HOMEWORK/CLASSWORK 2.1 (WATER–ALCOHOL SYSTEM)

We have a 50/50 wt. % mixture of water and *n*-hexanol. We plan to separate this mixture into its constituents and ultimately end up with almost pure streams of water and alcohols. Figure 2.24 shows the starting (i.e., simple) process flowsheet where we will mix water–hexanol stream with 1-octanol to end-up with a ternary mixture ("**TRI-MIX**").

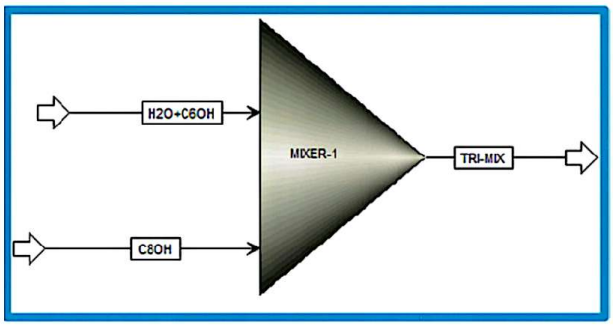


Figure 2.24 A simple process flowsheet for mixing water–hexanol mixture with 1-octanol.

Create an Aspen Plus flowsheet via selecting "**Specialty Chemicals and Pharmaceuticals | Specialty Chemicals with Metric Units**". The default property method assigned by Aspen Plus is "**NRTL**". We will use the mass as the flow-basis throughout the flowsheet, unless otherwise specified. Initially, add the following three components: water, 1-hexanol, and 1-octanol.

The total flow rate of "**H2O+C6OH**" stream is 100 kg/hr at 25°C and 2 atm. The flow rate of "**C8OH**" stream is also 100 kg/hr of pure octanol at 25°C and 2 atm. The mixer exists under the same conditions of pressure and temperature. Perform the following tasks:

1. Add the three components from the assigned component databanks.
2. Under "**Properties**" environment while in "**Analysis**" mode and using NIST/TDE experimental data, carry out the consistency tests on the binary VLE data of water–hexanol, water–octanol, and hexanol–octanol systems to see if it is possible to use the experimental VLE data instead of UNIFAC-estimated parameters for such binary interactions. Note: For all examined NIST data regarding the three binary systems, it was found that the maximum overall data quality was ≤0.364 and all failed relevant consistency tests.
3. If in Step #2, it is found that the experimental data fail the consistency tests and to avoid the little bit annoying warning appearing later in "**Control Panel**", select "**Estimate using UNIFAC**" option under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet. Click on "**Next**" button, select "**Run Property Analysis/Setup**" option from "**Properties Input Complete**" window, and click on "**OK**" button to estimate any missing property that is needed for further calculations.
4. Switching to "**Simulation**" environment and using the "**Model Palette**", add one mixer from "**Mixers/Splitters**" tab and three required material streams. Name the block and streams as shown in Figure 2.24.

5. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
6. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
7. Click on "**Next**" button and then on "**OK**" button found in "**Required Input Complete**" pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.
8. Watch out any simulation error or serious warning in "**Control Panel**" of Aspen Plus. If there is any warning or, error then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
9. Check for the results via inspecting "**TRI-MIX**" stream properties.
10. It is reported in literature that azeotropic conditions exist for some of those binary systems. Using the "**Azeotrope Search**" Azeotrope Search button found in "**Home**" ribbon, carry out an inspection for the possibility of azeotropic condition and if any report the azeotropic composition and temperature for such binary systems.

HOMEWORK/CLASSWORK 2.2 (WATER–ACETONE–EIPK SYSTEM WITH NIST/DTE DATA)

We have a 50/50 wt. % mixture of water and acetone. We plan to separate this mixture into its constituents and ultimately end up with almost pure streams of water and acetone. Figure 2.25 shows the starting (i.e., simple) process flowsheet where we will mix water–acetone stream with ethyl-isopropyl-ketone ("**EIPK**") stream to end-up with a ternary mixture ("**TRI-MIX**") product stream.

