manager

Suite 701, 110 Yeoksam-ro, Gangnam-gu, Seoul, 135-080 Korea

Phone: 82-2-2051-1533

Mobile: 82-10-4607-1224

E- mail: david.kim@cmsikorea.com

Out and About

VMG in Japan for the PIONA Reactive Refinery Seminar - May 24 to June 1, 2013



Kawasaki, JAPAN - Glen (top) and Norio present VMG's PIONA reactive refinery seminar on May 31st to Japanese attendees. Technical presentations were later followed by hands-on training at the daylong event. This marks another year of seminars from VMG Japan on new development technology of VMGSim.



VMG in Malaysia Training new Sales Reps

Juan Montelongo of VMG Calgary in Malaysia training the new VMG Sales Representatives for the South East Asia region on VMGSim. The intensive 5-day course covered all the basic and advanced features VMGSim, as well as some of the applications relevant to the region.



Pictured (Left to Right): Keane Cheng, Juan Montelongo, Lianne Choong, Diana Ann, Sharon Leong.

Characterizing and Installing Crude Oils in VMGSim

Characterizing and Installing Crude Oils in VMGSim: Gamma Distribution Example

Herbert Loria – Calgary

The objective of this article is to show how characterization of crude oils can be achieved using the Gamma Distribution option from the oil environment of VMGSim™ 7.0. The scenario of this example shows a situation where only bulk properties are available for characterization.

Gamma Distribution Example

Sometimes process or reservoir engineers face the challenge of characterizing oils with no TBP analysis and only few bulk properties. This example goes through the characterization of a reservoir oil for which the light ends and, the light ends free bulk molecular weight and standard liquid density are provided.

Oil Summary

Light Ends	Vol Fraction
Ethane	3.54E-04
Propane	0.0025
Iso-Butane	0.0014
n-Butane	0.0071
Iso-Pentane	0.0053
n-Pentane	0.0081
n-Hexane	0.0031
n-Heptane	0.0159

Light Ends free Molecular Weight = 170 g/gmol

Light Ends free Liquid Density @ 60 F = 857 kg/m³

To start the characterization, select a **Thermodynamic Model** and install the light ends compounds from the **Component** list in the **Thermo Model** form.

Properties of: RootThermo

Pure Compound Search | **Hypothetical Compound**

Compound

Family ALLComponents Detail Family Groups

Names
 Formula
 CASN

8 Selected Compound(s)

ETHANE	<input type="button" value="Sort ..."/> <input type="button" value="Compare Comp .."/> <input type="button" value="Delete"/> <input type="button" value="Delete All"/> <input type="button" value="Comp Group ..."/>
PROPANE	
ISOBUTANE	
n-BUTANE	
ISOPENTANE	
n-PENTANE	
n-HEXANE	
n-HEPTANE	

Property Package Components **Settings** Boiler Plate

Once this is done, open the Oil characterization environment. In the Light Ends tab, check the **Light Ends** box, set the **Light End Basis** to **Volume** and enter the light ends data. Note the **Use LE in Bulk Oil Props** check box remains blank, since the light end properties will not be taken into account in the properties of the light ends free fraction.

