



Thursday, February 14, 2013

VMGSim Courses

Hands on Introduction to VMGSim

February 20 and May 1 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

Dynamic Simulation with VMGSim

March 13 & 14 2013

Houston, TX, USA

The VMGSim dynamics course is a hands-on course where attendees will spend a significant amount of time building and running dynamics models in VMGSim. You are guided through the creation of a series of typical dynamics simulation case examples in VMGSim.

[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

March 27 & 28 and May 16 & 17 2013

Houston, TX, 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.

Upcoming Events

Webinars

Overview of the VMGSim Heat Exchanger and Air Cooler Rating Features
February 14

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

Advanced VMGSim Course

April 25 & 26 2013.

Calgary, AB, Canada

This two-day course is designed for those who are familiar with using VMGSim and are interested in learning new modeling techniques and more VMGSim features that will allow them to get more out of their simulation models.

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

To register or for more information, please email us at courses@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 February 14	11:00 to 12:00 pm	Overview of the VMGSim Heat Exchanger and Air Cooler Rating Features
Thursday March 7	11:00 to 12:00 pm	A practical guide to recycles in VMGSim

[Register here](#)

Out and About

VMG @ Laurance Reid Gas Conditioning Conference, February 24-27

Please be sure to stop by our hospitality room and visit with our team and partners. We will have plenty of food and drink to enjoy. Representatives from our Houston and Calgary offices will be attending. In addition representatives from our partner in Sulfur simulation, Sulfur Recovery Engineering will be in attendance.

<http://www.engr.outreach.ou.edu/lrgcc/>

Oil Characterization

Characterizing Crude Oils in VMGSim: Gamma Distribution in VMGSim™ 7.0

Herbert Loria - VMG Calgary

Introduction

A hydrocarbon fluid analysis sometimes shows a “plus” fraction where only bulk molecular weight and bulk standard liquid density are provided. Creating a single pseudo component with these average properties usually will not provide a good platform for fluid phase modeling. In particular, the usage of a single pseudo component tends to underestimate the molecular weight and specific gravity of the heaviest compounds that actually exist in the plus fraction, and therefore inaccurate dew points may result.

A flexible way of modeling C₇₊ (and higher) fractions is provided by Whitson’s gamma distribution approach [2]. This method is flexible enough to model exponential composition profiles as well as probabilistic (bell-shaped) molecular weight distributions. Whitson and Brulé [2] report a good fit between calculated and experimental cut molecular weights, with an average molecular weight error of 2.5 g/gmol for 44 oil samples.

The gamma probability density function is given by:

$$p(M) = \frac{(M - \eta)^{\alpha-1} e^{-\frac{M-\eta}{\beta}}}{\beta^{\alpha} \Gamma(\alpha)} \quad (1)$$

where Γ is the gamma distribution function. β is defined by equation 2.

$$\beta = \frac{M^+ - \eta}{\alpha} \quad (2)$$

The key parameters of the gamma distribution are:

α - Defines the shape of the distribution, and usually ranges between 0.5 and 2.5 for reservoir fluids, between 2.5 and 4 for resins and asphaltenes [3] and, between 25 and 30 for heavy oils and bitumen [2]. Note that if $\alpha = 1.0$, the distribution is exponential.

M^+ - Average molecular weight of fluid

η - Minimum molecular weight found in the distribution

Although the parameter η can be interpreted as the smallest molecular weight found in the distribution, from a practical point of view it can be considered an adjustable parameter that can be obtained from TBP data (if available). Approximate values for η are given by equation 3:

$$\eta = \frac{110}{1 + \left(1 + \frac{4}{\alpha^{0.7}}\right)} \quad (3)$$

Practically, η should be considered as a constant more than a physical property [2]. Recommended values for oils

and reservoir fluids are between 67 and 90 g/gmol and 1,500 g/gmol for resins and asphaltenes [3].

Different molecular weight distributions for several values of α are shown in Figure 1.

