



Tuesday, January 22, 2013

VMG USA New Address and Phone Number

We are pleased to announce our new office location in Houston's energy corridor. The office is located just off of I-10 on Park Row Drive.



17171 Park Row Drive
Suite 273
Houston, TX 77084
Phone: 281-944-9902

Our new location provides much needed room to grow, as well as the convenience of in-office training facilities for our VMG software training courses.

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.

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

Advanced VMGSim Course
Calgary
Feb 21 & 22

Dynamic Simulation with VMGSim
Houston
March 13 & 14

Overview of VMGSim
Houston
March 27 & 28

[Details...](#)

Connect with us:



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

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

Advanced VMGSim Course

February 21 & 22 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

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.

[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 February 14	11:00 to 12:00 pm	Overview of the VMGSim Heat Exchanger and Air Cooler Rating Features

[Register here](#)

Oil Characterization

Estimation of Heat of Combustion for Oil Pseudo Components in VMGSim™ 7.0

Herbert Loria - VMG Calgary

The main goal of this section is to describe the method for estimating enthalpies or heats of combustion inside the oil environment of VMGSim™ 7.0. The API procedure 14A1.3 [1] provides an accurate method for the estimation of enthalpies of combustion of petroleum fractions at 60 °F, this method is based on the liquid density at 60 °F, the molecular weight and, the percentage of sulfur and nitrogen present in the petroleum fraction. To validate the method, comparisons between enthalpies of combustion from the oil characterization environment and from a combustion reactor were done and they yielded small average absolute deviations (less than 1 %).

Enthalpies of combustion estimation

The standard heat of combustion is defined as the change in enthalpy resulting from the combustion of a substance, in the state that is normal at 77 °F and atmospheric pressure, beginning and ending at a temperature of 77 °F. The gross heat of combustion is the same as the standard heat of combustion except that the combustion begins and ends at 60 °F. The normal state for the water formed by the reaction is liquid in both cases.

The difference between the standard and the gross heat of combustion is the difference between the sensible heat changes of the products and reactants from 60 to 77 °F. This sensible heat difference is usually negligible in comparison with the heats of combustion, so the gross and standard heat of combustion are approximately equal [1].

The net heat of combustion is the heat evolved in a combustion beginning and ending at 60 °F with gaseous water in the products [2].

Combustion reactions proceed with a decrease in enthalpy, the enthalpy change is negative in sign. In the case of a petroleum fraction, the negative of the gross heat of combustion is known as the gross heating value (GHV) and the negative of the net heat of combustion is the net heating value (NHV), both quantities are therefore positive numbers [2].

Note that VMGSim 7.0 describes the Ideal Gas Enthalpy of Combustion at 298 K equal to the Net Heating Value (NHV), which is the negative of the net heat of combustion when gaseous water is present in the combustion products. In VMGSim 7.0, the Ideal Gas Enthalpy of Combustion at 298 K is a POSITIVE value equal to the Net Heating Value (NHV) and the negative of the net heat of combustion.

In VMGSim 7.0:

Ideal Gas Enthalpy of Combustion at 298 K [+] = NHV[+] = - Net heat of combustion[-]

The API Procedure 14A1.3 [1] defines the net heat of combustion for petroleum fractions as:

$$\begin{aligned} \Delta H_{C,60(net)} &= \left[- (16,796 + 54.5API - 0.217API^2 - 0.0019API^3) \right. \\ &\quad \left. - 0.01 \left[- (17,672 + 66.6API - 0.316API^2 \right. \right. \\ &\quad \left. \left. - 0.0014API^3) (\%S_e + \%I_e) \right] + 40.5(\%S_e) \right] * 2.326 * MW \end{aligned}$$

where:

$\Delta H_{C,60 (net)}$ = net heat of combustion in kJ/kmol

API = API gravity

$\%S_e$ = weight percent of sulfur (from chemical formula) minus average weight percent (from Table 14-0.1 in API Procedure 14A1.3[1])

$\%I_e$ = weight percent of inerts (from chemical formula) minus average weight percent (from Table 14-0.1 in API Procedure 14A1.3[1])

