Retrieve NIST Experimental Data within Aspen Plus® V8.0

1. Lesson Objectives

- Learn how to retrieve NIST experimental data for pure components in Aspen Plus.

2. Prerequisites

- Aspen Plus V8.0

3. Background

There are many reasons that we need physical properties of pure components.

When we look for a solvent for extractive distillation (a technology that uses a third component, the solvent, to separate two components in a mixture that are difficult to separate directly via distillation), we look for components with normal boiling point temperatures that are higher (but not too much higher) than the components to be separated. For such a case, we need to know the normal boiling point temperatures of candidate solvents during the search.

When we look for a solvent for extraction, we need to check the densities of candidate solvents to ensure the two liquid phases formed during extraction have enough differences in density. For the selected solvent, we also need to check its density against the existing liquid phase so that we know which liquid phase is heavier.

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Problem Statement and Aspen Plus Solution

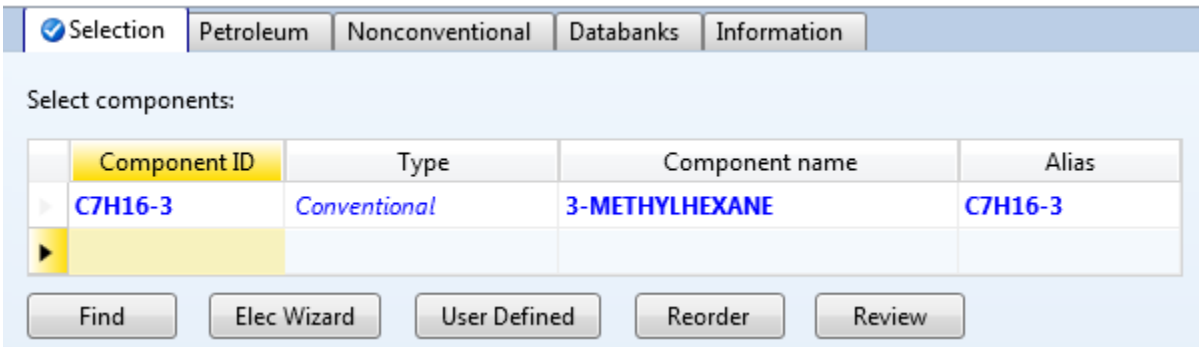
Problem Statement

The pre-condition of this example is that 3-methylhexane is now considered a promising candidate solvent for separation of acetone and water. The task is to determine whether the density of 3-methylhexane is different enough from the density of water. We also need to determine which of the two liquid phases formed mainly by these two components is heavier.