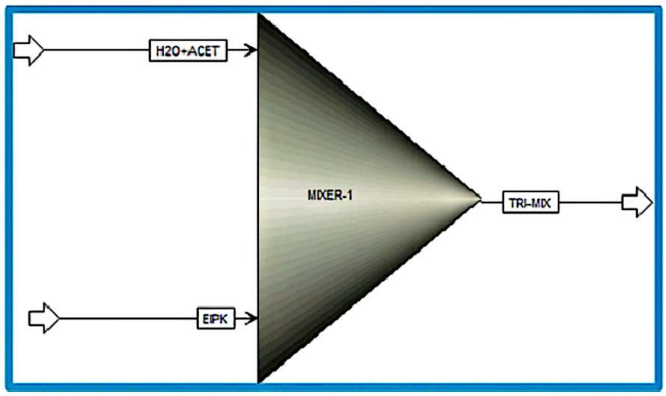
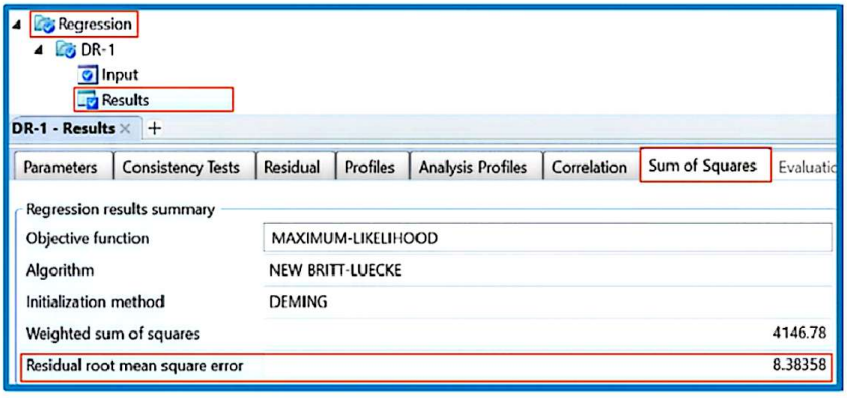


Figure 2.25 A simple process flowsheet for mixing water–acetone mixture with EIPK.

Create Aspen Plus flowsheet via selecting "**Specialty Chemicals and Pharmaceuticals | Specialty Chemicals with Metric Units**". The default property method assigned by Aspen Plus is "**NRTL**". We will use the mass as the flow-basis throughout the flowsheet, unless otherwise specified. Initially, add the following three components: water, acetone, and ethyl-isopropyl-ketone (EIPK).

The total flow rate of "**H2O+ACET**" stream is 100 kg/hr at 25°C and 1 atm. The flow rate of "**EIPK**" stream is also 100 kg/hr of pure EIPK at 25°C and 1 atm. The mixer exists under the same conditions of pressure and temperature. Perform the following tasks:

1. Add the three components from the assigned component databanks.
2. Under "**Properties**" environment while in "**Analysis**" mode and using NIST/TDE experimental data, carry out the consistency tests on the binary VLE data of water–acetone, water–EIPK, and acetone–EIPK systems to see if it is possible to use the experimental VLE data instead of UNIFAC-estimated parameters for such binary interactions.
3. For water–acetone system, you will find that the reliable VLE data sets are as shown earlier in Figure 2.18.
4. Save the data set in Step #3, following the steps shown earlier in Figure 2.19.
5. Using "**NRTL**" method, carry out the regression step under "**Properties**" environment while in "**Regression**" mode. Use the first entry in Table 2.2 and define parameters, under "**Parameters**" tab, as in Figure 1.38. You should be able to obtain the regressed NRTL parameters with RMMSE less than 10 for such VLE data sets as shown in Figure 2.26.



earlier in Figure 2.18.

4. Save the data set in Step #3, following the steps shown earlier in Figure 2.19.
5. Using "**NRTL**" method, carry out the regression step under "**Properties**" environment while in "**Regression**" mode. Use the first entry in Table 2.2 and define parameters, under "**Parameters**" tab, as in Figure 1.38. You should be able to obtain the regressed NRTL parameters with RMMSE less than 10 for such VLE data sets as shown in Figure 2.26.

