Oil Characterization

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Workshop

The petroleum characterization method in UniSim Design converts laboratory analyses of condensates, crude oils, petroleum cuts, and coal-tar liquids into a series of discrete hypothetical components. These petroleum hypo components provide the basis for the property package to predict the remaining thermodynamic and transport properties necessary for fluid modeling.

UniSim Design produces a complete set of physical and critical properties for the petroleum hypocomponents with a minimal amount of information. However, the more information you supply about the fluid, the more accurate these properties will be, and the better UniSim Design will predict the fluid's actual behaviour.

In this example, the Oil Characterization option in UniSim Design is used to model a reservoir fluid. The fluid is a combined gas and oil stream.

Learning Objectives

Once you have completed this section, you will be able to:

- Enter Oil data into UniSim Design and characterize an oil.

Building the Simulation

Before you start the characterization process, you must:

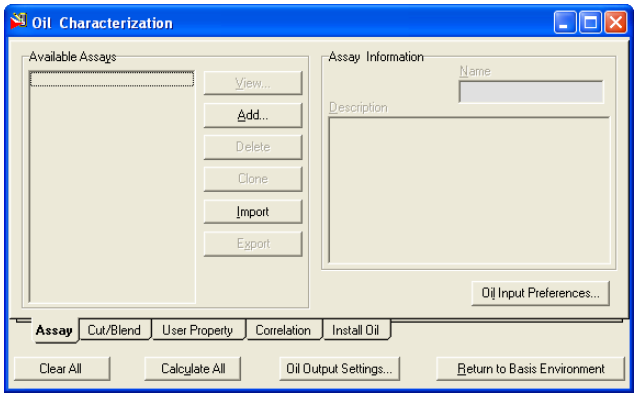
- Select a property package
- Add any non-oil components, specifically the light ends that are used in the characterization process

Defining the Simulation Basis

For this module, you will be building on the case that you saved at the end of the Getting Started Module.

1. Open the case that you saved at the end of the Getting Started Module.
2. Click the Enter Basis Environment button to return to the Basis environment.
3. Go to the **Oil Manager** tab and click the **Enter Oil Environment** button. You could also press the **Oil Environment** button on the tool bar. The oil characterization view appears.

Figure 1



Oil Characterization

The petroleum characterization in UniSim Design accepts different types of information about the oil. The more information you can supply about your sample, the more accurate the representation.

The Minimum amount of information that UniSim Design requires to characterize an oil:

- a laboratory distillation curve

or

- two of the following bulk properties: Molecular Weight, Density, or Watson K Factor.

There are three steps involved in characterizing any oil in UniSim Design:

1. Characterize the assay.
2. Generate hypocomponents.
3. Install the oil in the flowsheet.

Characterize the Assay

The assay contains all of the petroleum laboratory data, boiling point curves, light ends, property curves, and bulk properties. UniSim Design uses the supplied assay data to generate internal TBP, molecular weight, and density and viscosity curves (referred to as Working Curves). Just as with fluid packages, assays can be imported and exported to be used in different cases.

Assay Types

Accurate volatility characteristics are vital when representing a petroleum fluid in your process simulation. For all Distillation Curves, you are required to enter at least 5 data points. UniSim Design accepts the following standard laboratory analytical assay procedures:

- **True Boiling Point (TBP)**. Performed using a multi-stage batch fractionation apparatus operated at relatively high reflux ratios. TBP distillations conducted at atmospheric or vacuum conditions are accepted by the characterization.
- **ASTM D86**. Distillation employing batch fractionation but conducted using non-refluxed Engler flasks. Generally used for light to medium petroleum fluids. UniSim Design can correct for barometric pressure or cracking effects. You must provide the data on a liquid volume basis.
- **ASTM D1160**. Distillation employing batch fractionation but conducted using non-refluxed Engler flasks. Generally used for heavier petroleum fluids. Curves can be given at atmospheric pressure or corrected for vacuum conditions. You must provide the data on a liquid volume basis.
- **ASTM D86_D1160**. This is a combination of the D86/D1160 distillation data types. You can correct for thermal cracking and enable vacuum distillation for sub-atmospheric conditions. You must provide data on a liquid volume basis.
- **ASTM D2887**. Simulated distillation analysis from chromatographic data. Reported only on a weight percent basis at atmospheric conditions.
- **Equilibrium Flash Vaporization (EFV)**. Involves a series of experiments at constant atmospheric pressure, where the total vapour is in equilibrium with the unvapourized liquid.
- **Chromatographic Analysis**. A gas chromatograph analysis of a small sample of completely vapourized oil, analyzed for paraffin, aromatic, and naphthenic hydrocarbon groups from C6 to C30. Chromatographic analyses may be entered on a mole, mass or liquid volume basis.