Oil_1. Assay_1

Experimental Information
 Gamma Distribution
 Cn Compositional Analysis

Assay Information

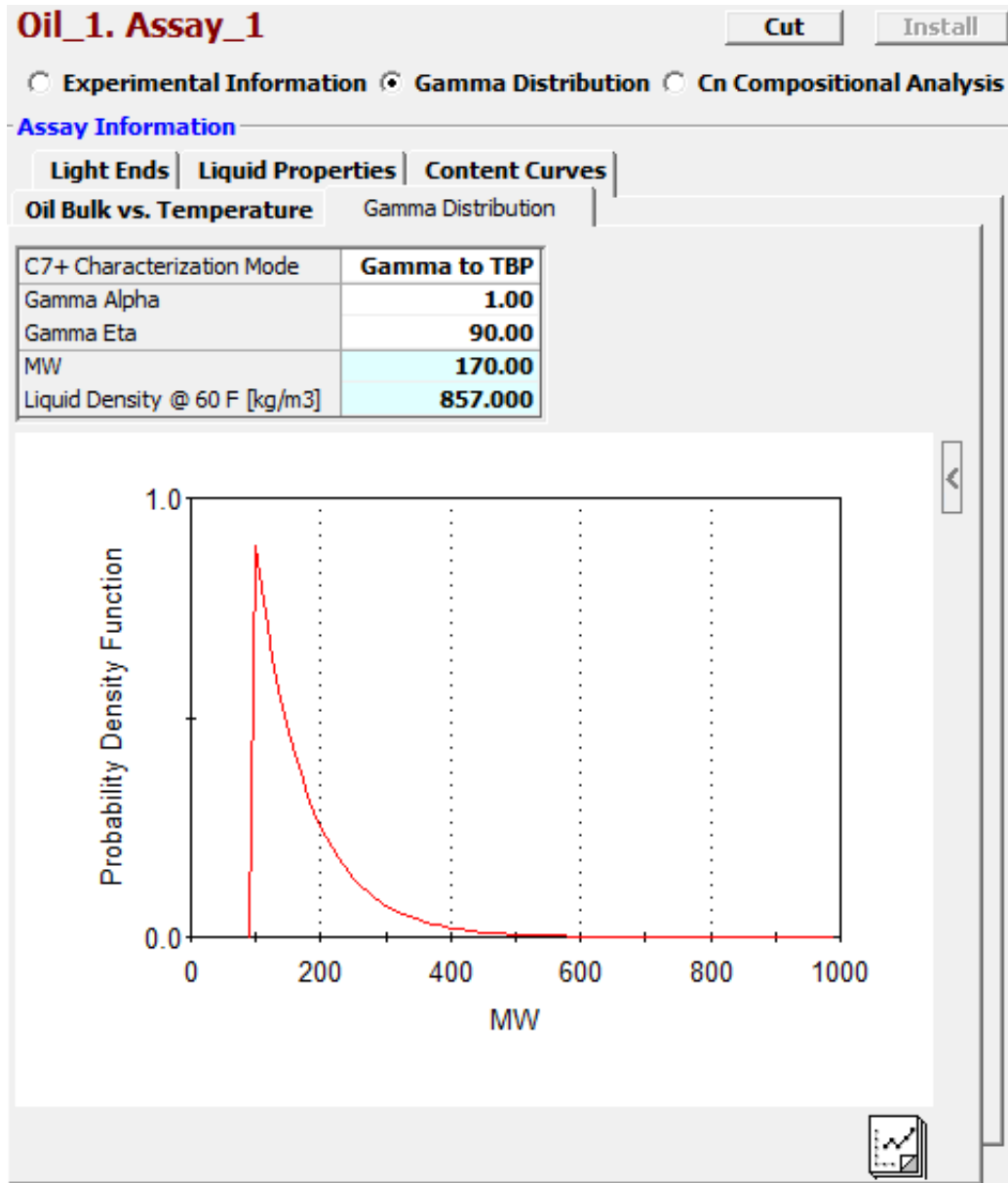
Light Ends
 Use LE in Bulk Oil Props

Light Ends Calculation Method
 Specify
 Auto Calculate
 Match

Sum = 4.382E-02 Light Ends Basis =

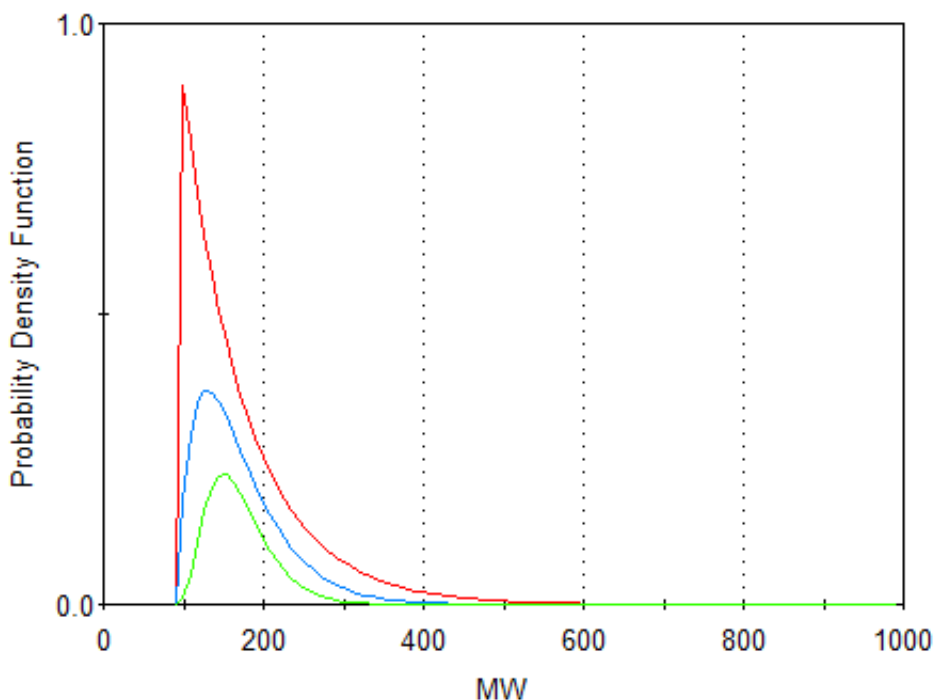
ETHANE	3.54E-04
PROPANE	0.0025
ISOBUTANE	0.0014
n-BUTANE	0.0071
ISOPENTANE	0.0053
n-PENTANE	0.0081
n-HEXANE	0.0031
n-HEPTANE	0.0159

Go to the **Gamma Distribution** tab, select the **Gamma to TBP** option and add the light ends free molecular weight and standard liquid density in their respective boxes.



Note that as soon as the molecular weight is entered, the probability density function (PDF) is plotted against the molecular weight. The shape of this curve gives an idea of the molar distribution for the Gamma characterization. Changing the parameters a and η produces a different distribution.

For example, changing a to 2.0 or 4.0 will produce the distributions shown in the following figure (red line $a = 1.0$, blue line $a = 2.0$, green line $a = 4.0$).



It can be observed how the molar distribution changes with the value of α . This type of parametric analysis can help to decide which molar distribution suits better the oil characterization, depending on the desired distribution of the molecular weight of the pseudo components.

In our example we will keep $\alpha = 1.0$ because this is the recommended value when dealing with reservoir oils according to Whitson and Brule [1]. The assay is now ready to cut, click on the **Cut** button to see the results.

Oil Case for RootThermo

Oil_1. Assay_1

Experimental Information | Gamma Distribution | Co Compositional Analysis

Assay Information: Light Ends | Liquid Properties | Content Curves | Oil Bulk vs. Temperature | Gamma Distribution

Results

Pseudo Components | Result Curves | Report

Dist [%]	T [C]
0.000	94.4
1.000	9.8
2.000	34.1
3.000	83.5
4.000	101.4
5.000	104.3
10.000	114.5
15.000	129.0
20.000	143.3
25.000	157.6
30.000	171.9
35.000	186.2
40.000	200.6
45.000	215.2
50.000	230.2
55.000	245.7
60.000	261.7
65.000	278.6
70.000	296.6
75.000	316.1
80.000	337.9
85.000	363.1
90.000	394.3
95.000	439.0
96.000	450.3
97.000	461.4