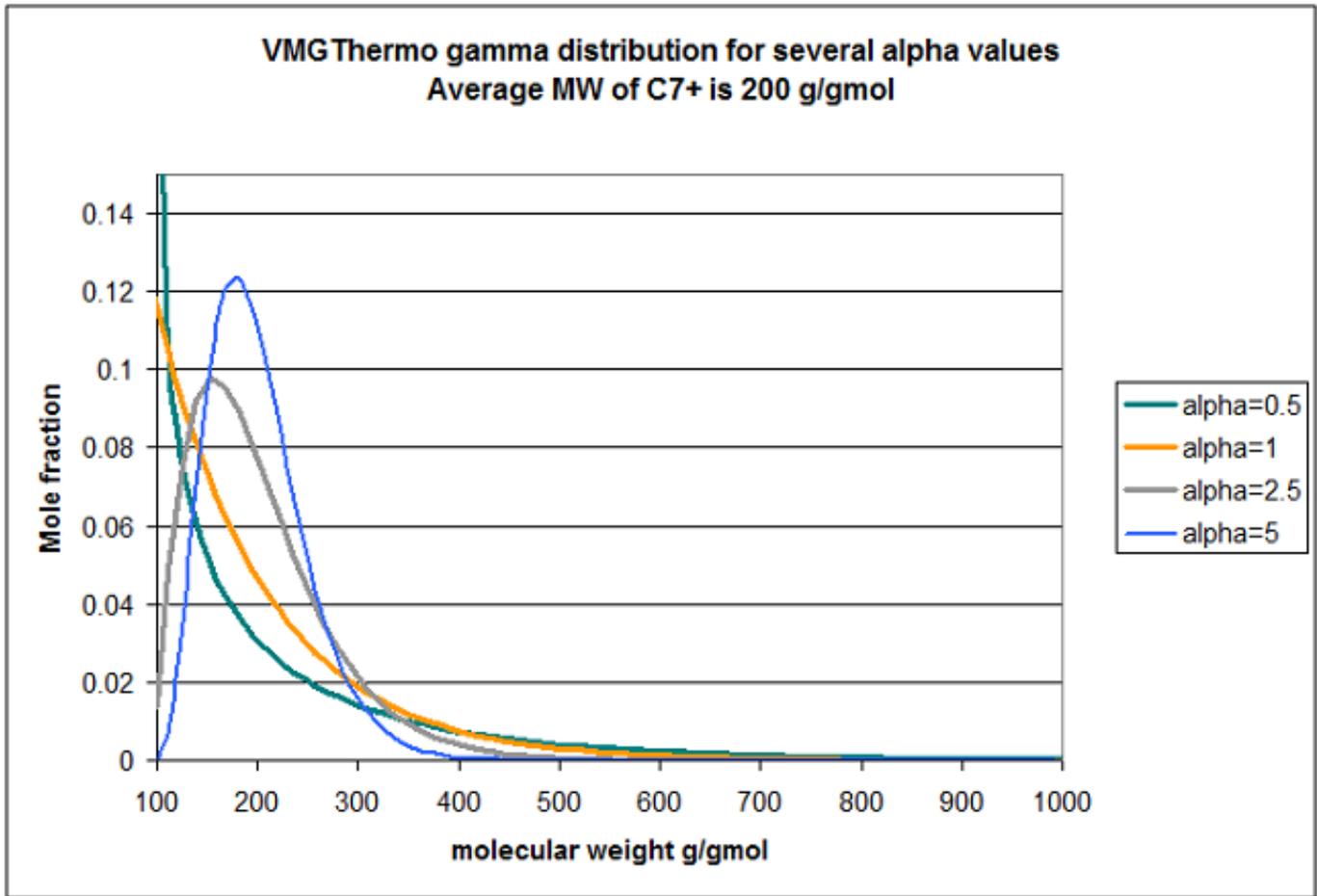


Figure 1 Whitson gamma distribution for C7+ fraction with $M = 200$ g/gmol, $\eta = 90$ g/gmol and several alpha parameter values

Equation 1 is applied to the plus fraction by dividing the area under the curve into sections, as shown in Figure 2.

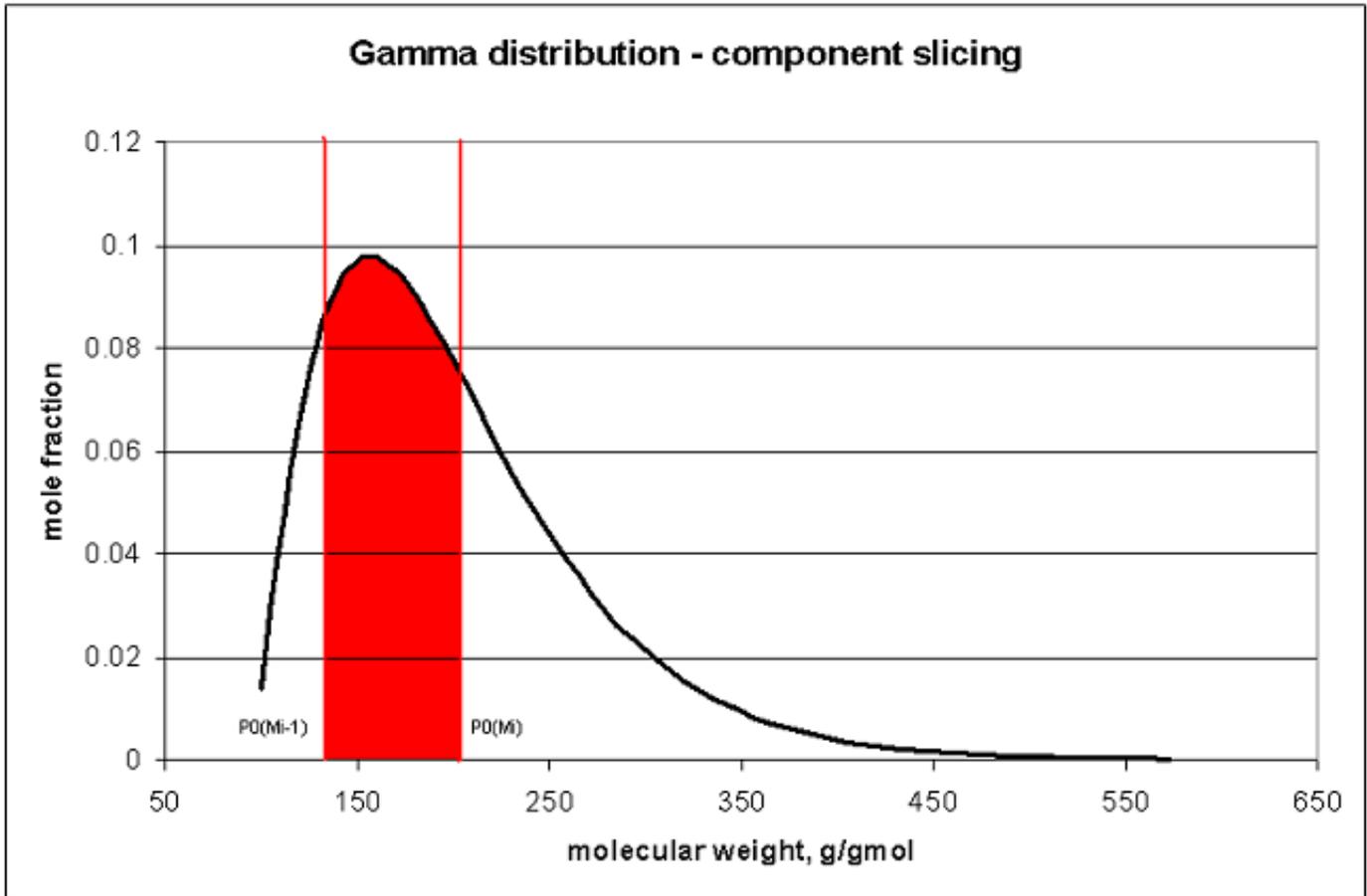


Figure 2 Determination of mole fraction of a component where mole fraction is equal to the area under the curve (shown in red)