Light Ends

Light Ends are defined as pure components with low boiling points. Components in the boiling range of C2 to n-C5 are most commonly of interest.

UniSim Design provides three options to account for Light Ends:

- **Ignore**. UniSim Design characterizes the Light Ends portion of your sample as hypocomponents. This is the least accurate method and as such, is not recommended.
- **Auto Calculate**. Select this when you do not have a separate Light Ends analysis but you want the low boiling portion of your assay represented by pure components. UniSim Design will only use the pure components you have selected in the fluid package.
- **Input Composition**. Select this when you have a separate Light Ends assay and your petroleum assay was prepared with the Light Ends in the sample. UniSim Design will provide a form listing the pure components you selected in the fluid package. This is the most accurate method of representation.

Bulk Properties

Bulk Properties for the sample may also be supplied. The bulk properties are optional if a distillation curve or chromatograph have been supplied.

- **Molecular Weight**. This is the Molecular Weight of the bulk sample. It must be greater than 16.
- **Mass Density**. The mass density must be between 250 and 2000 kg/m3. The units for density can be mass density, API or specific gravity, chosen from the drop down list in the Edit Bar.
- **Watson (UOP) K Factor**. This must be between 8 and 15. The Watson K Factor is an approximate index of paraffinicity. K = (Mean Avg BP)1/3/ (sp gr 60F/60F)
- **Bulk Viscosities**. Given at two reference temperatures, typically 37.78°C and 98.89°C (100°F and 210°F).

Physical Property Curves

UniSim Design accepts different types of physical property curves:

- Molecular weight curve
- Density curve
- Viscosity curve

Physical property analyses are normally reported from the laboratory using one of the following two conventions:

- Independent Assay Basis. A common set of assay fractions is not used for both the distillation curve and the physical property curve.
- Dependent Assay Basis. A common set of assay fractions is used for both the distillation curve and the physical property curve.

As you supply more information to UniSim Design, the accuracy of the petroleum characterization increases. Supplying any or all of the bulk molecular weight, bulk density, or bulk Watson K factor will increase the accuracy of your hypocomponent properties. You can also supply laboratory curves for molecular weight, density, and/or viscosity which will increase the accuracy further.

Adding Assay Data

On the Oil Characterizations view:

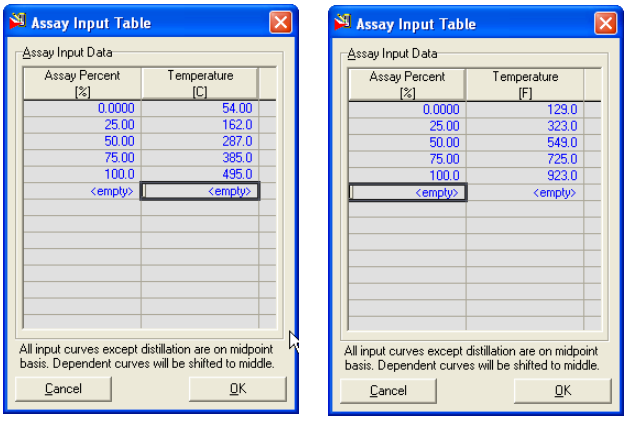
1. Select the **Assay** tab.
2. Click the **Add** button.
3. The **Input Data** tab of the Assay view appears.
4. In the **Name** cell, change the assay name to **Res-Fluid**.
5. For the Bulk Props cell, use the drop-down list to select **Used**.
6. From the Assay Data Type drop-down list, select **TBP**.
7. Once the correct Data Type is chosen, additional cells should appear. In the Light Ends cell; use the drop-down list to select **Input Composition**. The other cells will not be used in this example.
8. Select the **Light Ends** radio button in the Input Data group.
9. Specify the **Light Ends Basis** as **Mole %.**
10. Enter the following data. Note that the default basis for Light Ends is Liquid Volume %; this must be changed *before* the data is entered.