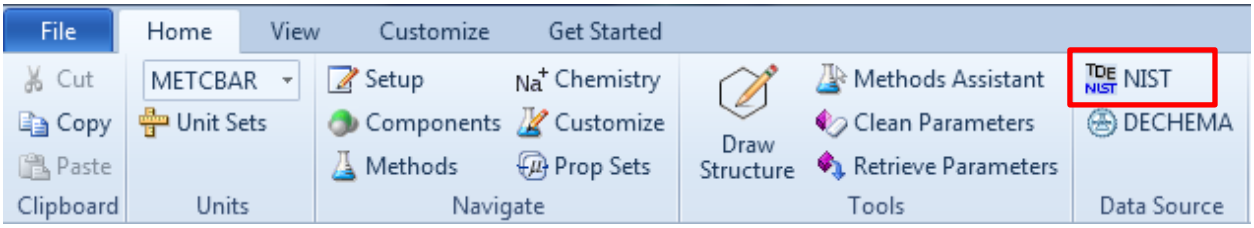
Aspen Plus Solution

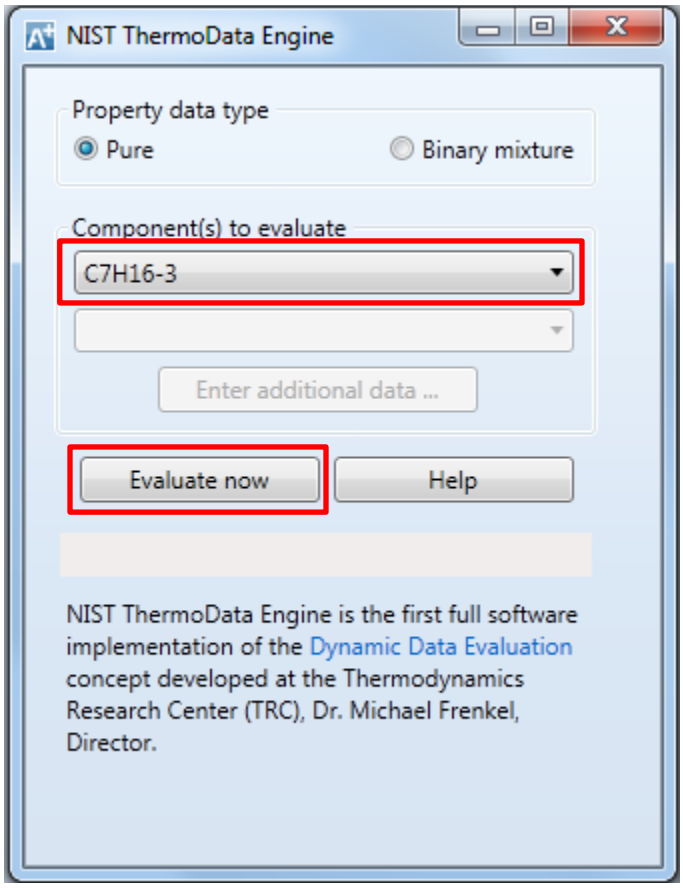
If you are unfamiliar with how to start Aspen Plus, select components, or define methods, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

4.01. Create a new simulation in Aspen Plus using the **Blank Simulation** template. The **Components | Specification | Selection** sheet is displayed. Enter **C7H16-3** for **Component ID**. Aspen Plus should auto-fill **Component name** as 3-methylhexane. If the component you are looking for does not appear, you can also use the **Find** button to search for the component.