The area under the curve between η and ∞ is equal to 1, and the area under a section is equal to the mole fraction of a slice. Mathematically we can write the mole fraction as shown in equation 4, and the average molecular weight of the slice is given by equation 5.

$$z_i = P(M_i) - P(M_{i-1}) \tag{4}$$

$$MW_i = \eta + \alpha\beta \frac{P_1(M_i) - P_1(M_{i-1})}{P_0(M_i) - P_0(M_{i-1})} \tag{5}$$

where:

$$P_0 = QS \tag{6}$$

$$P_1 = Q \left(S - \frac{1}{\alpha} \right) \tag{7}$$

$$Q = e^{-y} y^\alpha \Gamma(\alpha) \tag{8}$$

$$S = \sum_{j=0}^{\infty} y^j \left[\prod_{k=0}^j (\alpha + k) \right]^{-1} \quad (9)$$

$$y = \frac{M_i - \eta}{\beta} \quad (10)$$

With the molecular weight and compositions determined using the gamma distribution, the pseudo component liquid densities can be estimated using Soreide's correlation [2] adjusted to reproduce the user specified standard bulk liquid density. With the molecular weight and liquid densities defined for each fraction the normal boiling point can then be estimated using a another correlation developed by Soreide [2] (Note that Soreide's correlations are biased towards North Sea oil stocks [2]).

The Gamma Distribution characterization in VMGSim has two options: *Gamma to TBP* and *Gamma MW Distribution*. The following sections will explain their use and different features included in each option.

Gamma to TBP

The objective of the *Gamma to TBP* option is to characterize an oil fraction where only bulk physical properties are defined. Whitson's molar distribution is computed based on the provided α and η parameters and bulk molecular weight and standard liquid density. Figure 3 shows the Gamma Distribution form with the input parameters for the Gamma to TBP option.

Oil_1. Assay_1	
<input type="radio"/> Experimental Information <input checked="" type="radio"/> Gamma Distribution	
<input type="button" value="Light Ends"/> <input type="button" value="Liquid Properties"/> <input type="button" value="Content Curves"/>	
<input type="button" value="Oil Bulk vs. Temperature"/> <input type="button" value="Gamma Distribution"/>	
C7+ Characterization Mode	Gamma to TBP
Gamma Alpha	1.00
Gamma Eta	90.00
MW	
Liquid Density @ 60 F [lb/ft3]	

Figure 3 Gamma to TBP form from the Gamma Distribution characterization

The default values for the input parameters are $\alpha = 1.0$ and $\eta = 90.0$. For this option the boundary molecular weights are chosen arbitrarily at increments of 14.0 for the first 49 fractions, starting with η as the first lower boundary. The last fraction is calculated by setting the upper molecular weight boundary equal to 10,000. This produces 50 oil fractions.

The molecular weights and compositions that are determined using the gamma distribution model are used together with the bulk standard liquid density to obtain the standard liquid density of each fraction by means of the Soreide's correlation [2]. The boiling points of each fraction are then estimated from the calculated molecular weights and standard liquid densities with a correlation also developed by Soreide [2] based on 843 fractions from 68 reservoir C₇₊ samples.

Once these computations are done, a normal boiling point curve vs. cumulative mole fraction is obtained from the 50 defined fractions; this curve acts as TBP curve for the characterized oil.

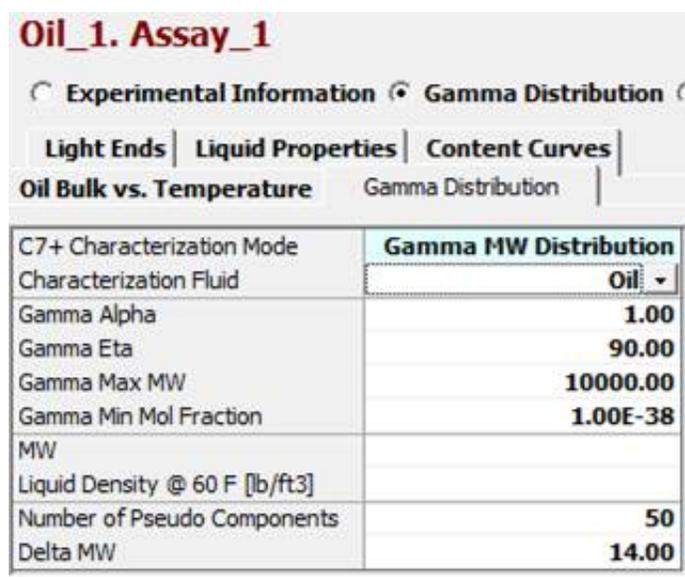
The next step is to convert these results to a TBP distillation analysis. A temperature step equal to the values defined by the temperature range in the Range Set section is taken. The amount of volume corresponding to this temperature step is associated with a pseudo component defined by the initial boiling point and the initial boiling point plus the temperature step. The arithmetic average temperature is used as the normal boiling point for this pseudo component. The procedure above is repeated until the entire distillation curve is transformed into pseudo components.

