

Updated May 4, 2021

OLI Chemistry Wizard is a Windows wizard-style application that leads you through the process of creating an OLI chemistry model file and associated model database file for use with any other OLI product or custom solution that incorporates OLI Engine. Chemistry Wizard includes both the Aqueous, mixed solvent electrolyte (MSE), and MSE-SRK databanks.

This manual is intended to give you a quick introduction to the Chemistry Wizard and lead you through the process of creating your first set of chemistry model files.

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1 Disclaimer

The OLI Chemistry Wizard document was created with version 11.0.1.5 of the software and images and values are subject to change as the software progresses. This document was created on May 4, 2021.

The product names of Aspen, Aspen Plus are registered trademarks of Aspen Technology.
The product names of ProII are registered trademarks of AVEVA.

2 A Quick Start

To launch Chemistry Wizard, double-click on the OLI Chemistry Wizard 11.0 icon on your desktop or, use your mouse to navigate to the Chemistry Wizard 11.0 menu entry in the Windows program menu:

Start -> OLI Systems -> Chemistry Wizard 11.0

Use a single left mouse button click on the Chemistry Wizard 11.0 menu entry to start the application.

For the programs Aspen Plus and ProII, you can find the path to the Chemistry Wizard in the following paths:

2.1.1 Aspen Plus

Start > OLI Systems > OLI Engine 11.0 for Aspen Plus

2.1.2 ProII

Start > OLI Systems > OLI Engine 11.0 for ProII

2.2 Welcome



Figure 1 Splash screen

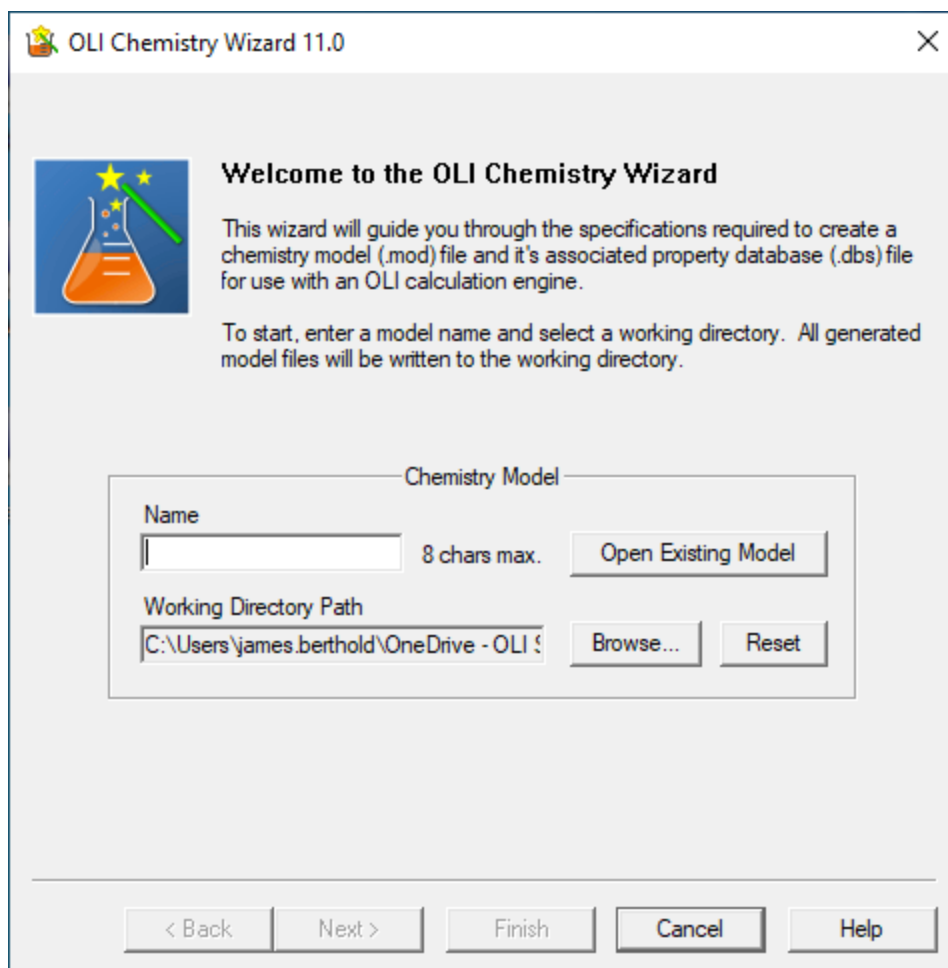


Figure 2 Welcome screen

The welcome dialog prompts to you specify a base name and a folder to use for all generated files.