Parameters/Methods

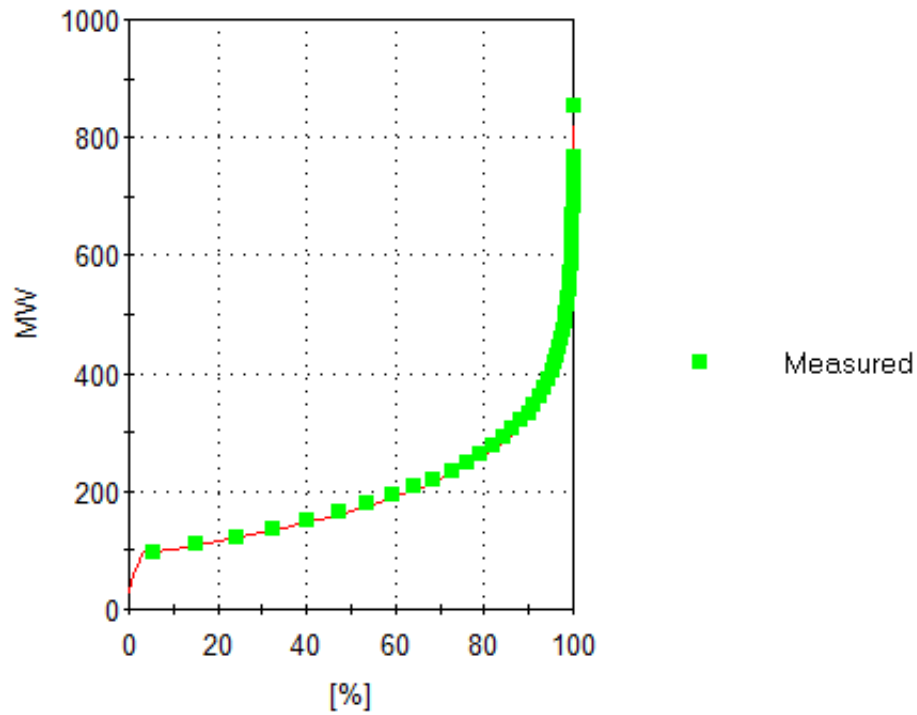
Bulk Information

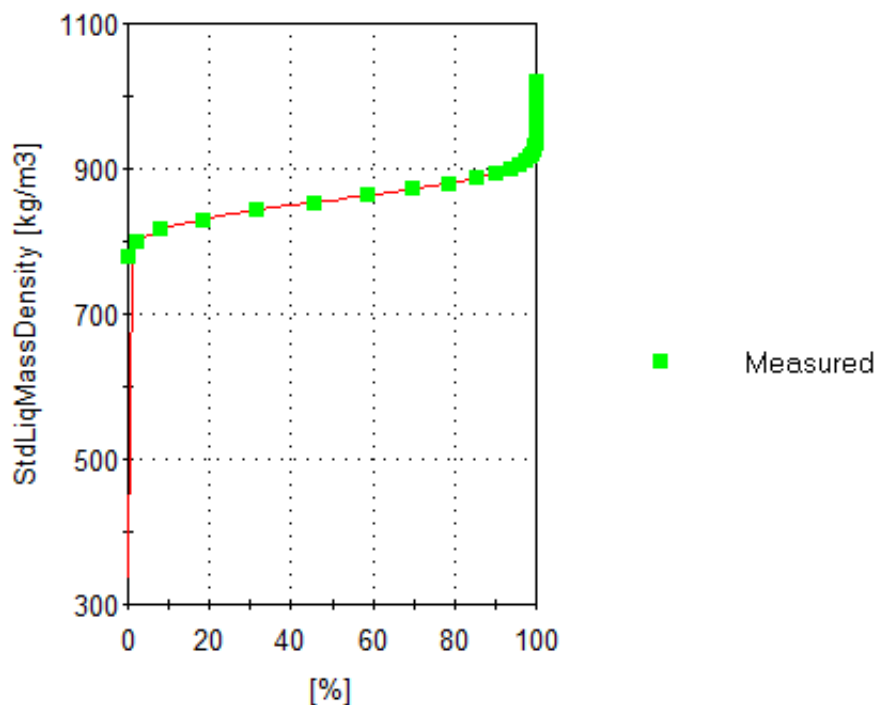
Liquid Density @ 60 F [kg/m ³]	857.000
MW	179.00
UCPK	11.36
Average Boiling Point [C]	248.4
Pressure [kPa]	101.33
NHR [kJ/mol]	6735945.9
NHMass [kJ/kg]	39944.54
Kinematic Visc. @ 100 F [m ² /s]	1.98E-06
Kinematic Visc. @ 210 F [m ² /s]	8.14E-07
Mode for Pseudo Names	Auto
Pseudo Base Name	OK_1_Assay_1
Prefix	ASP
Suffix	F

Active Range / Cut Set for : Assay_1

Name	Range-1	Range-2	Range-3
Number of Cuts	28	8	4
Cut Delta T [C]	13.90	27.75	55.53
Min. Temp [C]	37.8	427.0	649.0
Max. Temp [C]	427.0	649.0	873.1
Tc Est	Two	Two	Two
Pc Est	Two	Two	Two
Vc Est	Two	Two	Two
Acoustic Est	Lee-Kesler-Lee	Lee-Kesler-Lee	Lee-Kesler-Lee
Liq. Viscosity Est	API-VHG	API-VHG	API-VHG
Liq. Th. Cond. Est	API	API	API
Liq. Surf. Tension Est	API	API	API
Ideal Gas Cp Est	Lee-Kesler	Lee-Kesler	Lee-Kesler

The TBP, molecular weight and standard liquid density curves are calculated from the gamma distribution results and Soreide's correlations [1]. Go to the **Result Curves** tab and observe that the **TBP** curve is corrected to take into account the light ends fraction and, the **MW** and **Liq. Density @ 60 F** curves show the Gamma distribution results (green dots) that start where the light ends fraction finish (4.38 Vol%).





Result curves for other properties, including viscosity and thermal conductivity, can also be seen in the **Result Curves** tab. The pseudo component properties are calculated based on the Range Set estimation methods and can be explored in the **Pseudo Component** tab.

As seen before, in order to use the Gamma distribution it is necessary to have the molecular weight and standard liquid density of the characterized oil; however, sometimes these two properties are not always available. The oil environment of VMGSim has integrated correlations to calculate the average molecular weight and liquid density of an oil when only experimental transport properties data are available. The Tips and Tricks section of this issue deals with an example of this situation.

The **Gamma MW distribution** option can also be used to characterize fluids like resins or asphaltenes for which boiling point experimental information is usually not available; in this case a molecular weight distribution can be used to characterize these fluids. The only information that is needed for the characterization of a resin or asphaltene is its molecular weight, since its standard liquid density will be calculated using Yarranton et al. [2] correlation.

More examples on how to use the Gamma Distribution option to characterize oils with different combinations of available experimental data can be found in the **Oil Characterization** section of the **User's Manual** of VMGSim 7.0.

References

1. Whitson, C. H. and Brule, M. R. Phase Behavior. Richardson, TX: Society of Petroleum Engineers, 2000
2. Alboudwarej, H.; Akbarzadeh, K.; Beck, J.; Svrcek, W.Y.; and Yarranton, H.W.; "Regular Solution Model for Asphaltene Precipitation from Bitumens and Solvents", AIChE Journal, 49, 2948-2956, 2003

Thermodynamic Modeling and Process Simulation through PIONA Characterization

Glen Hay, Herbert Loria, and Marco A. Satyro - VMG Calgary

ABSTRACT

Individual components may not be able to represent the structure of heavy hydrocarbons because these materials are formed by several chemical species that are difficult to characterize with the current analytical techniques. Lumped component techniques can be applied to model these types of hydrocarbons; this procedure is often based on combining many pure compounds into groups with average physical properties.

Nevertheless, this technique fails for separations that are chemically driven due to the lack of chemical information in the lumped component groups. A new approach of the lumped characterization technique is shown in this work. This technique consists of using constant slates of selected compounds to cover the carbon number ranges of interest for the modeling of different refinery reactors.

The different combinations of these component slates allow matching the experimental distillation curve of a given feed and calculating its chemical characteristics ranging from simple properties such as molecular weight and standard density to PIONA (n-paraffin, iso-paraffin, olefin, naphthene, and aromatic) characterization data. The key advantage of this new method is the capture of the essential chemistry of the feedstock that affects property calculations while keeping a constant and consistent component list.

[Full article.](#)

Tips and Tricks

Characterization of Oils with the Minimum amount of Data

Herbert Loria - Calgary

The objective of this section is to show how to obtain a comprehensive oil characterization with a reduced amount of oil pseudo components when only experimental transport properties of a crude oil are available.

From a Gamma Distribution to a TBP Distillation Curve

Sometimes Process engineers face the problem of characterizing crude oils when distillation data and bulk experimental properties are missing and the only information available is transport properties data.

VMGSim has integrated correlations to calculate a complete oil characterization based on transport properties data using the Gamma distribution. The results of this type of characterization are very interesting from an academic point of view since they can provide lots of information due to the large quantity of pseudo components that can be created. However; a large number of pseudo components can increase several times the convergence time of a flowsheet.

The following example will show how to characterize an oil when minimum quantity of experimental data are provided and how to obtain a reduced number of pseudo components that can define the TBP distillation curve of such oil.

In this case, a heavy oil, for which the only experimental information available is the bulk kinematic viscosities at 100 and 210 °F, will be characterized.

Oil Summary

Kinematic Visc @ 100 °F = 1.424 e-03 m²/s

Kinematic Visc @ 210 °F = 3.458 e-05 m²/s

To start the characterization, open a new case in VMGSim and select **Advanced Peng-Robinson** as the **Thermodynamic Model**. Then, open the oil environment and select **Gamma MW distribution** as the C7+ Characterization Mode and **Oil** as the characterization Fluid.

Now, it is necessary to change the default values for the Whitson's Gamma model in the Gamma Distribution form in order to have the recommended values for a heavy oil.