The number of pseudo components depends on the number of cuts defined in the Range Set section. Standard liquid density and molecular weight for the pseudo components are calculated from the standard liquid density and molecular weight curves from the gamma distribution. The rest of the physical properties for the pseudo components are then calculated based on the selected estimation methods in the Range Set section.

If this option is selected, the "Default" Range Set is automatically assigned to the characterization; however, it can always be modified for any other Range Set of preference.

Gamma MW Distribution

To access this option in the Gamma Distribution form, select *Gamma MW Distribution* as the C7+ Characterization Mode. The objective of the Gamma MW Distribution option is to characterize a hydrocarbon fraction (oil, resin or asphaltene) for which only physical properties are defined. The molar distribution is computed based on the provided parameters for Whitson's model and the bulk molecular weight and standard liquid density from the hydrocarbon. Figure 4 shows the Gamma Distribution form with the necessary input parameters for the Gamma MW Distribution option.



Oil_1. Assay_1	
Experimental Information Gamma Distribution	
Light Ends Liquid Properties Content Curves	
Oil Bulk vs. Temperature Gamma Distribution	
C7+ Characterization Mode	Gamma MW Distribution
Characterization Fluid	Oil
Gamma Alpha	1.00
Gamma Eta	90.00
Gamma Max MW	10000.00
Gamma Min Mol Fraction	1.00E-38
MW	
Liquid Density @ 60 F [lb/ft3]	
Number of Pseudo Components	50
Delta MW	14.00

Figure 4 Gamma MW Distribution form from the Gamma Distribution characterization

The default values for α and η are 1.0 and 90.0, respectively. In this option the user has the liberty to set up all the parameters to compute Whitson's model. In this case, the boundary molecular weights are chosen based on the given values for η and Gamma Max MW, which are the lower and upper molecular weights of the distribution. Delta MW is the molecular weight increment for the Gamma distribution. Default values for Gamma Max MW and Delta MW are 10,000 and 14.0, respectively.

The number of pseudo components to be characterized is also an input option, the default value is 50. The minimum mole fraction to be computed for each pseudo component (Gamma Min Mol Fraction) can also be set up in this form; the recommended values are between 1e-04 and 1e-38. In the case of heavy fluids, components with very small fractions are important for phase behaviour computations.

An extra feature in the Gamma MW Distribution option is the possibility of choosing different types of fluids for

characterization as shown in Figure 5. The physical properties calculations will depend on the selected fluid type.

Oil_1. Assay_1

Experimental Information **Gamma Distribution**

Light Ends | Liquid Properties | Content Curves

Oil Bulk vs. Temperature | Gamma Distribution

Gamma MW Distribution	
C7+ Characterization Mode	
Characterization Fluid	Oil
Gamma Alpha	1.00
Gamma Eta	90.00
Gamma Max MW	10000.00
Gamma Min Mol Fraction	1.00E-38
MW	
Liquid Density @ 60 F [lb/ft ³]	
Number of Pseudo Components	50
Delta MW	14.00

Figure 5 Gamma MW Distribution form showing the different types of characterization fluids

Characterization fluid - Oil

It is important to notice that when using this option or the Gamma to TBP option the bulk molecular weight must be between 30 and 2,000 g/gmol and the standard liquid density between 500 and 1,500 kg/m³.

The number of pseudo components that is set up in the form defines the actual number of pseudo components created for this type of characterization. The molecular weights, liquid densities and normal boiling points calculated during the gamma distribution are assigned to each pseudo component.

The rest of each pseudo component physical properties are calculated based on the selected estimation methods in the Range Set section. In this option, the pseudo components are named accordingly to their estimated molecular weight.

The default Range Set for this option is "SingleRange", this Range Set can be modified by the user for any other option.

Characterization fluid – Resin/Asphaltene

In the case of this type of fluids, the provided bulk molecular weight can be higher than 2,000 g/gmol. Asphaltenes can have molecular weights larger than 3,000 g/gmol [3], and the bulk standard liquid density is not a mandatory parameter to be provided for resins or asphaltenes. If standard liquid density value is missing, it will be calculated using a correlation developed by Yarranton et al. [4] which is based on the resin or asphaltene molecular weight.

The number of pseudo components set up in the form defines the actual number of pseudo components created for the characterization. Molecular weights and compositions are determined using the gamma distribution model and assigned to each pseudo component. The standard liquid density for each pseudo component is calculated based on Yarranton's correlation [4]. In this case the user has the option of selecting the pseudo components normal boiling point estimation method as shown in Figure 6.

Oil_1. Assay_1

Experimental Information **Gamma Distribution**

Light Ends | Liquid Properties | Content Curves

Oil Bulk vs. Temperature | Gamma Distribution

C7+ Characterization Mode	Gamma MW Distribution
Characterization Fluid	Asphaltene
Normal Boiling Point Estimation	Soreide
Gamma Alpha	Lee-Kesler
Gamma Eta	Soreide
Gamma Max MW	10000.00
Gamma Min Mol Fraction	1.00E-38
MW	
Number of Pseudo Components	50
Delta MW	14.00

Figure 6 Gamma MW Distribution form showing the options for the normal boiling point estimation methods for resins and asphaltenes

The normal boiling point estimation options are Lee-Kesler [5] and Soreide [2] estimation methods. The default method is Soreide. Once these properties are calculated, the remaining physical properties of each pseudo component are calculated based on the selected estimation methods in the Range Set section.

The chemical family assigned to each pseudo component will be the same as the selected fluid, i.e. Resin or Asphaltene. In this option the pseudo components are named accordingly to their estimated molecular weight.

When this option is selected the "Resin-Asphaltene" Range Set is automatically assigned to the characterization, this can be modified for any other Range Set of preference.