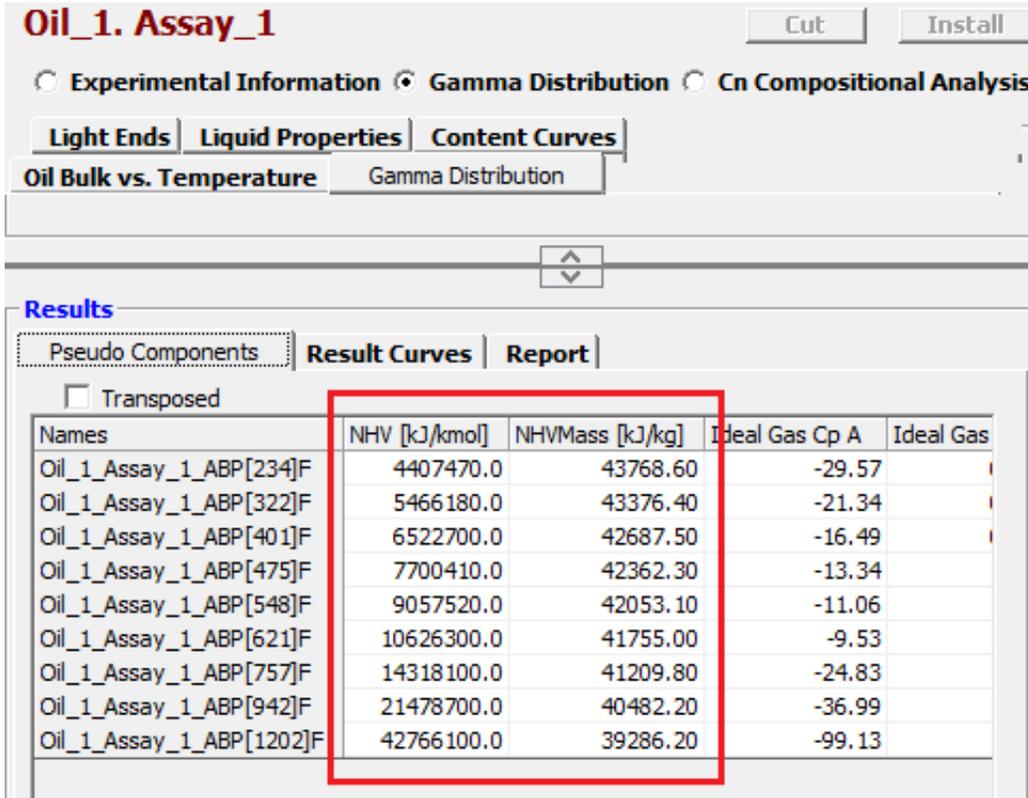
MW = molecular weight

Then, $NHV = - \Delta H_{C,60 (net)}$

This procedure is applied during the calculation of the pseudo component physical properties inside the Oil Characterization environment of VMGSim 7.0. Molecular weight and API gravity are obtained directly from the pseudo component properties and, the sulfur and nitrogen (inerts) weight percent are obtained from the chemical formula of the pseudo component. For more information about the chemical formula estimation for oil pseudo components please refer to our previous newsletter.

The NHV can also be calculated in enthalpy mass units; this value is obtained by dividing the enthalpies in mole basis by the pseudo component molecular weight.

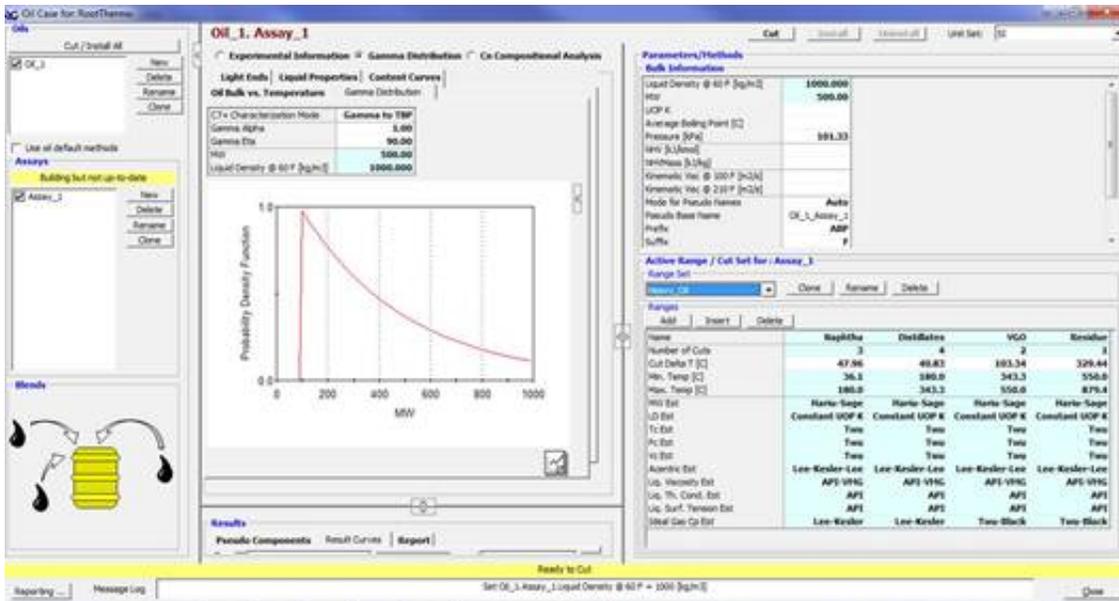
In the Oil Characterization environment, the enthalpy of combustion at 77 °F in molar enthalpy units is called NHV in order to be consistent with VMGSim 7.0. The enthalpy of combustion at 77 °F in mass enthalpy units is called NHV_{Mass} . Two extra columns in the Pseudo Components tab from the Results view in the Oil Characterization environment were added in order to display the heat of combustion of the oil pseudo components.