The working directory defaults to your temporary directory. Use the **Browse** button to change the working directory. Your new working directory will be saved as a preference and will be used whenever you start Chemistry Wizard. If you do change the working directory and would like to revert to the default, simply click the Reset button.

Notice the **Open Existing Model** button. Whenever you use Chemistry Wizard to create a chemistry model, a special file with a '.cws' extension is created¹. This file enables you to return to a case that you created with the Chemistry Wizard, view current settings, make revisions, and regenerate chemistry model files.

After you supply a model name (no extension) the Next button will become active. Click **Next** to proceed.

¹ Users of Aspen Plus and the OLI Chemistry Wizard will have a file extension of "cwa"

2.3 Databank Selection

Chemistry Wizard includes several optional databanks. The “Public” databank is always selected and cannot be removed from the **Selected** databanks list.

You can add an optional databank by selecting (with a single left click) an entry in the **Available** list. As soon as an entry in the **Available** list is selected, the right arrow button will become active. When you click the right arrow button, the databank will be moved to the **Selected** list.

You can remove an optional databank by highlighting it in the **Selected** list and clicking the (now active) left arrow button.

When 2 or more optional databanks are added to the **Selected** list, they can be re-sorted using the up and down arrows. The databanks are searched top-down. So, the first entry in the **Selected** databanks will be searched first, the second entry is next, etc. The “Public” databank is always searched last².

For now, do not add any optional databanks and select **Next**.

² For the MSE thermodynamic framework, the “Public” databank is MSEPUB.