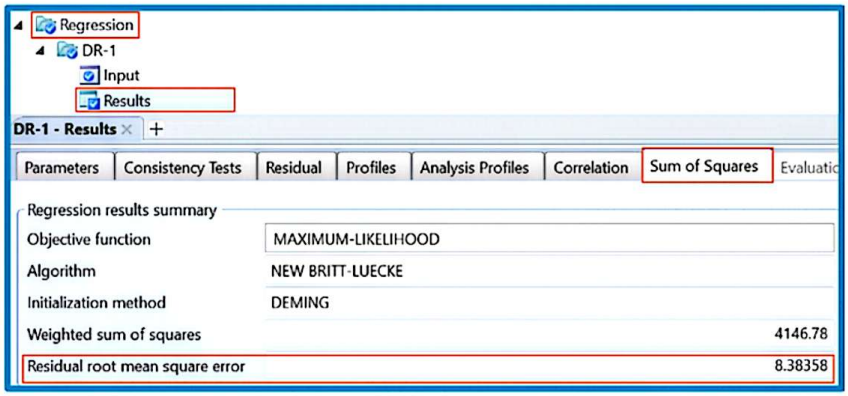


Figure 2.26 Regressing water–acetone VLE data using a 2-parameter "**NRTL**" model.

6. After successfully completing the regression step, click on "**Yes to all**" button appearing in the pop-up window to replace the existing binary interaction parameters with the newly regressed ones, for water–acetone system as shown in Figure 2.27.

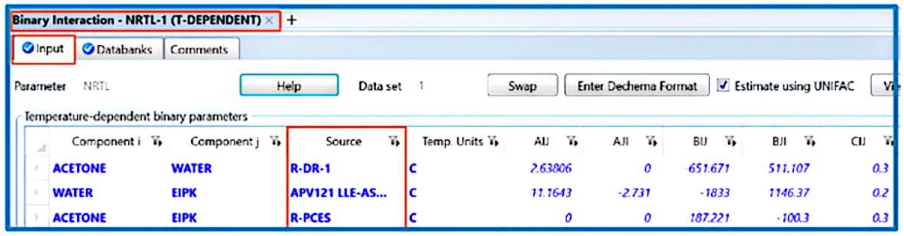


Figure 2.27 The binary interaction parameters for acetone–water system based on the regression step (R-DR-1).

7. To avoid the little bit annoying warning appearing later in "**Control Panel**", select "**Estimate using UNIFAC**" option under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet. Click on "**Next**" button, select "**Run Property Analysis/Setup**" option from "**Properties Input Complete**" window, and click on "**OK**" button to estimate any missing property that is needed for further calculations.
8. Switching to "**Simulation**" environment and using the "**Model Palette**", add one mixer from "**Mixers/Splitters**" tab and three required material streams. Name the block and streams as shown in Figure 2.25.
9. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
10. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
11. Click on "**Next**" button and then on "**OK**" button found in "**Required Input Complete**" pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.
12. Watch out any simulation error or serious warning in "**Control Panel**" of Aspen Plus. If there is any serious warning or error, then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
13. Check for the results via inspecting "**TRI-MIX**" stream properties.
14. Using the "**Azeotrope Search**" Azeotrope Search button found in "**Home**" ribbon, carry out inspection for the possibility of an azeotropic condition and if any report the azeotropic composition and temperature for such binary systems.

HOMEWORK/CLASSWORK 2.3 (WATER–ACETONE–EIPK SYSTEM WITHOUT NIST/DTE DATA)

Consider the same problem of Homework/Classwork 2.2 and trace all steps except for those pertaining to using NIST/DTE experimental data.

1. Add the three components from the assigned component databanks.
2. To avoid the little bit annoying warning appearing later in "**Control Panel**", select "**Estimate using UNIFAC**" option under "**Methods**" | "**Parameters**" | "**Binary Interaction**" | "**NRTL-1**" sheet. Click on "**Next**" button, select "**Run Property Analysis/Setup**" option from "**Properties Input Complete**" window, and click on "**OK**" button to estimate any missing property that is needed for further calculations.
3. Switching to "**Simulation**" environment and using the "**Model Palette**", add one mixer from "**Mixers/Splitters**" tab and three required material streams. Name the block and streams as shown in Figure 2.25.
4. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams.
5. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
6. Click on "**Next**" button and then "**OK**" button found in "**Required Input Complete**" pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.

7. Watch out any simulation error or serious warning in "**Control Panel**" of Aspen Plus. If there is any serious warning or error, then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
8. Check for the results via inspecting "**TRI-MIX**" stream properties. See if the results here are different from that in Homework/Classwork 2.2.
9. Using the "**Azeotrope Search**" Azeotrope Search button found in "**Home**" ribbon, carry out inspection for the possibility of an azeotropic condition and if any report the azeotropic composition and temperature for such binary systems. See if the azeotropic condition reported here is different from that in Homework/Classwork 2.2.