Validation

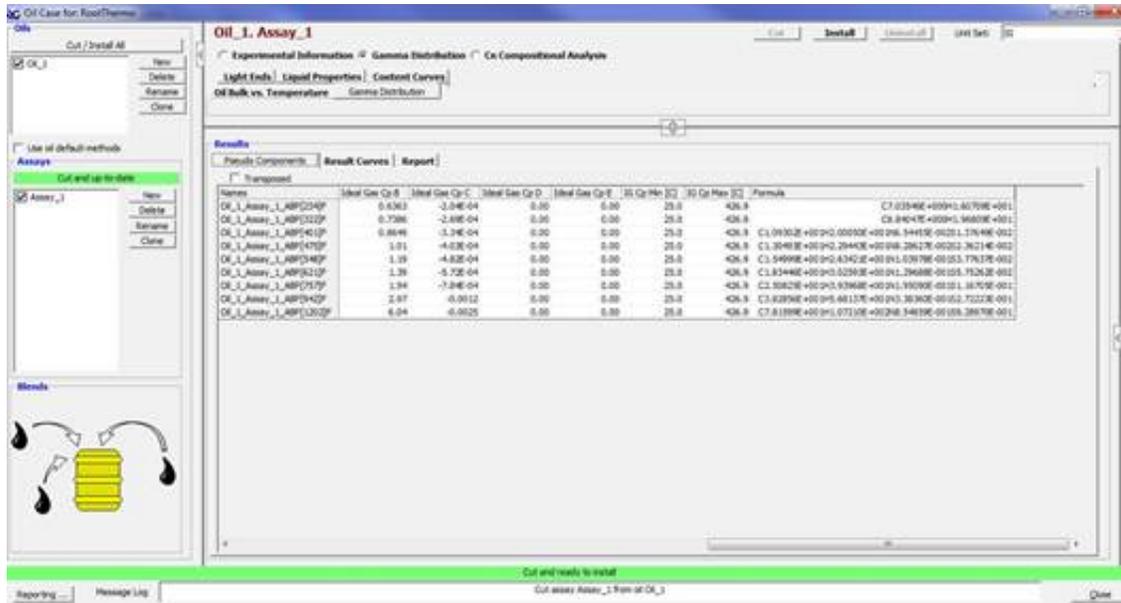
In order to validate this procedure, a VMGSim 7.0 simulation can be done. Open VMGSim 7.0 and start a case selecting the **Advanced Peng Robinson** property package. Change the Unit Set to **SI** and go to the **Oil Characterization** environment.

In this case, a heavy oil (standard liquid density = 1000 kg/m³ and MW = 500) is cut and installed using the **Gamma Distribution** and the **Gamma to TBP** characterization mode. In order to reduce the number of pseudo components, the "Heavy_Oil" Range Set is employed to cut this oil.



Once the oil is cut and installed, the enthalpy of combustion for each pseudo component can be obtained from the

Pseudo Components tab in the Result Section.

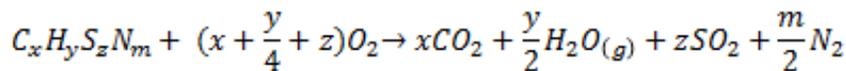


The formulas and enthalpies of combustion for each oil pseudo component are presented in the following table:

n	NHV [kJ/kmol]	NHVMass [kJ/kg]	Formula
0	4407470	43768.6	C7.03546E+000H1.60709E+001
1	5466180	43376.4	C8.84047E+000H1.96809E+001
2	6522640	42687.1	C1.09416E+001H2.00258E+001N6.55136E-002S1.37793E-002
3	7700330	42361.8	C1.30623E+001H2.29673E+001N8.29458E-002S2.36451E-002
4	9057410	42052.6	C1.55149E+001H2.63677E+001N11.04079E-001S3.78004E-002
5	10626200	41754.5	C1.83619E+001H3.02879E+001N11.29611E-001S5.75806E-002
6	14317800	41209.1	C2.51051E+001H3.94323E+001N11.95266E-001S1.16811E-001
7	21478200	40481.4	C3.83182E+001H5.68620E+001N3.38648E-001S2.72455E-001
8	42764800	39285	C7.82211E+001H11.07294E+002N8.55528E-001S9.29697E-001

The next step is to compare the NHV values from the characterization to those obtained from a combustion reaction. In order to do this, a stream containing 1 kgmole/h at 25 °C of each pseudo component is mixed with another stream containing oxygen at the same temperature with the stoichiometric quantity based on the combustion formula, the mixed stream is connected to an equilibrium reactor and the balanced combustion reaction is provided. The reactor is solved as isothermal and isobaric and the heat of reaction at 25 °C is recorded.

The combustion reaction is represented by:



The following table shows the stoichiometric coefficients for the combustion reaction of each oil pseudo component (PC) characterized in the Oil environment:

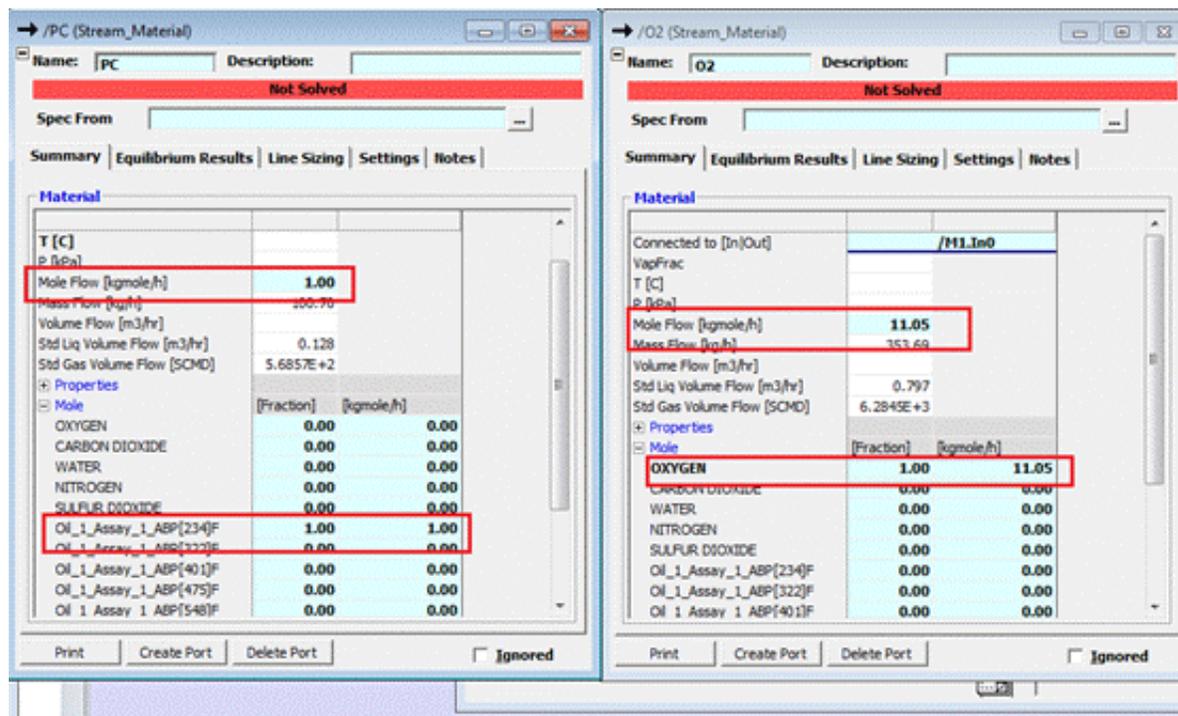
n	PC	+	O2	=	CO2	+	H2O	+	N2	+	SO2
0	1		11.05319		7.03546		8.03545		0		0
1	1		13.7607		8.84047		9.84045		0		0
2	1		15.96183		10.9416		10.0129		0.032757		0.013779
3	1		18.82777		13.0623		11.48365		0.041473		0.023645
4	1		22.14463		15.5149		13.18385		0.05204		0.0378
5	1		25.99146		18.3619		15.14395		0.064906		0.057581
6	1		35.07999		25.1051		19.71615		0.097633		0.116811
7	1		52.80616		38.3182		28.431		0.169324		0.272455
8	1		105.9743		78.2211		53.647		0.427764		0.929697

The heat of reaction at 25 °C (HR_{xn} 25 C) from the combustion reactor was compared to the negative of the NHV (i.e., the net heat of combustion) calculated in the oil characterization for each pseudo component.

To calculate the heat of reaction at 25 °C or 77 °F in VMGSim 7.0, follow the next steps:

Add the following compounds to the case: **O₂**, **CO₂**, **H₂O**, **N₂** and **SO₂**.

Assign the first oil pseudo component (**Oil_1_assay_1_ABP[234]F**) to a material stream named PC and enter 1 kgmole/h to the mole flow, assign **O₂** to a second material stream named O2 and enter the corresponding stoichiometric coefficient from the previous table as the mole flow, in this case 11.05319 kgmole/h.



Mix both streams using a **Mixer** unit operation and set the temperature and pressure of the mixed stream to 298.15 K (25 °C) and 101.325 kPa (1 atm).

/M1 (Mixer)

Name: **M1** Description:

Not Solved

Inlets: **2**

Summary | Equilibrium Results | Notes

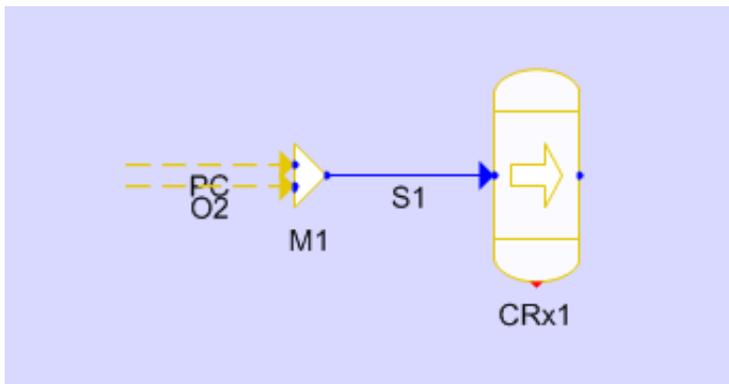
Main Data

Calc P Mode: **LowestPInOutlet**

Material

PortName	In0	In1	Out
Is Recycle Port	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Connected Stream/Unit Op	/O2.Out	/PC.Out	/S1.In
VapFrac			0.9558
T [C]			25.0
P [kPa]			101.33
Mole Flow [kgmole/h]	11.05	1.00	12.05
Mass Flow [kg/h]	353.69	100.70	454.39

Now connect a **Conversion Reactor** to the mixed stream.



Open the Conversion Reactor and go to the **Reactions** tab. Click on **Add/Edit** and fill the stoichiometric coefficients of the combustion reaction.