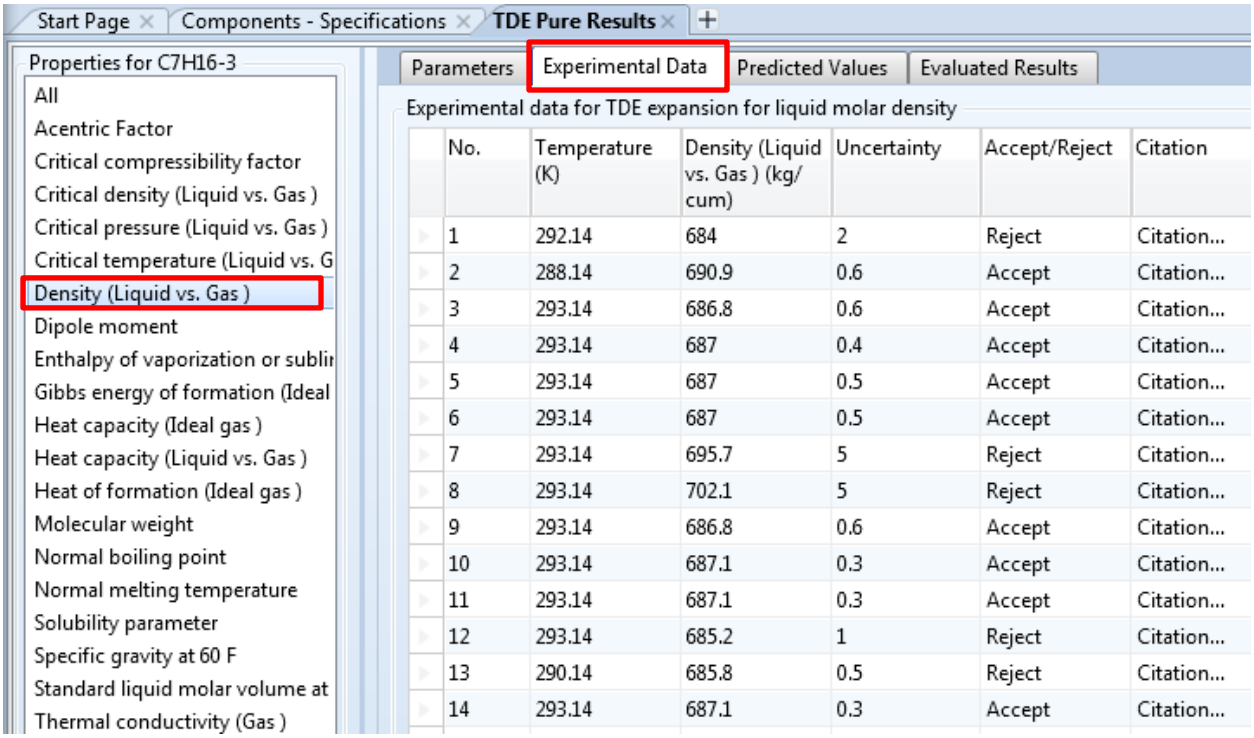


4.02. To retrieve and view the NIST experimental data and perform property evaluation, click the **Data Source | NIST** button in the **Home** tab of the ribbon. Select **C7H16-3** under **Component(s) to evaluate**. Click the **Evaluate now** button and wait for the search engine to retrieve the data.



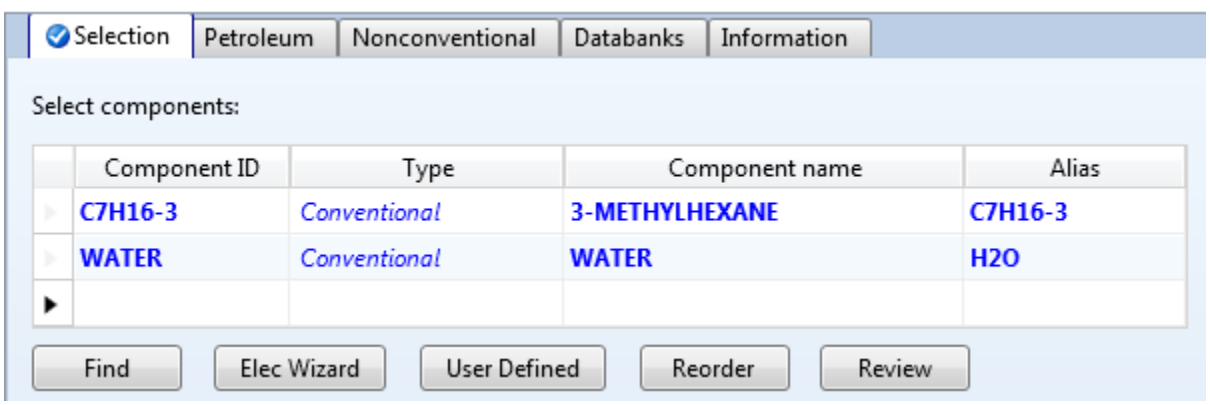


4.03. Close the **NIST ThermoData Engine** window after the search is complete. Select the **Density (Liquid vs. Gas)** option under **Properties for C7H16-3** and then click the **Experimental Data** sheet. You will see a list of experimental data from NIST, sorted by temperature, density, uncertainty, accept/reject, and citation. The **Accept/Reject** column indicates whether or not the specific experimental data point serves as an outlier. Note that the density for 3-methylhexane is approximately 685 kg/m^3 at room temperature.