For this component...	Enter this Mole %...
N2	0.48
H2S	0.00
CO2	0.87
C1	41.83
C2	8.87
C3	7.11
i-C4	1.47
n-C4	3.75

For this component...	Enter this Mole %...
i-C5	1.25
n-C5	1.63
C6	0.00
H2O	0.00

11. Select the **Distillation** radio button. Change the curve basis from Mole to **Liquid Volume**.
12. Click on the **Edit Assay** button to enter the curve as shown below.

Figure 2



13. Select the **Bulk Props**. radio button to enter the following bulk property data:
    - The Molecular Weight is **79.6**
    - The Standard Density is **0.6659 SG_60/60api**

14. Click on the **Light Ends Handling & Bulk Fitting Options** button, and un-check the option for Curve Includes L.E. for the distillation curve. This is required because the curve data does not include the light ends components.
15. Once you have entered all of the data, click the **Calculate** button. The status message at the bottom of the assay window should change to **Assay was Calculated**.

Once the assay is calculated, the working curves are displayed on the **Working Curves** tab. The working curves are regressed from the entered data. The calculation of the blend will be based on these curves.

16. Close the Assay window to return the **Oil Characterization** view. You should still be on the **Assay** tab of the view.

Notice that all of the buttons are now accessible.

Hypocomponent Generation/Oil Blending

The Cut/Blend characterization in UniSim Design splits the internal working curves for one or more assays into hypocomponents. The Cut/Blend tab of the Oil Characterization view provides two functions, cutting the oil into Hypocomponents and blending two or more Assays into one set of hypocomponents.

Cut Ranges

You have three choices for the Cut Option Selection:

- **Auto Cut** - UniSim Design cuts the assay based on internal values.

Range...	Cuts...
37.78 - 425 ^{o}C (100-800 ^{o}F)	28 (4 per 37.78 ^{o}C or 100 ^{o}F)
425 - 650 ^{o}C (800-1200 ^{o}F)	8 (2 per 37.78 ^{o}C or 100 ^{o}F)
650-870 ^{o}C (1200-1600 ^{o}F)	4 (1 per 37.78 ^{o}C or 100 ^{o}F)

- **User Points** - You specify the number of hypocomponents required. UniSim Design proportions the cuts according to an internal weighting scheme.

Range...	Cuts...
IBP - 425 ^{o}C (IBP-800 ^{o}F)	4 per 37.78 ^{o}C or 100 ^{o}F
425 - 650 ^{o}C (800-1200 ^{o}F)	2 per 37.78 ^{o}C or 100 ^{o}F
650 - FBP (1200-FBP)	1 per 37.78 ^{o}C or 100 ^{o}F

- **User Ranges** - You specify the boiling ranges and the number of cuts per range.

Cutting the Assay

Once the Assay has been calculated, you can cut the Assay into individual hypocomponents.

1. Move to the **Cut/Blend** tab of the Oil Characterization view. Click the **Add** button to create a new Blend.
2. In the Name cell, change the name from the default, Blend-1 to **Res-Fluid**.
3. From the list of Available Assays (there should only be one), select **Res-Fluid** and click the **Add** button. This adds the Assay to the Oil Flow Information table and a blend (cut) will automatically be calculated. The Blend is calculated using the default Cut Option, **Auto Cut**.
4. Instead of using the default Auto Cut option, change the Cut Option Selection to **User Points** and change the Number of Cuts to **5**.

The results of the calculation can be viewed on the **Tables** tab of the Blend view.

Installing the Oil in the Flowsheet

The final step of the characterization is to transfer the hypocomponent information into the flowsheet.

1. Move to the **Install Oil** tab of the Oil Characterization view. The blend, Res-Fluid appears in the Oil Install Information group.
2. In the Stream Name column, enter the name, **GasWell 4**, to which the oil composition will be transferred. UniSim Design will assign the composition of your calculated Oil and Light Ends into this stream, completing the characterization process.
3. Return to the Basis Environment by clicking the **Return to Basis Environment** button.