For a heavy oil, the recommended Whitson's parameters are:

α = 25.0

η = 90 g/gmol

Gamma Max MW = 1210 g/gmol

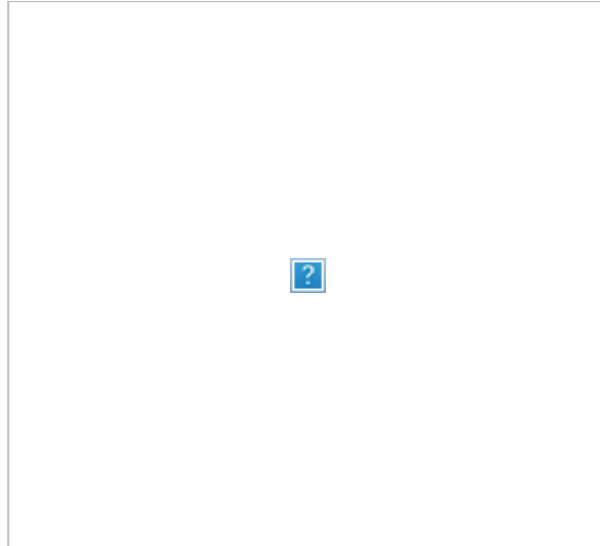
Number of Pseudo Components = 80

Delta MW = 14 g/gmol

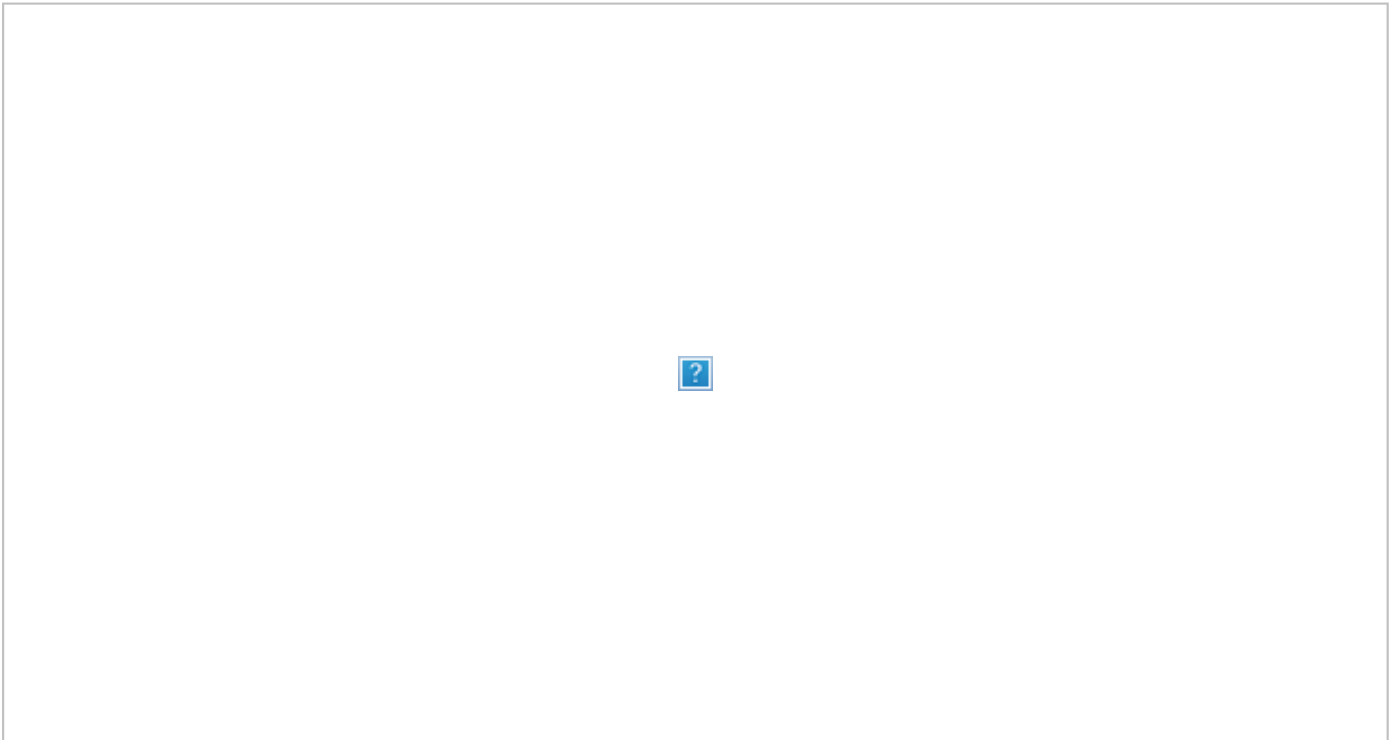
The values of **Gamma Max MW** and **Delta MW** were selected in order to have 80 pseudo components distributed in intervals of 14 g/gmol. 80 pseudo components will guarantee a smooth molecular weight distribution.



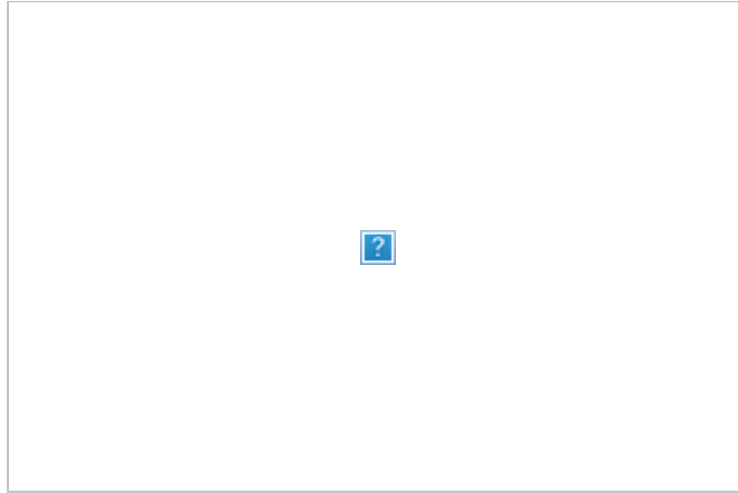
Now add the kinematic viscosity values in the **Bulk Information** grid in the right hand side of the oil environment.



The assay is now ready to cut, click on the **Cut** button to see the results. Click the **Install** button to install the characterized pseudo components.