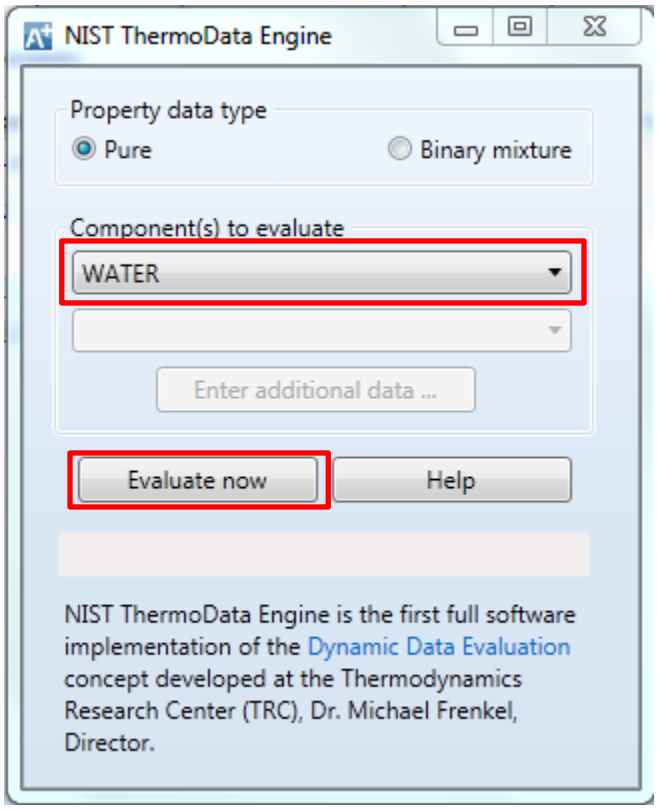
No.	Temperature (K)	Density (Liquid vs. Gas) (kg/cum)	Uncertainty	Accept/Reject	Citation
1	292.14	684	2	Reject	Citation...
2	288.14	690.9	0.6	Accept	Citation...
3	293.14	686.8	0.6	Accept	Citation...
4	293.14	687	0.4	Accept	Citation...
5	293.14	687	0.5	Accept	Citation...
6	293.14	687	0.5	Accept	Citation...
7	293.14	695.7	5	Reject	Citation...
8	293.14	702.1	5	Reject	Citation...
9	293.14	686.8	0.6	Accept	Citation...
10	293.14	687.1	0.3	Accept	Citation...
11	293.14	687.1	0.3	Accept	Citation...
12	293.14	685.2	1	Reject	Citation...
13	290.14	685.8	0.5	Reject	Citation...
14	293.14	687.1	0.3	Accept	Citation...

4.04. In the navigation pane, go to the **Components | Specifications | Selection** sheet. Enter **WATER** for **Component ID** in the second row on the grid.