Gamma PDF plot

A feature that complements all the options in the Gamma Distribution characterization is the addition of the Gamma Probability Density Function (PDF) vs. molecular weight. This plot is automatically calculated once the bulk molecular weight is entered and it is based on the specified α and η parameters.

This plot helps on visualizing the shape of the gamma molar distribution before cutting the oil. Figure 7 shows the different shapes of the PDF for different α values (0.5, 1.0, 2.0 and 5.0) with MW = 200 g/gmol and η = 90 g/gmol.

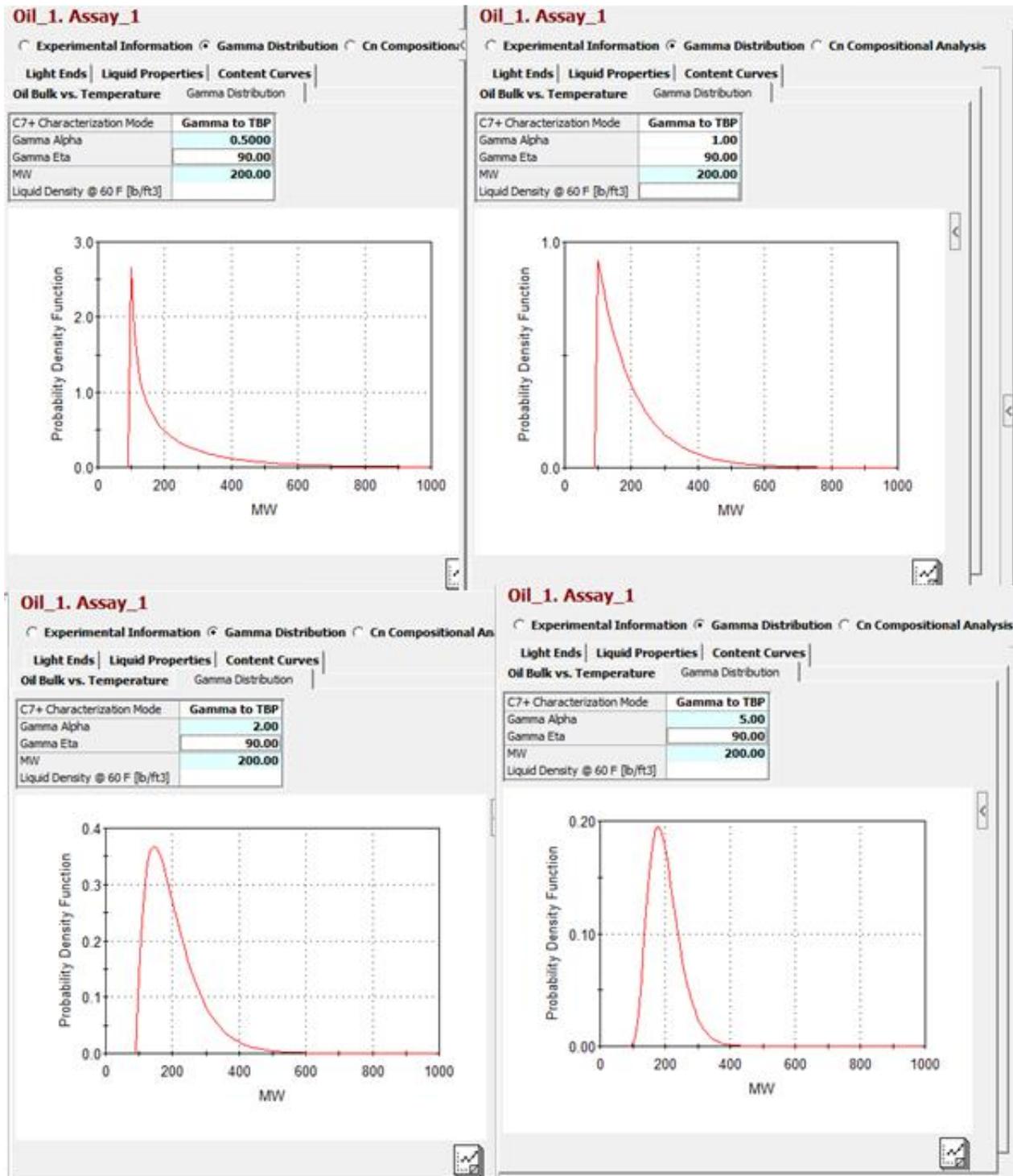


Figure 7 Gamma PDF plot with MW = 200 g/gmol, η = 90 g/gmol and several α parameter values (0.5, 1.0, 2.0, 5.0)

Gamma Distribution Report

The Report tab in the Results section will show important information regarding the different steps followed to cut an oil using the Gamma Distribution. Figure 8 shows an example of the Gamma Distribution information in the Report tab.