HOMEWORK/CLASSWORK 2.4 (WATER–SUCROSE SYSTEM)

We plan to mix sugar with water to evaluate the final mix product properties. Figure 2.28 shows the starting (i.e., simple) process flowsheet where we will mix water with sugar stream to end up with the product stream. Add the two components water and sucrose, the selected component databanks.

1. Change the default property method from "**NRTL**" to "**SOLIDS**". Click on "**Next**" button, select "**Run Property Analysis/Setup**" option from "**Properties Input Complete**" window, and click on "**OK**" button to estimate any missing property that is needed for further calculations.
2. Switching to "**Simulation**" environment and using the "**Model Palette**", add one mixer from "**Mixers/Splitters**" tab and three material streams. Name the block and streams as shown in Figure 2.28.

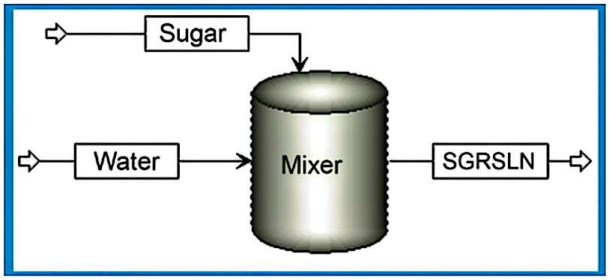


Figure 2.28 A simple process flowsheet for mixing water–sugar mixture.

HOMEWORK/CLASSWORK 2.4 (WATER–SUCROSE SYSTEM)

We plan to mix sugar with water to evaluate the final mix product properties. Figure 2.28 shows the starting (i.e., simple) process flowsheet where we will mix water with sugar stream to end up with the product stream. Add the two components water and sucrose, the selected component databanks.

1. Change the default property method from "**NRTL**" to "**SOLIDS**". Click on "**Next**" button, select "**Run Property Analysis/Setup**" option from "**Properties Input Complete**" window, and click on "**OK**" button to estimate any missing property that is needed for further calculations.
2. Switching to "**Simulation**" environment and using the "**Model Palette**", add one mixer from "**Mixers/Splitters**" tab and three material streams. Name the block and streams as shown in Figure 2.28.

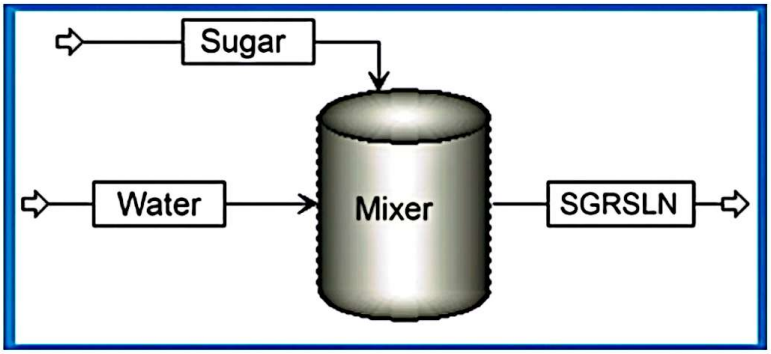


Figure 2.28 A simple process flowsheet for mixing water–sugar mixture.

3. Add the feed stream conditions in terms of pressure, temperature, and compositional flow rate for both feed streams. For sugar stream, enter $T = 25°C$, $P = 1$ atm, and flow rate of 100 kg/hr sucrose. On the other hand, for water enter 1 m^3/hr of pure water at 25°C and 1 atm.
4. For the first mixer, you do not have to enter any input data; Aspen Plus will do the job for you.
5. Click on "**Next**" button and then "**OK**" button found in "**Required Input Complete**" pop-up window, where the latter confirmation lets Aspen Plus run the simulation immediately.

6. Watch out any simulation error or serious warning in "**Control Panel**" of Aspen Plus. If there is any serious warning or error, then you need to fix the problem. Aspen Plus will not give you error-free results unless you do everything correctly.
7. Check for the results via inspecting "**SGRSLN**" stream properties. Report the following solution properties: Mass density (kg/m^3), total mass flow rate (kg/hr), total volumetric flow rate (m^3/hr), mass fraction of sugar, the average molecular weight (kg/kmol), total molar flow rate (kmol/hr), and the mole fraction of sucrose.