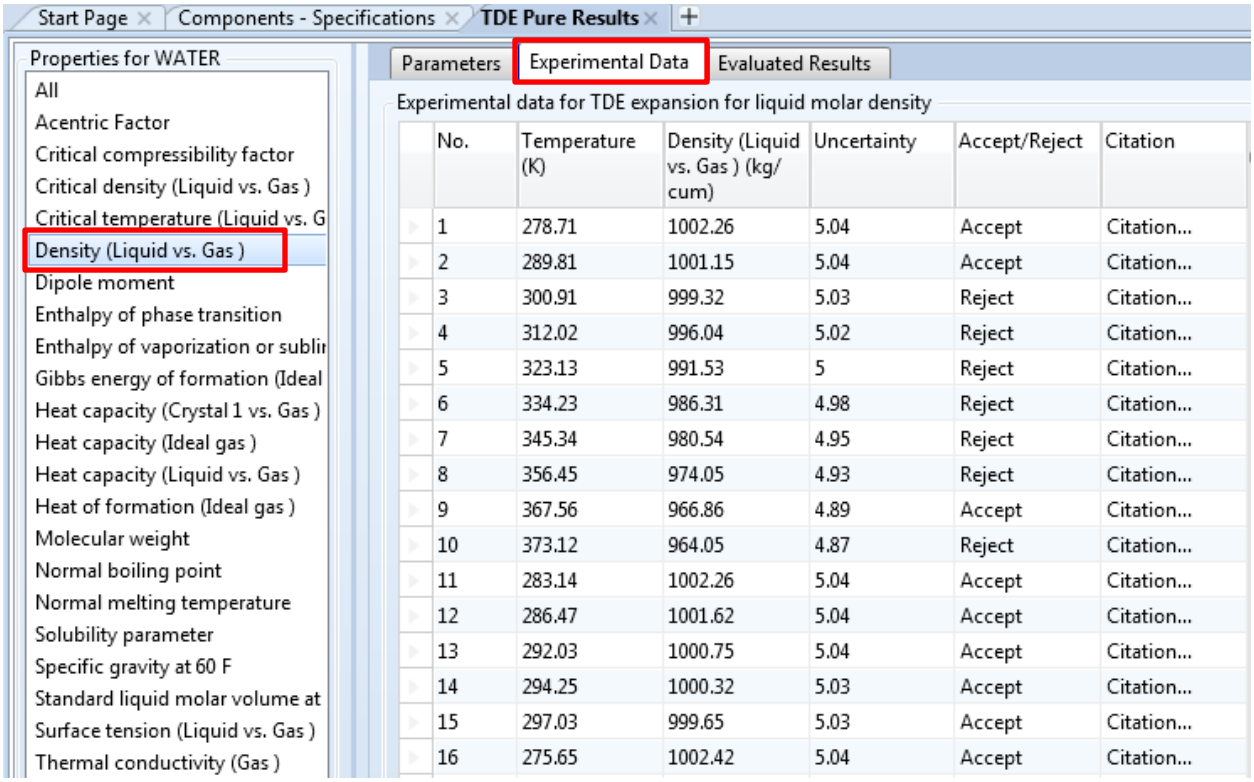


Component ID	Type	Component name	Alias
C7H16-3	Conventional	3-METHYLHEXANE	C7H16-3
WATER	Conventional	WATER	H2O

4.05. Click the **Data Source | NIST** button in the **Home** tab of the ribbon. Select **WATER** as the **Component(s) to evaluate**. Click the **Evaluate now** button to retrieve experimental data of water from NIST.



4.06. Close the **NIST ThermoData Engine** window after the search is complete. Select the **Density (Liquid vs. Gas)** option under the **Properties for WATER** and go to the **Experimental Data** sheet. You will see a list of experimental data from NIST, sorted by temperature, density, uncertainty, accept/reject, and citation. Note that the density of water is approximately 1000 kg/m^3.



No.	Temperature (K)	Density (Liquid vs. Gas) (kg/cum)	Uncertainty	Accept/Reject	Citation
1	278.71	1002.26	5.04	Accept	Citation...
2	289.81	1001.15	5.04	Accept	Citation...
3	300.91	999.32	5.03	Reject	Citation...
4	312.02	996.04	5.02	Reject	Citation...
5	323.13	991.53	5	Reject	Citation...
6	334.23	986.31	4.98	Reject	Citation...
7	345.34	980.54	4.95	Reject	Citation...
8	356.45	974.05	4.93	Reject	Citation...
9	367.56	966.86	4.89	Accept	Citation...
10	373.12	964.05	4.87	Reject	Citation...
11	283.14	1002.26	5.04	Accept	Citation...
12	286.47	1001.62	5.04	Accept	Citation...
13	292.03	1000.75	5.04	Accept	Citation...
14	294.25	1000.32	5.03	Accept	Citation...
15	297.03	999.65	5.03	Accept	Citation...
16	275.65	1002.42	5.04	Accept	Citation...

5. Conclusions

The density of 3-methylhexane is around 685 kg/m^3, which is clearly less than the density of water (1000 kg/m^3). The liquid phase formed mainly by 3-methylhexane should be lighter than the phase formed mainly by water and, thus, the aqueous phase should be at the bottom and the other liquid phase should be at the top.

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