12. Petroleum Calculations

Overview

Calculations with the OLI Software can be used to characterize crude oils. Here is a quote from the OLI Tricks of the Trade manual (AQSim):

Crude oils are complex groups of organic molecules containing hundreds, perhaps thousands of pure components in a single oil. Modeling crude oils using pure components is impractical, because analyzing for each pure component is cost prohibitive and the number of species would make calculations overwhelming. A convenient solution to this problem and to modeling the properties of a crude oil is to create pseudo components. Crude Oil properties may be defined through a distillation curve, where each boiling point range is a progression of molecular weights, densities, solubilities, viscosities and other properties associated with that section. It is reasonable for low boiling point molecules to be low molecular weight, low density, low viscosity, and more soluble in water. We can dice boiling point curves using well accepted methods standard to create pseudocomponents that in combination reflect the property of the whole oil.

There are two ways to create a crude oil stream on the Analyzers. The first is to start with a PVT curve and create pseudocomponents using one of the three thermodynamic methods coded into the software. The second is to enter the pseudocomponent data directly and using the same thermodynamic methods to predict the component properties.

The three thermodynamic methods are API, Lee Kesler, and Cavett. At the time of writing, the software implementation specifications for these methods were not in hand.

This involves taking distillation data (such as ASTM D86) and converting that information into properties that the OLI software can use. This is generally referred to as “Creating Pseudo Components.”

There are two classes of this type of data. Actual assay (or distillation data) in which we cut the boiling point curves up into individual components or the actual entering of a pseudocomponent.

This section shows you how to enter each method.

Assays

For this example we will enter a distillation curve for a sample crude oil. This sample used ASTM method D86 to characterize the crude oil (see Chapter 13 on page 224 for a description of the distillation methods). The data for the distillation curve can be found in Table 12-1 on page 211.
Table 12-1 Sample Distillation data using ASTM method D86, API Gravity of 31

<table>
<thead>
<tr>
<th>Volume Percent Distilled</th>
<th>Temperature, C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td>5</td>
<td>30</td>
</tr>
<tr>
<td>10</td>
<td>50</td>
</tr>
<tr>
<td>20</td>
<td>60</td>
</tr>
<tr>
<td>40</td>
<td>80</td>
</tr>
<tr>
<td>60</td>
<td>120</td>
</tr>
<tr>
<td>80</td>
<td>150</td>
</tr>
<tr>
<td>90</td>
<td>180</td>
</tr>
<tr>
<td>95</td>
<td>200</td>
</tr>
<tr>
<td>99</td>
<td>220</td>
</tr>
<tr>
<td>100</td>
<td>240</td>
</tr>
</tbody>
</table>

Create a standard OLI Studio stream at the following conditions

Stream Name  Crude
Temperature  25 °C
Pressure  1.0 atmospheres
H₂O  5 moles

You will need to enter the name of the assay. In our example we are using the name “Assay”. You are limited to only 5 characters for the name of the assay.

**After entering the name Assay Do Not (repeat Do Not) press any other key! See Figure 12-1**
The OLI Analyzer requires a different series of key strokes to enable the entering of the assay data.

After typing the name “Assay” you will need to use the following key combination

**Shift – Enter**

Press both of these keys together. You should be able to view the screen as shown in Figure 12-2 on page 213.
We will begin by defining the type of assay data. Click in the cell next to the **Assay Data Type** to see a list of distillation types.

There are four types, select **ASTM D86**

Next click in the cell next to the **Average Bulk Density Type**
There are three types (see 13 on page 224)

Select **API Gravity**

Finally we need to select the thermodynamic method. Click in the cell next to **Thermo Method**

There are four types (see 13 on page 224)

![Thermodynamic methods](image)

Select **API-8** (Default)

We are now ready to enter the distillation data. Click the **Edit** button next to the **Distillation Data** cell. You should see Figure 12-6 below.

![Blank Distillation Data](image)

Enter the data from Table 12-1 on page 211
Figure 12-7 Completed Data

When done click the **OK** button.

We can now finish the entering of the data.

Temperature  25.0  °C
Pressure   1.0    Atm
H2O       5.0    mole
Assay     1000.0  mole
Density (API)  31
Distillation Curve Cuts  5
The Distillation Curve Cuts will eventually become individual pseudocomponents, each with its own critical parameters and thermodynamic reference data.

After entering the data, select an Isothermal calculation and click the **Calculate** button.

Figure 12-9 below shows the range of composition.
You can see that the program calculated a Liquid-Liquid case in which we have some organic liquid and some aqueous liquid. Our crude oil named “Assay” has been split apart into 5 individual components (remember the “Cuts” above?). Each component has the parent assay name and temperature of the cut in Kelvin.
Pseudocomponents

There are times when the user does not have (or does not want to use) distillation data. Rather the user had the individual properties for a single pseudocomponent. OLI allows the user to enter the individual pseudocomponents.

We will start by creating a standard stream. On the input grid we will enter our pseudocomponent name. In Figure 12-10 below we are entering the name PC1.

Press the Control-Enter keys to open the dialog.

Figure 12-10 Starting to enter a pseudocomponent
This will create an empty data grid for the pseudocomponent. As with the assays, we need to enter some data for the pseudocomponent.

For this example we will have 100 moles of the component which has a normal boiling point of 20°C and a specific gravity of 0.72. The third parameter, molecular weight, will be calculated in this example. In general, only two of the three parameters need be entered.

After entering the pseudocomponent, please enter the remaining pseudocomponents as found in Table 12-2 below.

**Table 12-2 Sample pseudocomponent data**

<table>
<thead>
<tr>
<th>Pseudocomponent</th>
<th>Amount (moles)</th>
<th>Method</th>
<th>Normal Boiling Point, °C</th>
<th>Specific Gravity</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC1</td>
<td>100</td>
<td>API</td>
<td>20</td>
<td>0.72</td>
</tr>
<tr>
<td>PC2</td>
<td>200</td>
<td>API</td>
<td>60</td>
<td>0.76</td>
</tr>
<tr>
<td>PC3</td>
<td>250</td>
<td>API</td>
<td>100</td>
<td>0.8</td>
</tr>
<tr>
<td>PC4</td>
<td>250</td>
<td>API</td>
<td>140</td>
<td>0.85</td>
</tr>
<tr>
<td>PC5</td>
<td>180</td>
<td>API</td>
<td>190</td>
<td>0.9</td>
</tr>
</tbody>
</table>
Figure 12-13 below shows the completed input grid.

Notice that at the bottom of each pseudo component there is a “+” and a field called calculated properties. OLI Studio immediately predicts all the calculated properties for each pseudocomponent. Click the “+” sign next to PC1.
The values in the green boxes can be changed to match data from other programs.

Create a single point calculation, set the conditions to 15°C and 1.0 atmospheres and press the calculate button.
Figure 12-15 PC Output