Reaction Data for CRx1

Enter data on the <New> column to add a reaction, <Delete> key to delete a reaction

	Rxn0	
Rxn Name	R1	<New>
Base Comp	Oil_1_Assay_1_ABP[234]F	
Conversion (%)	100.00	
Solution Order	0	
0 Oil_1_Assay_1_ABP[234]F	-1.00	
1 Oil_1_Assay_1_ABP[322]F		
2 Oil_1_Assay_1_ABP[401]F		
3 Oil_1_Assay_1_ABP[475]F		
4 Oil_1_Assay_1_ABP[548]F		
5 Oil_1_Assay_1_ABP[621]F		
6 Oil_1_Assay_1_ABP[757]F		
7 Oil_1_Assay_1_ABP[942]F		
8 Oil_1_Assay_1_ABP[1202]F		
9 OXYGEN	-11.0532	
10 CARBON DIOXIDE	7.0355	
11 WATER	8.0355	
12 NITROGEN		
13 SULFUR DIOXIDE		
Balance	0.0021	
H Rx'n(25 °C)[kJ/kmol]	-4408827.2151	

Selection reaction : Rxn0

R1:7.0355*CARBON_DIOXIDE+8.0355*WATER-!Oil_1_Assay_1_ABP[234]F-11.053;

Buttons: OK, Set Soln Order, Cancel

Now observe the heat of reaction at 25 °C (H Rx'n (25 C) = -4408827 kJ/kgmole) and compare it to the one obtained from the characterization (NHV = - Heat of Combustion @ 25 C = -4407470 kJ/kgmole). The average absolute deviation of the results is 0.0307 %.

The same procedure can be repeated for the rest of the characterized oil pseudo components. The required stoichiometric coefficients to solve the combustion equations were presented in the previous table. The comparison of the enthalpies of combustion for each pseudo component calculated in the oil characterization and those calculated from the combustion reactor are shown in the following table.

Heat of combustion reaction @ 25 °C:

n	-NHV [kJ/kmol] (H Comb @ 77 F)	HRxn 25 C [kJ/kmol]	AAD %
0	-4407470	-4408827	0.030794
1	-5466180	-5467831	0.030204
2	-6522640	-6524288	0.025271
3	-7700330	-7702206	0.02436
4	-9057410	-9059575	0.023904
5	-10626200	-10628664	0.02319
6	-14317800	-14321050	0.022701
7	-21478200	-21482858	0.021685
8	-42764800	-42773590	0.020554

As it can be seen in this table, the average absolute deviation between the heats of combustion from the oil characterization and those calculated in the combustion reactor are very small (less than 1 %).

Adjustment of pseudo component enthalpies of combustion from bulk oil values

The adjustment of the pseudo components enthalpies of combustion in the Oil characterization environment of VMGSim 7.0 with respect to the bulk oil values is performed in a similar way as the molecular weight adjustment. Once the pseudo components properties are calculated, a molar average bulk value is calculated; then, a normalization procedure is performed with respect to the provided (experimental) bulk value.

In order to be consistent with the units in VMGSim 7.0, the enthalpies of combustion can be provided in mass or molar basis. If the bulk molar basis value is provided, the mass bulk value is calculated using the available bulk molecular weight and the bulk molar basis value is used for the rest of the calculations.

If the bulk mass basis value is provided, the mole bulk value is calculated using the available bulk molecular weight and the bulk molar basis value is used for the rest of the calculations.

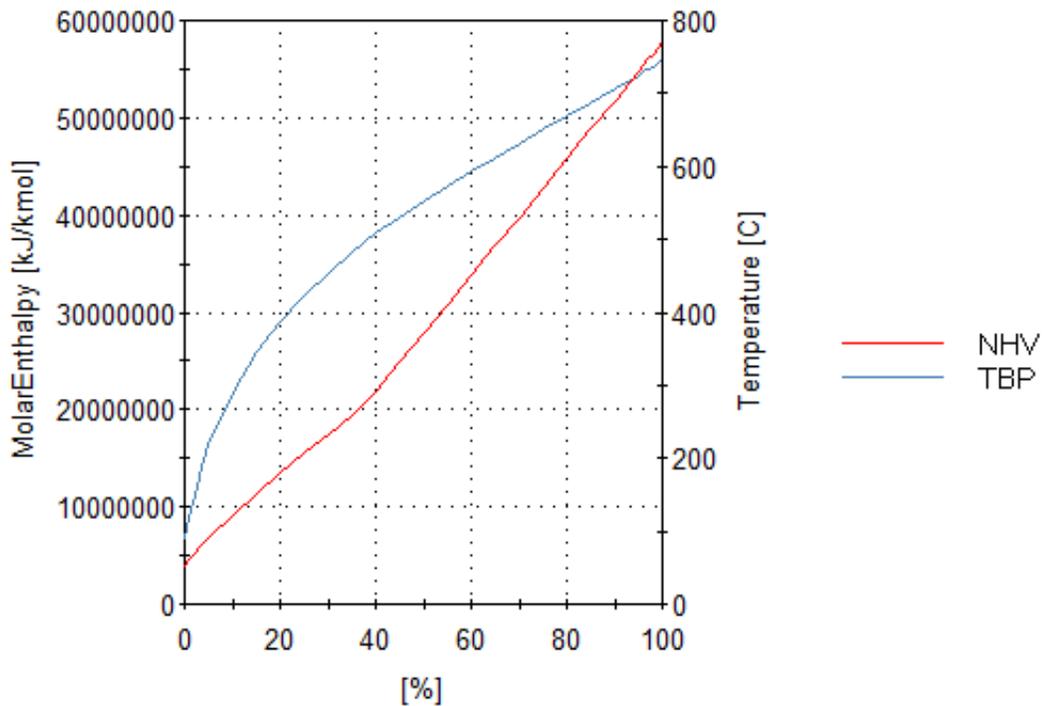
In the case of both, molar and mass basis, values are specified; the molar basis value will override the bulk mass basis.