When you return to the Basis Environment, the hypocomponents that you have generated in the Oil Characterization are placed in the current fluid package. You can view the fluid package and examine the individual hypothetical components which make up your oil.

Save your case!

Analyzing the Results

Once you have calculated a blend, you can examine various property and flow summaries for the generated hypocomponents that represent a calculated oil.

Return to the Oil Environment and open the view for the blend, Res-Fluid.

Tables Tab

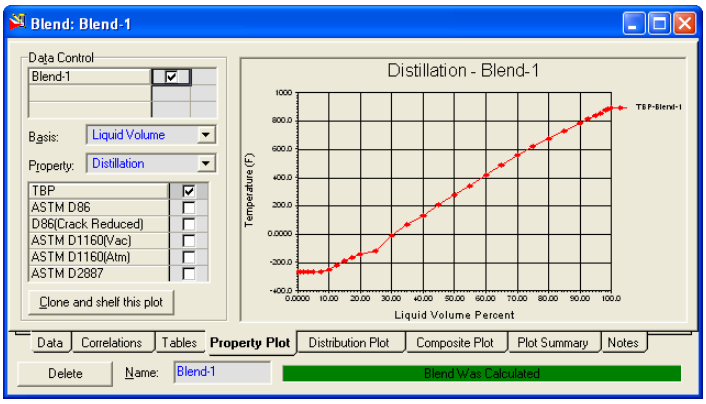
The Tables tab of the blend contains various information, representing the oil and the components. From the **Table Type** drop down, you can select different information to display.

- **Component Properties**. When this is selected, choose either Main Properties or Other Properties from the Table Control.
- **Main Properties**. Provides the normal boiling point, molecular weight, density, and viscosity information for each component in the oil.
- **Other Properties**. Provides the critical temperature, critical pressure, acentric factor, and Watson K Factor for each individual hypocomponent.
- **Component Breakdown**. For the input light ends and each hypocomponent, this provides individual liquid volume %, cumulative liquid volume %, volume, mass, and mole flows.
- **Molar Compositions**. Provides the molar fractions of each light ends component and each hypocomponent in the oil.
- **Oil Properties**. Choose the Basis (Mole, Mass, Liquid Volume) and then the property you want to display.
- **Boiling Points**. Provides TBP, D86, D86 Corr, D1160 Vac, and D1160 Atm temperature ranges for the oil.
- **Other Properties**. Provides critical temperature, critical pressure, acentric factor, molecular weight, density, and viscosity ranges for the oil.
- **User Properties**. Provides all user property ranges for the oil.
- **Oil Distributions**. Provides tabular information of how your assay would be distributed in a fractionation column. You can use standard fractionation cuts or user defined cuts.

Property Plot Tab

UniSim Design can plot various properties versus liquid volume, mole, or mass percent distilled.

Figure 3



From the Basis drop-down list, choose Mass, Mole, or Liquid Volume for the X-axis.

From the Property drop-down list, choose the property to be plotted on the Y-axis.

- Distillation. You can plot one or more of the following: TBP, D86, D86 (Crack Reduced), D1160 (Vac), D1160 (Atm), or D2887.
- Molecular Weight
- Density
- Viscosity
- Critical Temperature
- Critical Pressure
- Acentric Factor
- User Properties

Composite Plot Tab

The Composite Plot tab allows you to visually check the match between the input assay data and the calculated property curves. The choice for the graphical comparison is made from the Property drop-down list.

- TBP or ASTM Distillation Curve
- Molecular Weight Curves
- Mass Density Curves
- Viscosity Curves
- Any User Property Curve

Viewing the Stream in the Simulation

1. Leave the Oil Environment to return to the Basis Environment.
2. Enter the Simulation Environment.
3. Move to the Workbook to view the stream that you created, **GasWell 4**. You can view the stream composition on the Compositions tab.

If you determine that some of the hypocomponents parameters need to be recalculated, you can return to the Oil Environment at any time to make changes.

The following parameters need to be added to the stream GasWell 4:

- Temperature = **35°C (95°F)**
- Flowrate = **545 kgmole/h (1200 lbmole/hr)**

Save your case!