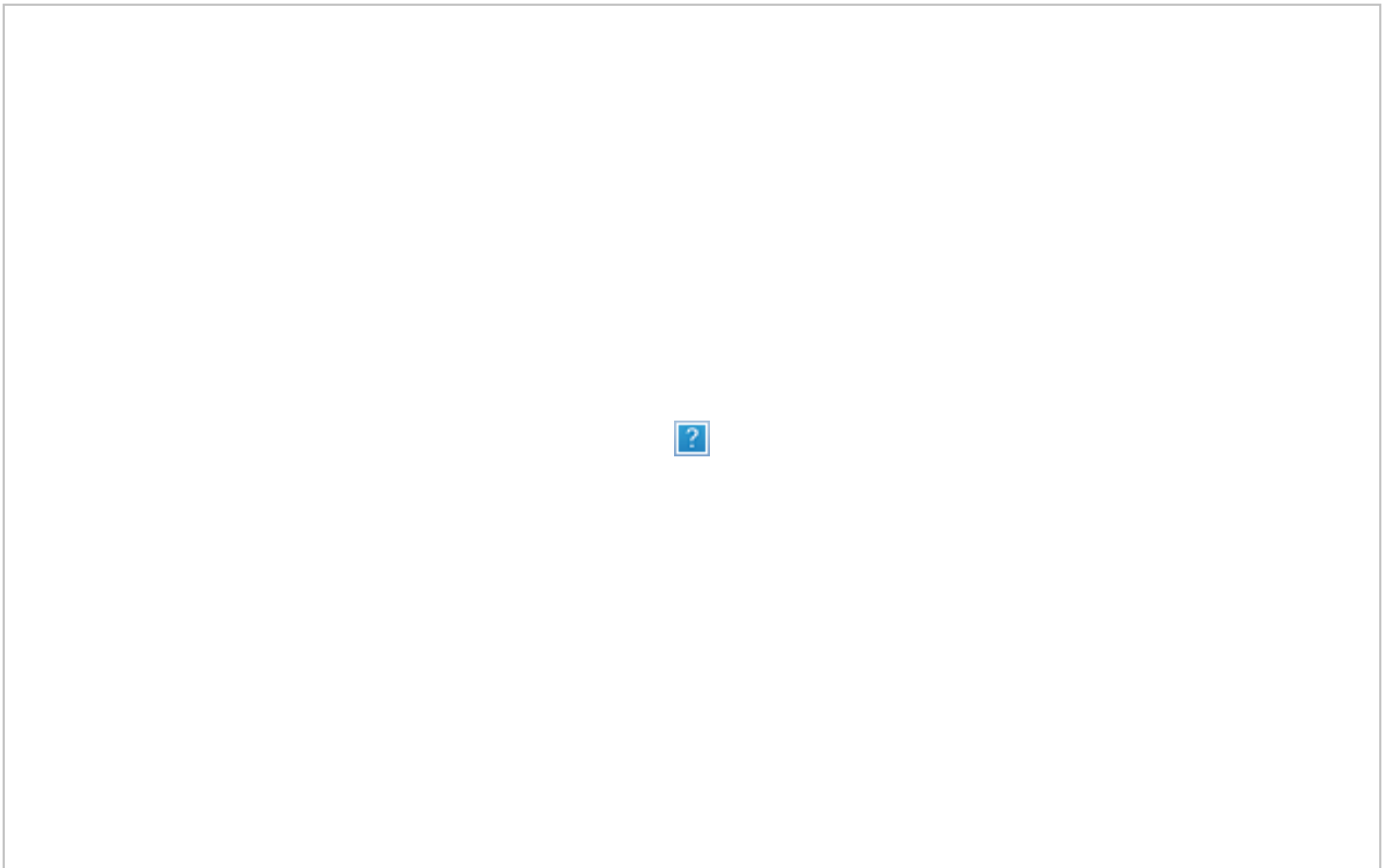


Go to the Result curves and select the Fraction vs Cn curve in Mole basis.



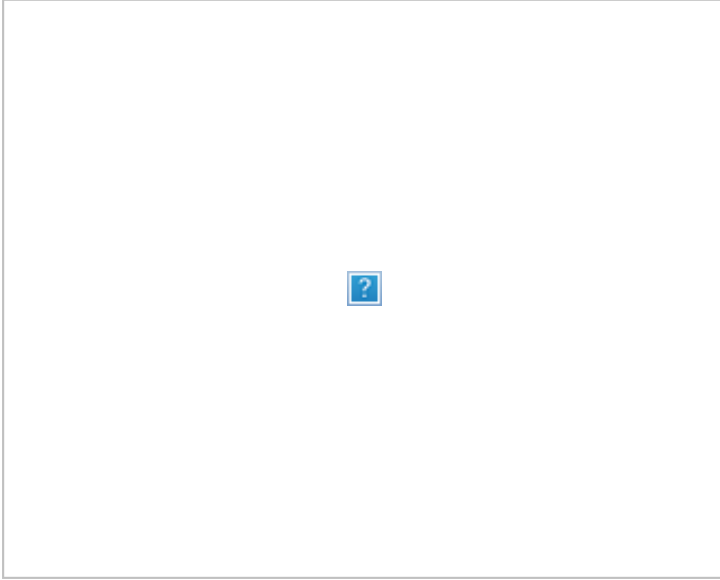
It can be observed that the characterization follows a modal distribution based on the entered Whitson's parameters. This oil is characterized based on just two kinematic viscosity points and contains 80 pseudo components; however, using this oil with this large amount of pseudo components could slow down the solution of some unit operations.

The first reaction would be to change the number of pseudo components to be created in the Gamma Distribution, but in this case the fine resolution achieved with 80 pseudo components will be lost, as it is shown in the following figure. In this figure the oil was re-cut with the Gamma Distribution using the same parameters as before but with only 8 pseudo components and **Delta MW = 140 g/gmol**.