In order to demonstrate how this adjustment works, see the following example in VMGSim 7.0.

Return to the oil that was characterized in the previous case (standard liquid density = 1000 kg/m³, MW = 500, Gamma Distribution, Gamma to TBP option and "Heavy_Oil" Range Set). As it can be seen in the following figure the bulk NHV in mole and mass basis is calculated from the pseudo components values.

Bulk Information	
Liquid Density @ 60 F [kg/m ³]	1000.000
MW	500.00
UOP K	11.23
Average Boiling Point [C]	516.0
Pressure [kPa]	101.33
NHV [kJ/kmol]	20097003.0
NHVMass [kJ/kg]	41125.99
Kinematic Visc @ 100 F [m ² /s]	5.53E-04
Kinematic Visc @ 210 F [m ² /s]	1.86E-05
Mode for Pseudo Names	Auto
Pseudo Base Name	Oil_1_Assay_1
Prefix	ABP
Suffix	F

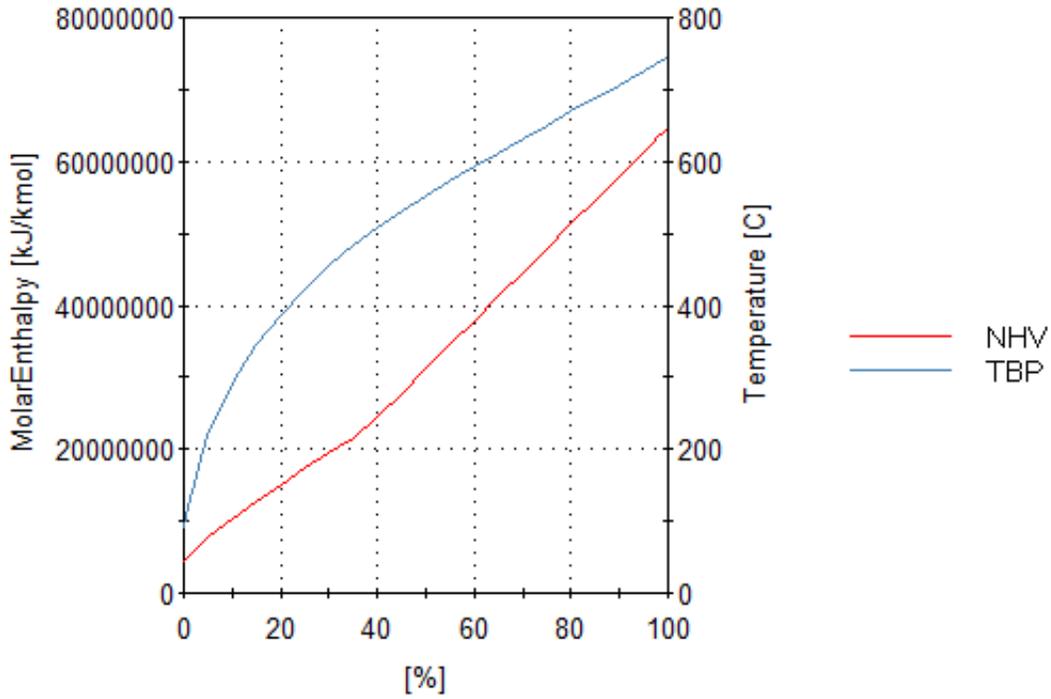
Go to the Results section and select NHV as the type of the Result Curves. Take a look to the NHV vs. %Dist plot (volume basis) based on the calculated NHV from the oil pseudo components.



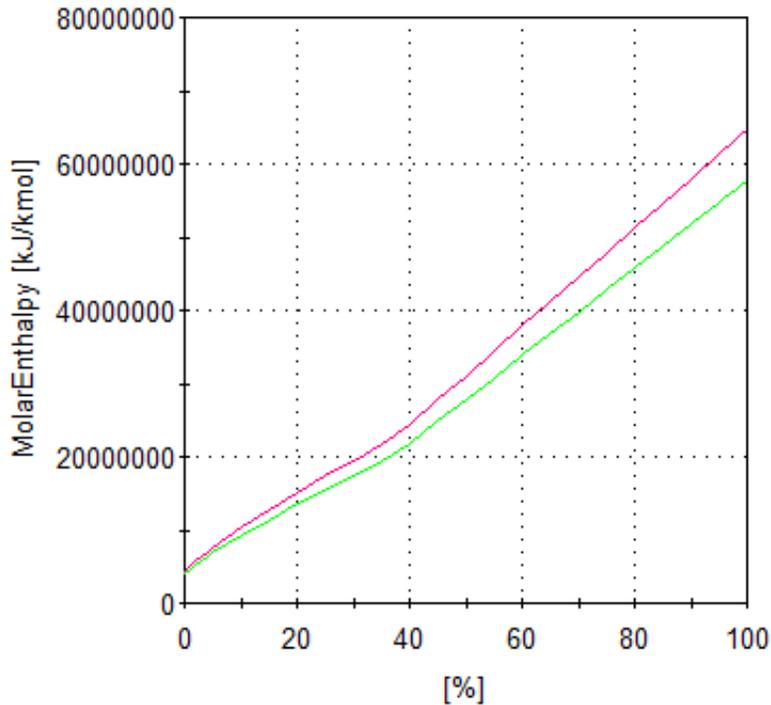
Now provide the NHVMass bulk value for this oil, let's assume that it is 45,000 kJ/kg and cut the oil.