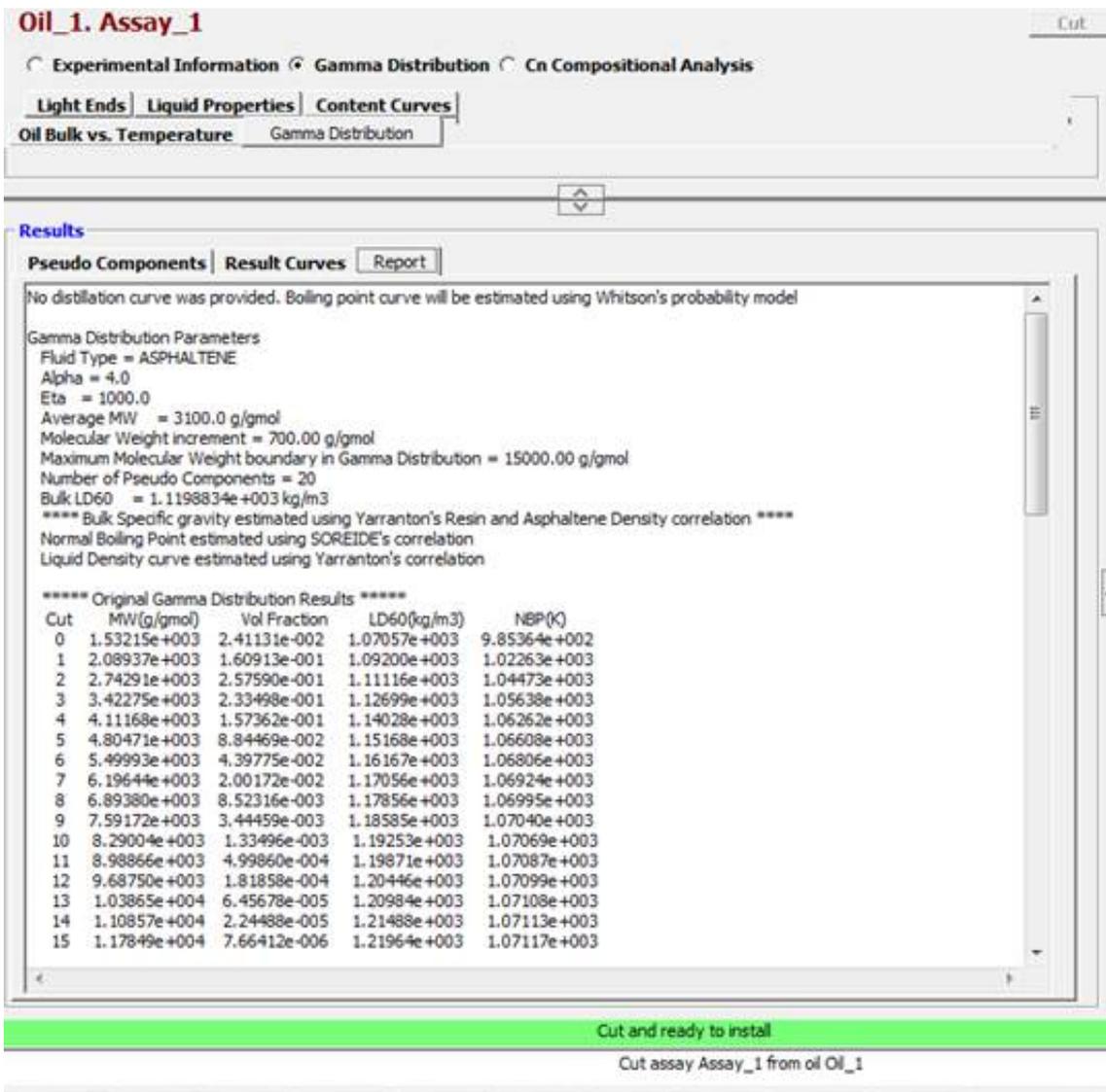


Figure 8 Report tab from Gamma Distribution characterization

This report will inform about all the Gamma distribution parameters and results as well as any error and its cause in case that the oil was not cut. It will also tell the user about any change in the number of characterized pseudo components. For example, in the Gamma MW Distribution, the Gamma Min Mol Fraction parameter can be set to a value that is higher than a computed mole fraction for the n pseudo component, in this case the number of pseudo component is reset to $n - 1$ and the user is warned in the Report tab.

In our following issue we will present some examples on how to use the Gamma Distribution characterization and its different options.

References

1. Whitson, C.H.; "Characterizing Hydrocarbon Plus Fractions", European Offshore Petroleum Conference & Exhibition, London, England, October 1980
2. Whitson, C.H. and Brulé, M.R. "Phase Behavior", SPE Monograph, Vol. 20, 2000
3. Akbarzadeh, K.; Alboudwarej, H.; Svrcek, W.Y.; and Yarranton, H.W.; "A Generalized Regular Solution Model for Asphaltene Precipitation from n-Alkane Diluted Heavy Oils and Bitumens", Fluid Phase Equilibria, 232, 159-170, 2005

4. 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
5. Whitson, C.H.; "Effect of Physical Properties Estimation on Equation of State Predictions"; *SPE Journal*, SPE 11200, 1982

Heavy Hydrocarbons Critical Property Estimation

VMGSim pure component review

Carl Landra - VMG Calgary

Introduction

Periodically, VMG's pure component databank undergoes internal audits for quality assurance. In the last audit we concentrated on the consistency of paraffin and iso-paraffin physical properties, specially the consistency of physical properties with carbon number above 20 due to the use of VMGSim and VMGThermo for modeling heavier and heavier feedstocks and related upgrading problems.

This physical property review showed some inconsistencies in the physical properties of paraffins and iso-paraffins. VMG's pure component database is based on data published by Yaws¹ and NIST/TDE. After the review we identified two areas for improvement. Firstly, we revisited values for critical temperature, pressure, volume, acentric factor, specific gravity and ideal gas heat capacities for consistency with respect to hydrocarbon type and carbon number. Secondly the database was extended to cover n-paraffins up to n-decacontane (C₁₀₀H₂₀₂), ensuring a consistent platform for the modeling of processes where large distributions of paraffins are important such as gas-to-liquids. A brief example using the specific gravity physical property is provided below. Detailed information is available to clients upon request.

Specific Gravity

While reviewing the properties of hydrocarbons in VMGSim 6.5 it was found that for a limited number of components (2,2,15,15-tetramethylhexadecane, octadecane, 2,6-dimethyl-, 5,14-dimethyloctadecane, eicosane, 2-methyl-, 7,14-dimethyleicosane, heneicosane, 2-methyl-, docosane, 2-methyl-, (-)-10,13-dimethyldocosane, 7,9-dibutyl-9-methylpentadecane, 11-nonylheneicosane, and 9,11-dihexyl-11-methylnonadecane) the specific gravity from the Yaws or NIST/TDE was incorrect. The data points that were found to be in error can be seen in the plots below. The data is for components starting from hydrocarbons C₂₀H₄₂ and heavier. There are a select few data points that are large outliers, as shown in Figure 1. Consistency is important to ensure rational VLE simulations resulting from any thermodynamic model.