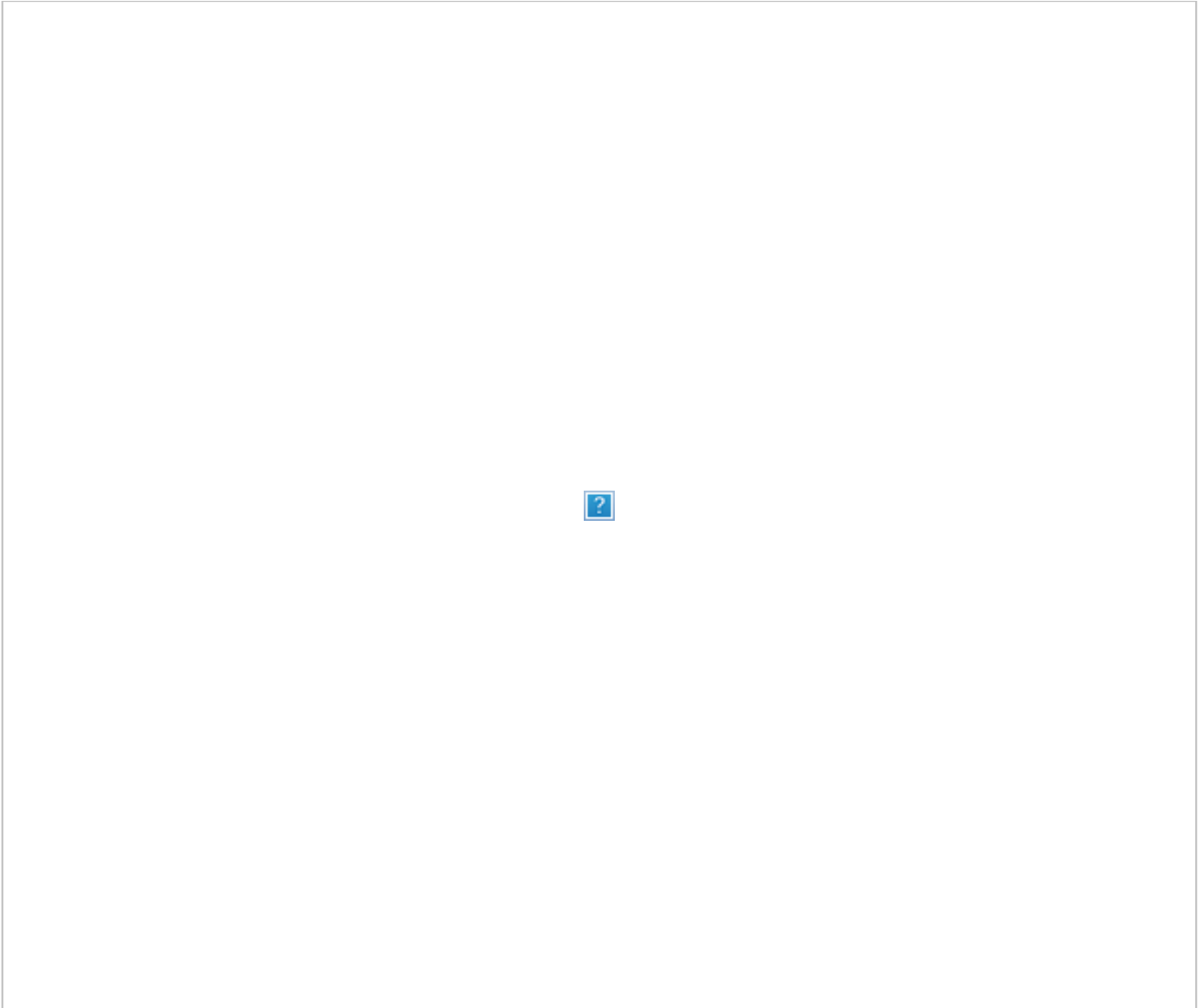


The oil environment of VMGSim allows characterizing this oil with less pseudo components without losing the achieved resolution with the Gamma distribution. To do this, follow the next procedure.

Return to the original Gamma Distribution assay with 80 pseudo components and **Clone** the assay as Assay 2. Now, select **Experimental information** as the characterization type and go to the **Distillation Curve** tab.

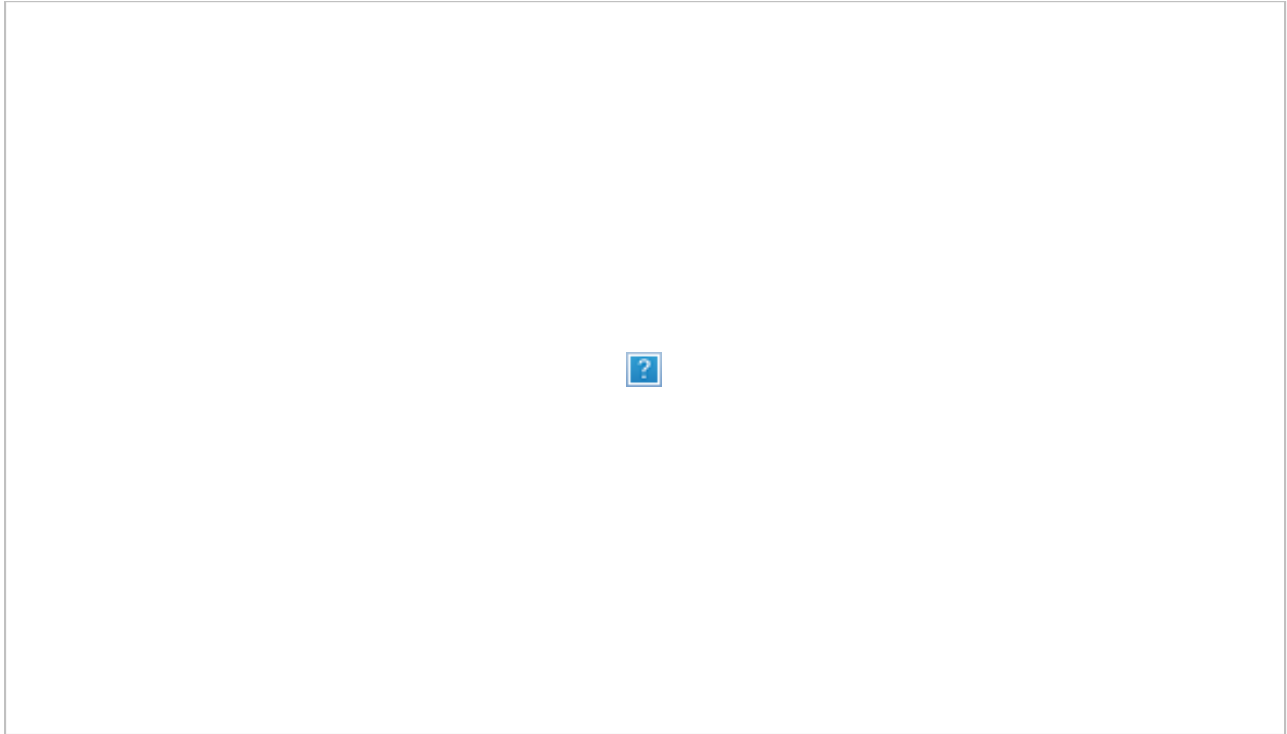


It can be seen that the TBP curve that was created during the Gamma distribution characterization is available in the Distillation Curve tab; this curve will be used as the TBP for the new oil. Click on the **Liquid Properties** tab and it will be seen that the **Molecular Weight** and **Standard Liquid Density** curves are also available.

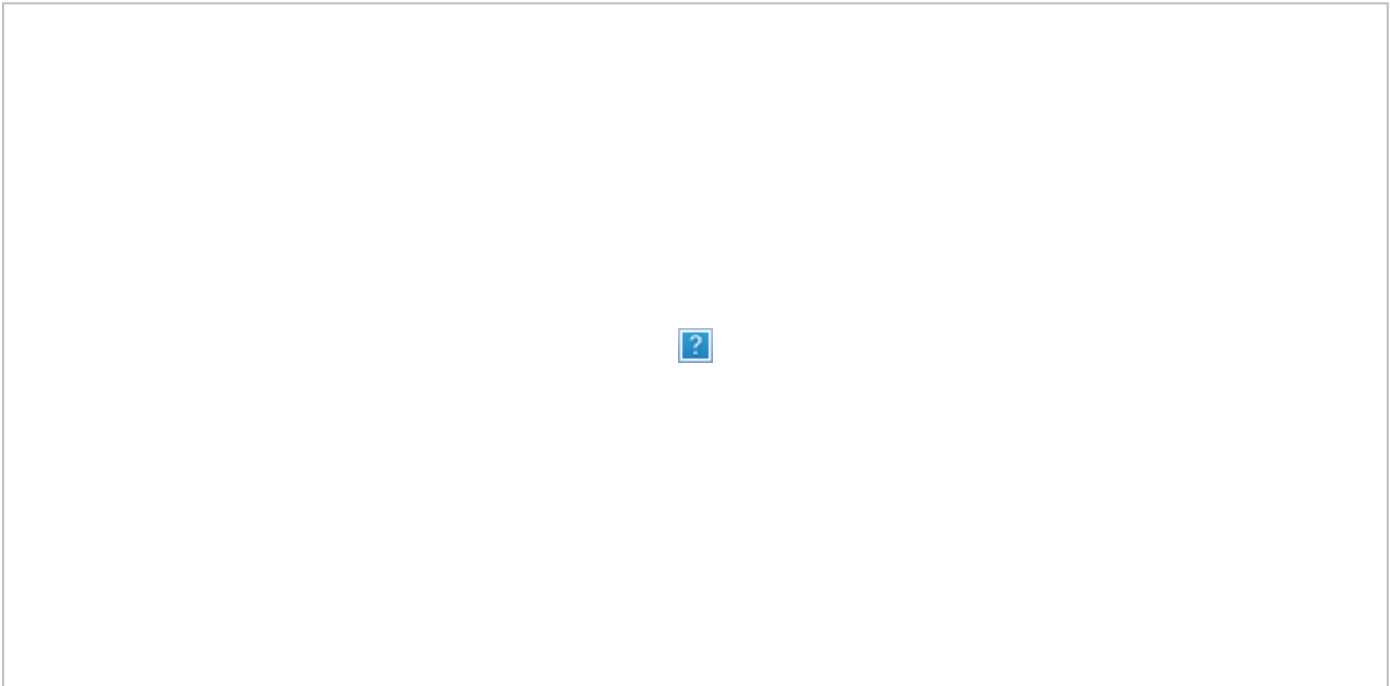


It can also be noticed that the kinematic viscosities that were added in the previous assay are also available as specifications for the new one.