Bulk Information	
Liquid Density @ 60 F [kg/m3]	1000.000
MW	500.00
UOP K	11.23
Average Boiling Point [C]	516.0
Pressure [kPa]	101.33
NHV [kJ/kmol]	20097003.0
NHVMass [kJ/kg]	45000.00
Kinematic Visc @ 100 F [m2/s]	5.53E-04
Kinematic Visc @ 210 F [m2/s]	1.86E-05
Mode for Pseudo Names	Auto
Pseudo Base Name	Oil_1_Assay_1
Prefix	ABP
Suffix	F

Go to the Results section and select NHV as the type of the Result Curves. Take a look to the NHV vs. %Dist plot (volume basis).



After cutting the oil with the new bulk NHV value, the NHV for the pseudo components are shifted to the left, because they were adjusted to a higher NHVMass bulk value than the one predicted before. The following figure compare both cases (the green line corresponds to the characterization without the bulk value and the pink one has the results from the characterization that adjusts the NHV of the pseudo components to the bulk value).



The opposite behaviour is expected if the NHV bulk value is lower than the predicted one.

References

1. API Technical Data Book: Petroleum Refining, 5th Edition, American Petroleum Institute, 1992
2. Himmelblau, D.M.; "Basic Principles and Calculations in Chemical Engineering", 7th Edition, Prentice Hall, Upper Saddle River, NJ, 2004

Tips and Tricks

Tower form - VMGSim™ 7.0

James van der Lee - VMG Calgary

Auto-create specifications from the configuration tab

Under the Configuration tab it is possible to enter tower specs by entering them into the appropriate value. For example, if you'd like to specify the std liquid volume flow rate in the condenser liquid simply expand the Details tab of the Draw frame and then type the desired spec value.

Name: T1_1 **Description:**

Configuration | Spec/Estimates | Efficiencies | Profile | Convergence | Settings | Notes | Add/RemoveStages ... | Schematic ...

Condenser: Partial Degree Subcool [F]: 0.00
 Reboiler: None Tower Sizing ...

Total stages = 39					
FEED		feed	bottomFeed	<New>	
Stage		29	30		
Connected Obj		/Crude_Feed_...			
+ Details					
DRAW		draw	condenserL	condenserV	bottomL <New>
Stage		1	1	1	30
Type		WaterDraw	LiquidDraw	VapourDraw	LiquidDraw
Connected Obj					
+ Details					
VapFrac					
T [F]					
P [psia]					
MoleFlow [lbmole/h]					
MassFlow [lb/h]					
VolumeFlow [ft3/s]					
StdLiqVolumeFlow [ft3/s]					
StdGasVolumeFlow [MMSCFD]					
+ Properties					
+ Molar Composition					
+ Mass Composition					
+ StdLiqVolume Composition					
+ Comp Mole Flow [lbmole/h]					

Print Always Restart from Last Conv **Feed 'bottomFeed' is not fully specified Not Converged** Ignored

Solve Restart Last Conv

As soon as the Enter key is pressed the value will be entered into the tower as a specification. Notice that the value now appears as a specified value, and the number of Degrees of Freedom has been reduced. This feature is of particular value when dealing with towers with a large number of degrees of freedom.

/T1_1 (RefluxedAbsorber): 39 Stages, Degree of Freedom = 12
Name: T1_1 **Description:**

Configuration | **Spec/Estimates** | Efficiencies | Profile | Convergence | Settings | Notes | |

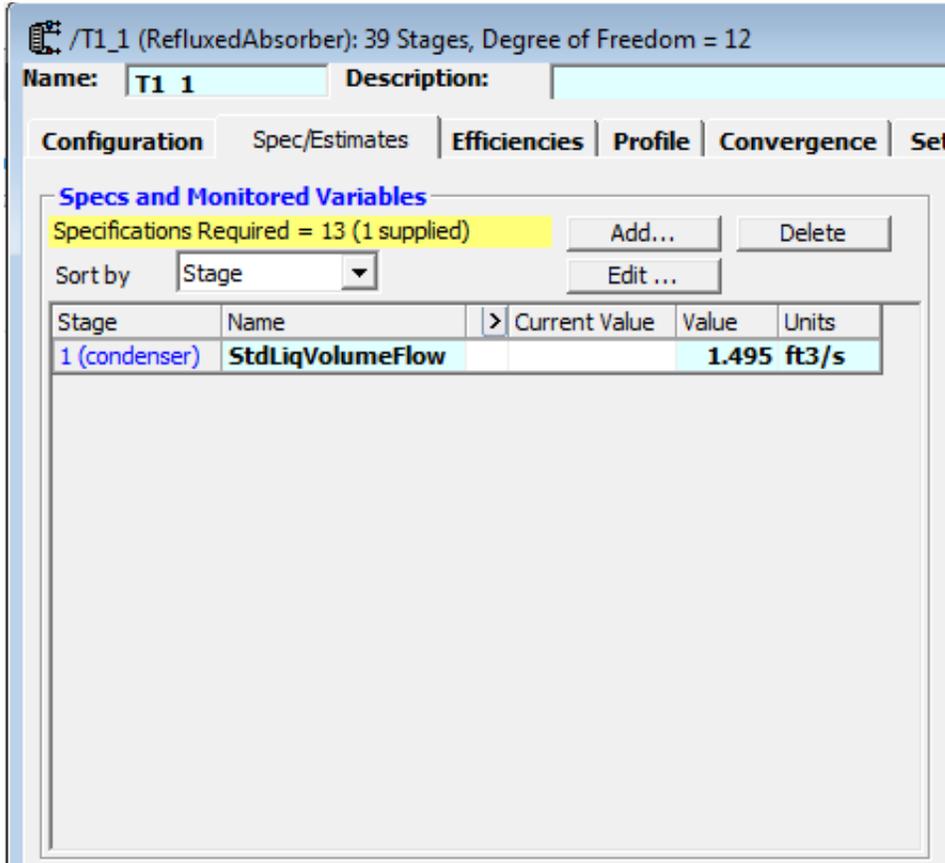
Condenser: Partial **Degree Subcool [F]:** 0.00
Reboiler: None