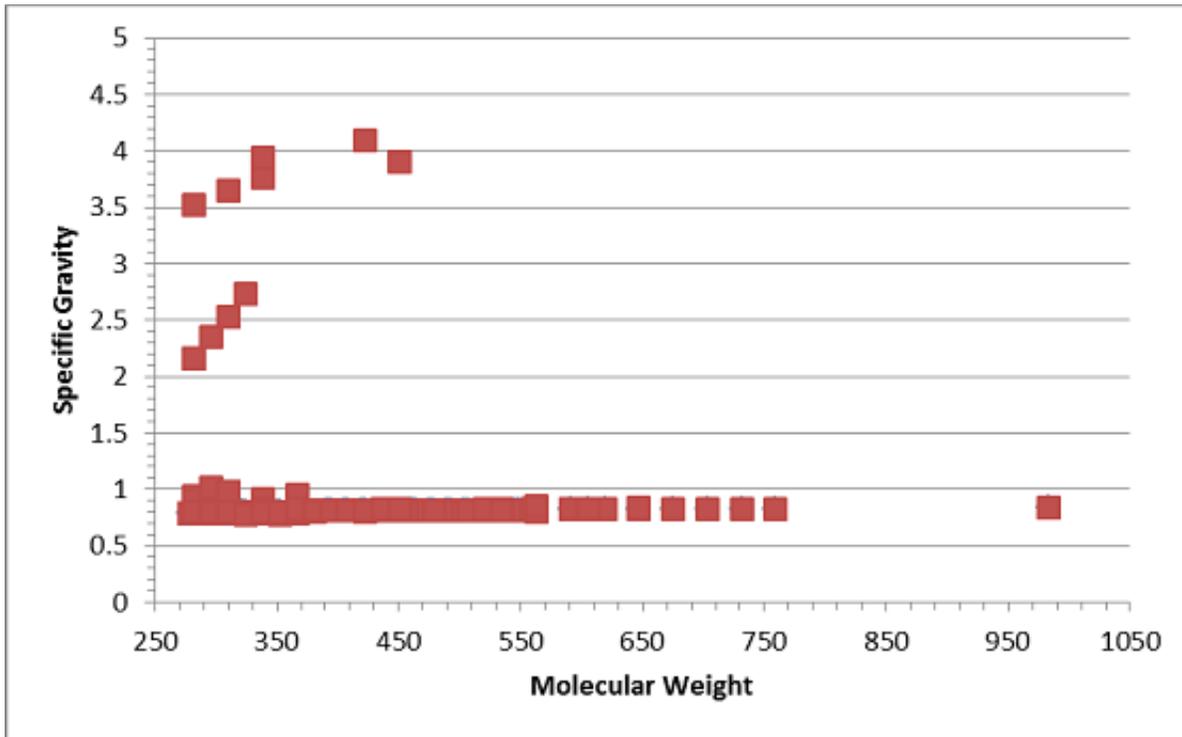


Figure 1: Specific Gravity of hydrocarbons in VMGSim 6.5

In order to keep the specific gravity values consistent and continuous, the specific gravity was updated for all components used in this study using Riazi²'s equation.

$$SG = 0.85 - \exp(92.22793 - 89.82301MW^{0.01})$$

1

The improvements to these values can be seen in the figure below.