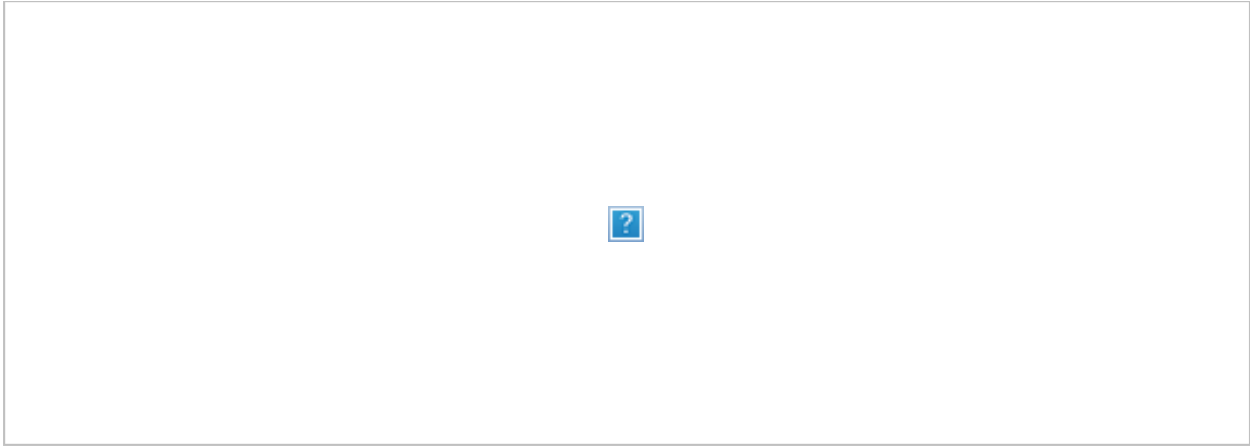
Before cutting the oil, let's use the "**Heavy_Oil**" Range Set to specify the different cuts for this oil, by inspecting the TBP, it can be seen that most of the pseudo components are present in the Distillates and VGO ranges of the oil. Then, set the number of cuts of the "Heavy_Oil" Range as: Naphtha = 1, Distillates = 2, VGO = 4 and Residue = 1.



Assay 2 is now ready to cut, click on the **Cut** button to see the results. Click the **Install** button to install the characterized pseudo components.

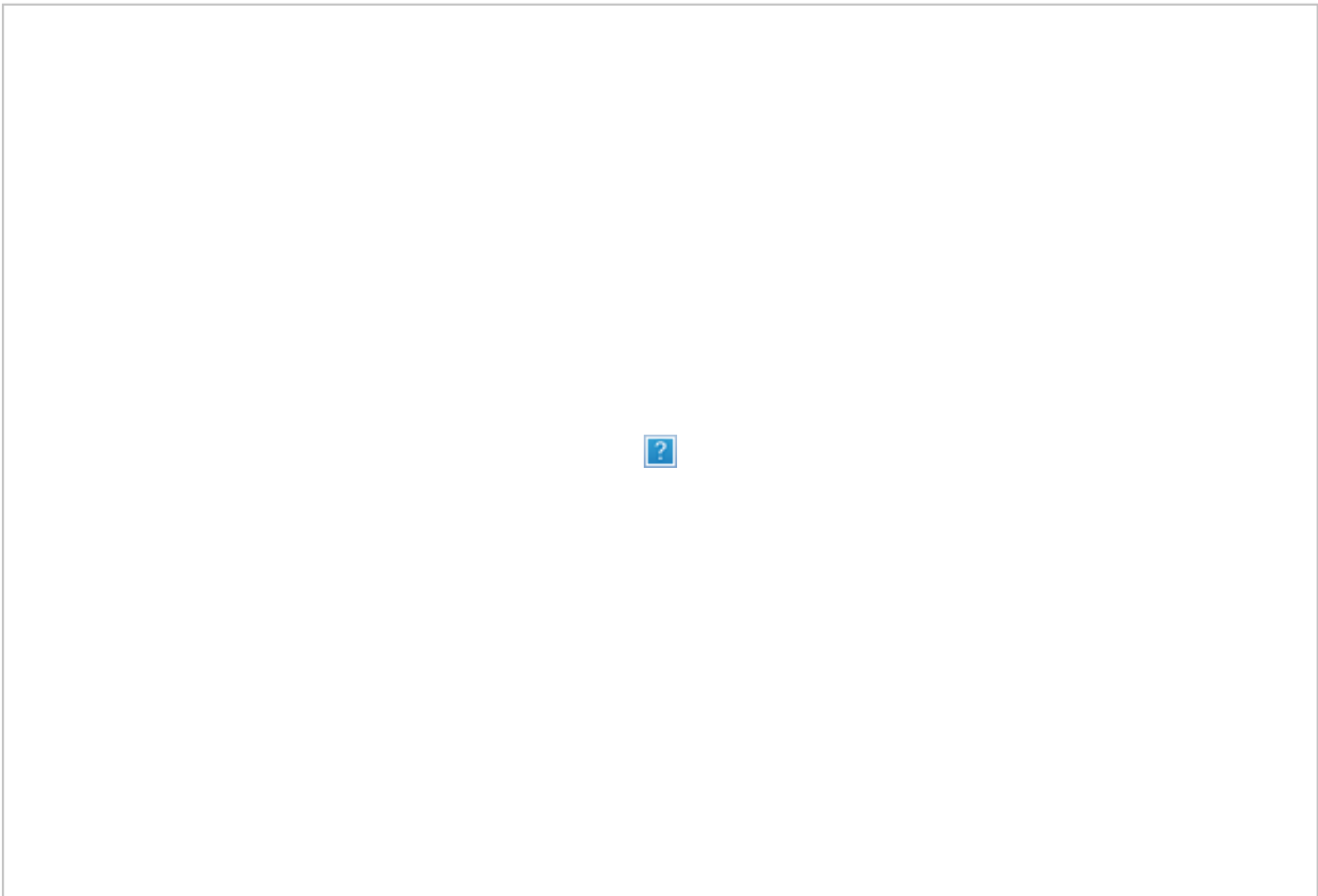


Note that the resulting TBP is similar to the one provided by the Gamma Characterization; however, in this case we have only 7 pseudo components defining the curve as compared with the 80 obtained from the previous assay.