Total stages = 39					
FEED		feed	bottomFeed	<New>	
Stage		29	30		
Connected Obj		/Crude_Feed_...			
+ Details					
DRAW		draw	condenserL	condenserV	bottomL <New>
Stage		1	1	1	30
Type		WaterDraw	LiquidDraw	VapourDraw	LiquidDraw
Connected Obj					
+ Details					
VapFrac					
T [F]					
P [psia]			19.70	19.70	32.70
MoleFlow [lbmole/h]					
MassFlow [lb/h]					
VolumeFlow [ft3/s]					
StdLiqVolumeFlow [ft3/s]					
StdGasVolumeFlow [MMSCFD]					
+ Properties					
+ Molar Composition					
+ Mass Composition					
+ StdLiqVolume Composition					
+ Comp Mole Flow [lbmole/h]					

 Always Restart from Last Conv

Feed 'bottomFeed' is not fully specified
 Not Converged Ignored

Moving to the Spec/Estimates tab you will notice that the specs entered in the Configuration tab have also been added to the Specs and Monitored Variables section of the Spec/Estimates tab.



Create specifications directly in the specs section

The Specs and Monitored Variables section will allow you to add specifications directly (this is especially helpful if you cannot find the desired specs under the Configuration tab), and edit existing specs or delete them using the appropriate button. You can also convert a spec into a monitored variable by simply deleting the value of the spec.

Specify display units

Another useful feature of the Specs and Monitored Variables section is the ability to change units of each of the specs and monitored variables. For example, in the following figure the std liquid volume flow can be changed from ft3/s to bbl/day by clicking on the pull down menu and selecting bbl/day.

Specs and Monitored Variables
 Specifications Required = 13 (13 supplied) Add... Delete
 Sort by Stage Edit...

Stage	Name	>	Current Value	Value	Units
1 (condenser)	Reflux		0.8305	0.8305	
1 (condens...	StdLiqVolumeFlow	...	1.495	1.495	ft3/s
1 (condenser)	MoleFlow	...	0.00	0.00	ft3/s
2	Energy	...	5.500E+7	5.500E+7	gal(US)/...
3	StdLiqVolumeFlow		3.249	3.249	m3/s
17	Energy	...	3.500E+7	3.500E+7	gal(US)/hr
18	StdLiqVolumeFlow		1.950	1.950	bbl/day
22	Energy	...	3.500E+7	3.500E+7	bbl/hr
23	StdLiqVolumeFlow		1.950	1.950	ft3/hr
28	StdLiqVolumeFlow		0.227	0.227	Mbbl/day
3 (Strip_1)	StdLiqVolumeFlow	...	0.604	0.604	m3/d
3 (Strip_1)	Energy	...	7.500E+6	7.500E+6	ml/h
3 (Strip_2)	StdLiqVolumeFlow	...	1.251	1.251	l/h
3 (Strip_3)	StdLiqVolumeFlow	...	0.292	0.292	cm3/min

Specs and Monitored Variables
 Specifications Required = 13 (13 supplied) Add... Delete
 Sort by Stage Edit...

Stage	Name	>	Current Value	Value	Units
1 (condenser)	Reflux		0.8305	0.8305	
1 (condenser)	StdLiqVolumeFlow	...	23000.000	23000.000	bbl/day
1 (condenser)	MoleFlow	...	0.00	0.00	lbmole/h
2	Energy	...	5.500E+7	5.500E+7	Btu/hr
3	StdLiqVolumeFlow		3.249	3.249	ft3/s
17	Energy	...	3.500E+7	3.500E+7	Btu/hr
18	StdLiqVolumeFlow		1.950	1.950	ft3/s
22	Energy	...	3.500E+7	3.500E+7	Btu/hr
23	StdLiqVolumeFlow		1.950	1.950	ft3/s
28	StdLiqVolumeFlow		0.227	0.227	ft3/s
3 (Strip_1)	StdLiqVolumeFlow	...	0.604	0.604	ft3/s
3 (Strip_1)	Energy	...	7.500E+6	7.500E+6	Btu/hr
3 (Strip_2)	StdLiqVolumeFlow	...	1.251	1.251	ft3/s
3 (Strip_3)	StdLiqVolumeFlow	...	0.292	0.292	ft3/s

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