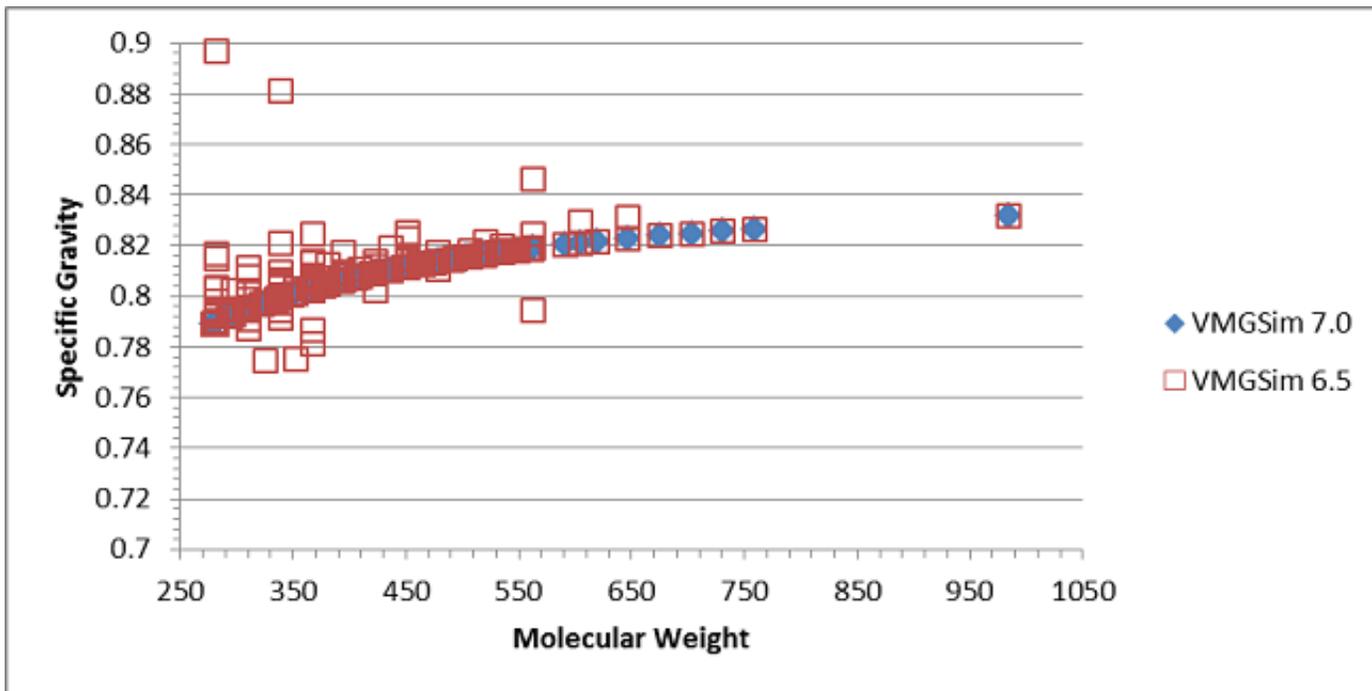


Figure 2: Specific Gravity of hydrocarbons in VMGSim 7.0

Figure 2 shows that the original trendline in VMGSim 6.5 was correct and that only the few outliers needed to be corrected and updated. The work done to update these values was also used to calculate the specific gravity for the list of new components in VMGSim 7.0.

Conclusions

As the work above shows, the majority of data points for specific gravity in VMGSim 6.5 matched the anticipated values. However several paraffins required small changes to ensure consistency with recommended values and a few paraffins had incorrect specific gravities that required corrections. Similar work was done for critical temperature, pressure and volume, acentric factor, ideal gas heat capacity, liquid density and normal boiling point. The calculations used to update these properties were also extended to the new components added in VMGSim 7.0. Clients can request the complete report by contacting your local support office.

References

1. Yaws, C. L. *Chemical Properties Handbook*; McGraw-Hill: New York, 1999
2. Riazi, M. R. *Characterization and Properties of Petroleum Fractions*; ASTM International: W. Conshohocken, PA, 2005

Tips and Tricks

New PFD border and information shapes in VMGSim™ 7.0

Luis Duhne - VMG Calgary

VMGSim™ 7.0 features the new ID blocks and border shapes that make easier the identification and formatting of your PFD. To add ID information to your flowsheet, simply drag and drop the ID block shapes from the Utility stencil. These blocks contain information such as Case Name, Customer and Project Name. Borders can be easily added as well. The new border shapes will automatically adjust to the size of your flowsheet.

The new PFD borders and the ID block shapes are located in the Utility stencil. Simply drag and drop them to add them to your flowsheet.

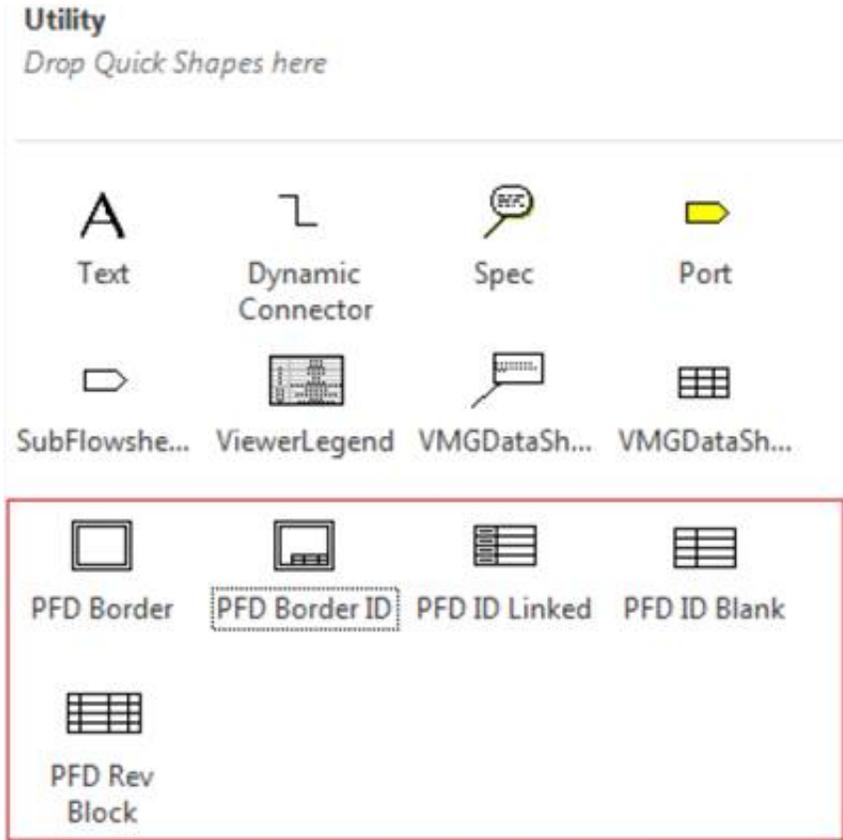


Figure 1 Utility Stencil with the new shapes.

PFD ID Linked

This shape displays common identification fields from the VMGSim case. The fields are already linked to variables from the reporting system which can be specified through the Reporting menu.

File Name	MDEAExample Documentation
Company	Virtual Materials Group
Customer	Gas Global Inc.
Project	MDEA Application
Job No.	MDEA 3
Prepared By	L.D.
Date	6/18/2012

Figure 2 PFD ID Linked Shape

PFD ID Blank

This shape is a customizable ID block. It contains blank fields that can be used to manually type information or to link information to variables from the case. The fields that can be used from the simulator include:

Approved By, Checked By, Comments, Company, Customer, Date, Drawn By, FileName, JobNo, Location, Prepared By and Project.