To compare both assays, close the oil characterization environment and go to the VMGSim flowsheet. Create two material streams, **S1** and **S2**; connect **S1** to Assay 1 and **S2** to Assay 2 and assign a pressure of 101.325 kPa to each stream.

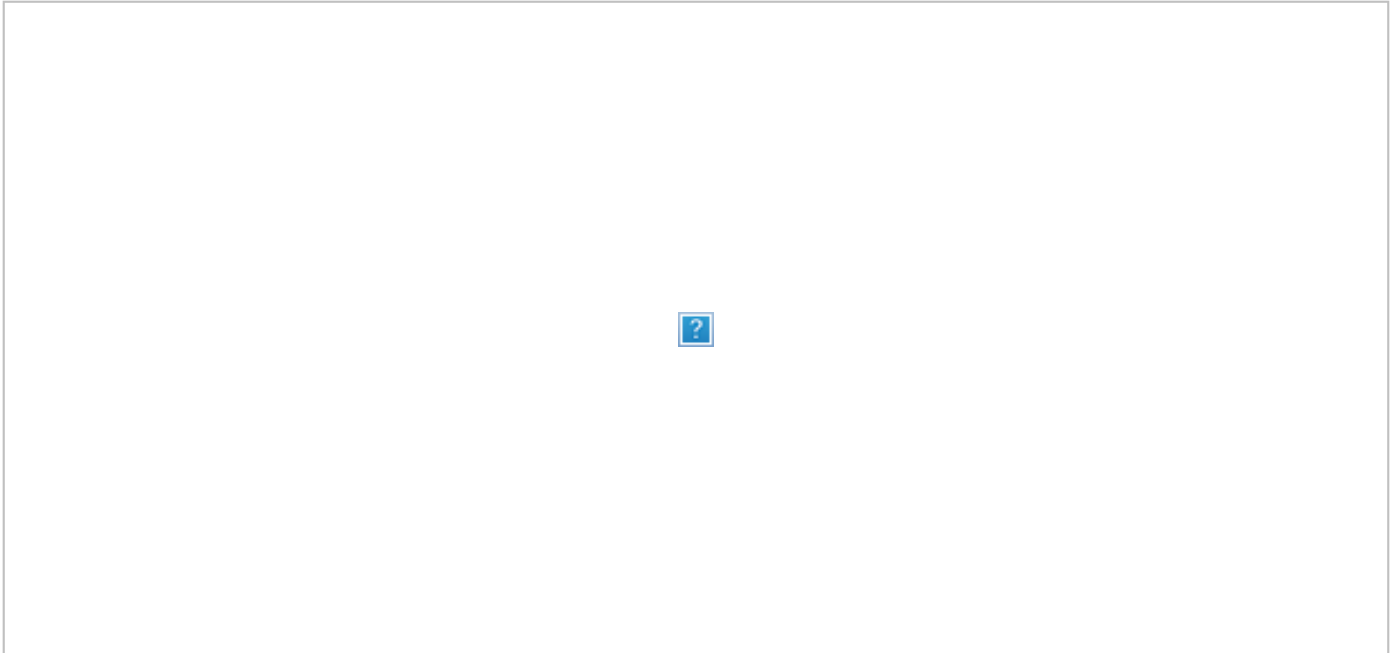
Open a **Case Study** and connect the **Temperature** of each stream as the **Independent Variable** and the **Kinematic Viscosity** of each stream as the **Dependent Variable**. Set the minimum and maximum values of the **Temperature** to 0 and 200 °C, respectively with 20 points. Be sure that the **Run All Combination** box is not checked to avoid running all the different combination of the stream temperatures.



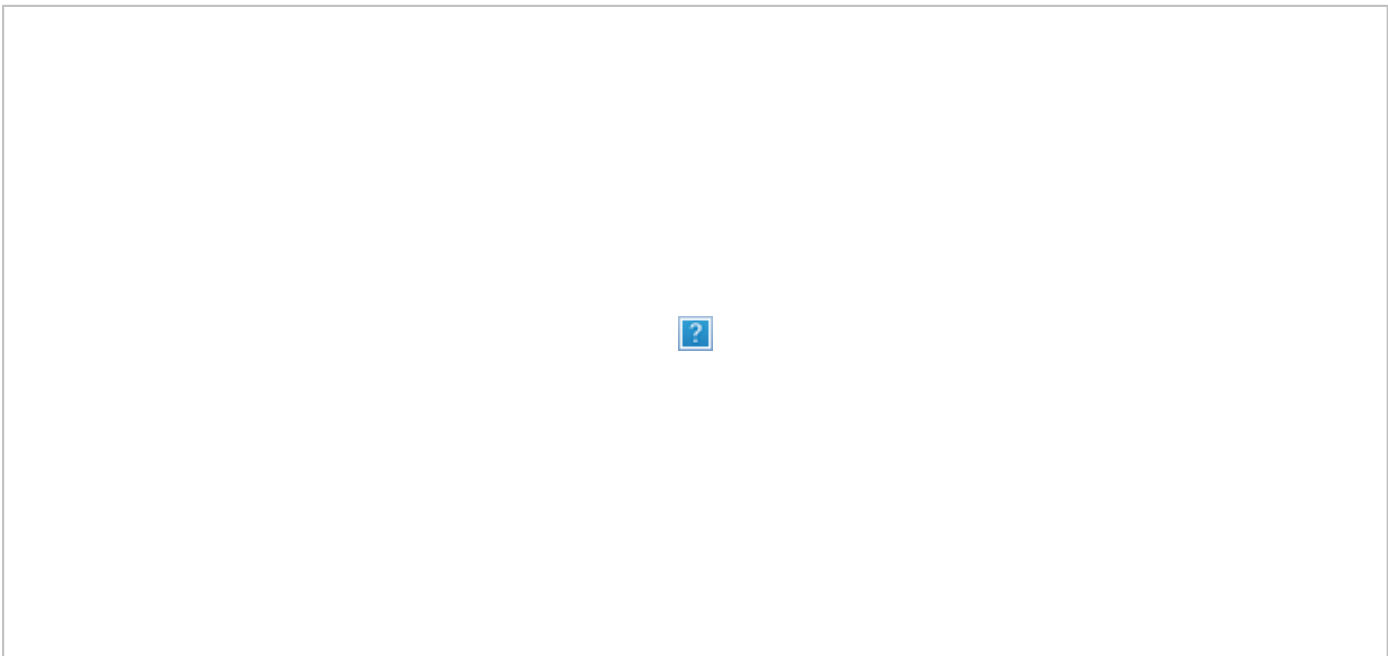
Run the **Case Study** and select the **Plot** tab to compare the kinematic viscosities predicted for each assay.

As it can be seen in the following figure, both predictions are similar (the pink line represents Assay 1 and the

green one Assay 2); meaning that both assays will yield same results for this property; however, Assay2 with 7 pseudo component will give faster answers when used in more complicated flowsheets.



The same procedure can be repeated for different properties and the results will be similar. For instance, the following figure shows the same type of analysis using the **Liquid Density**.



This exercise exemplified the use of the Gamma Distribution to characterize an oil with the minimum amount of experimental data and, how to covert that characterization into another one with a reduced amount of pseudo components.

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