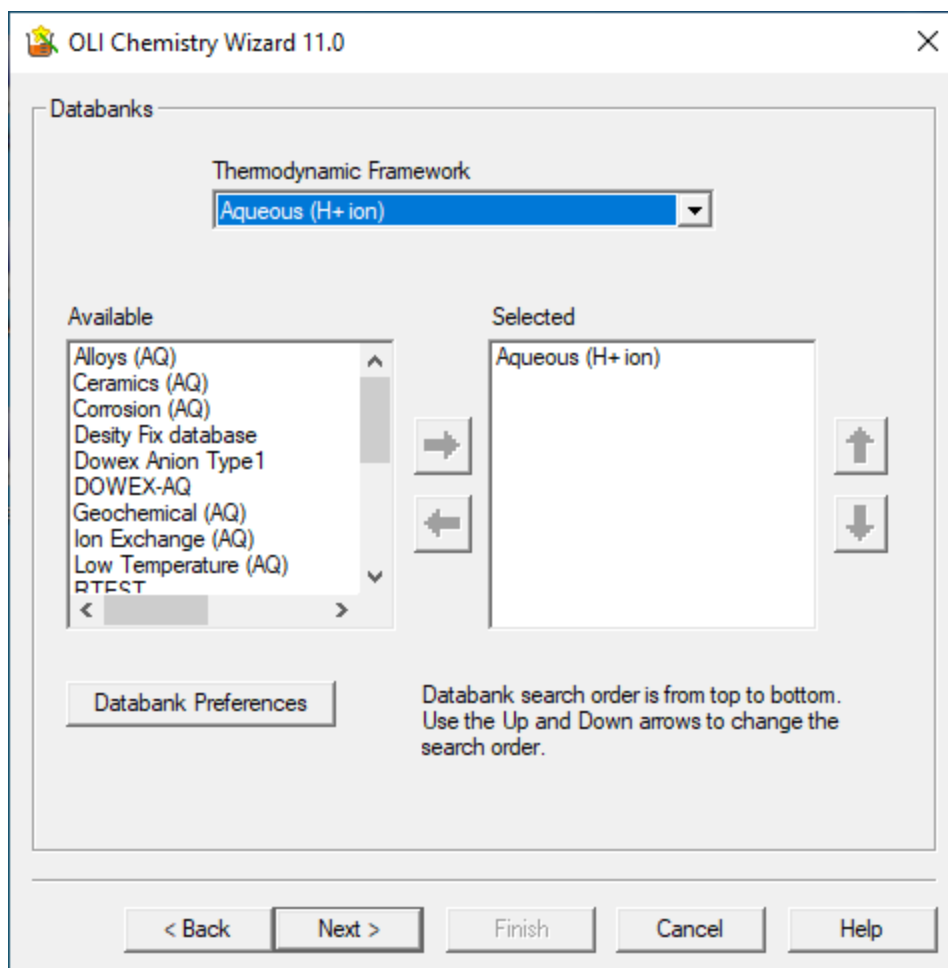


Figure 3 Selected Databanks

2.4 Component Selection

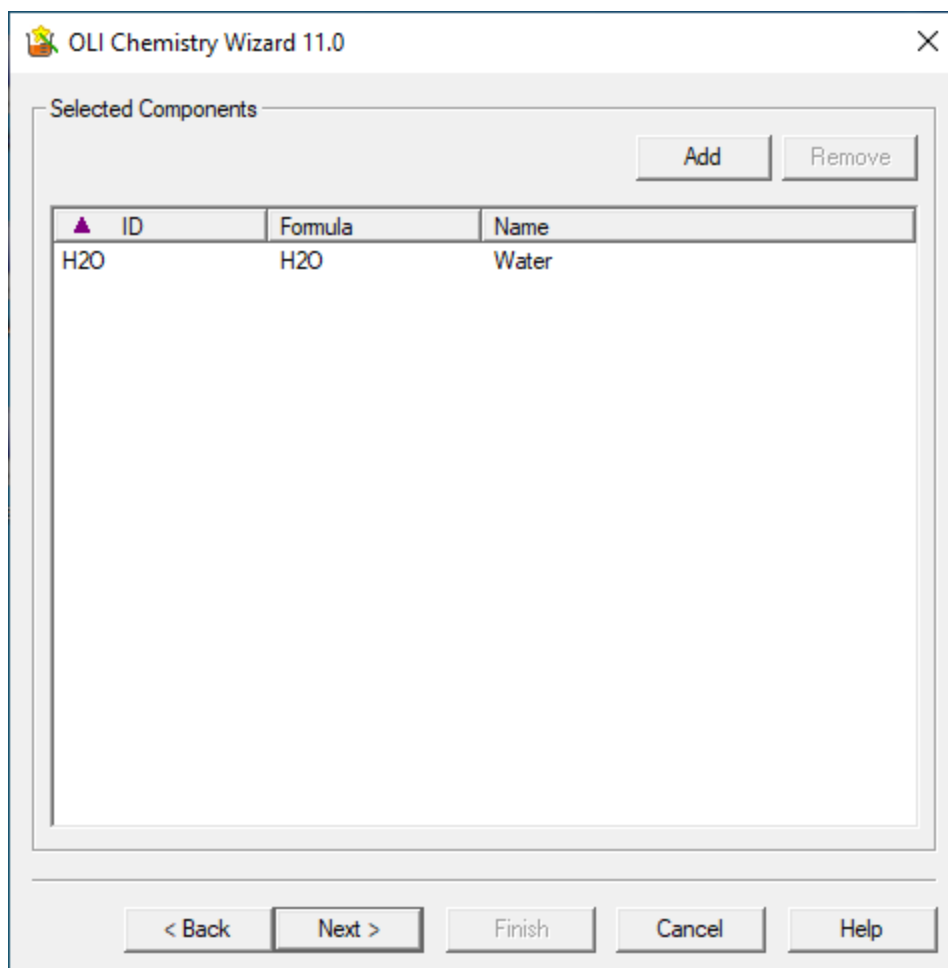


Figure 4 Component Addition

This page shows the **Selected Components** for this case. By default, water is always included. More components can be selected by clicking the **Add** button in the top-right corner:

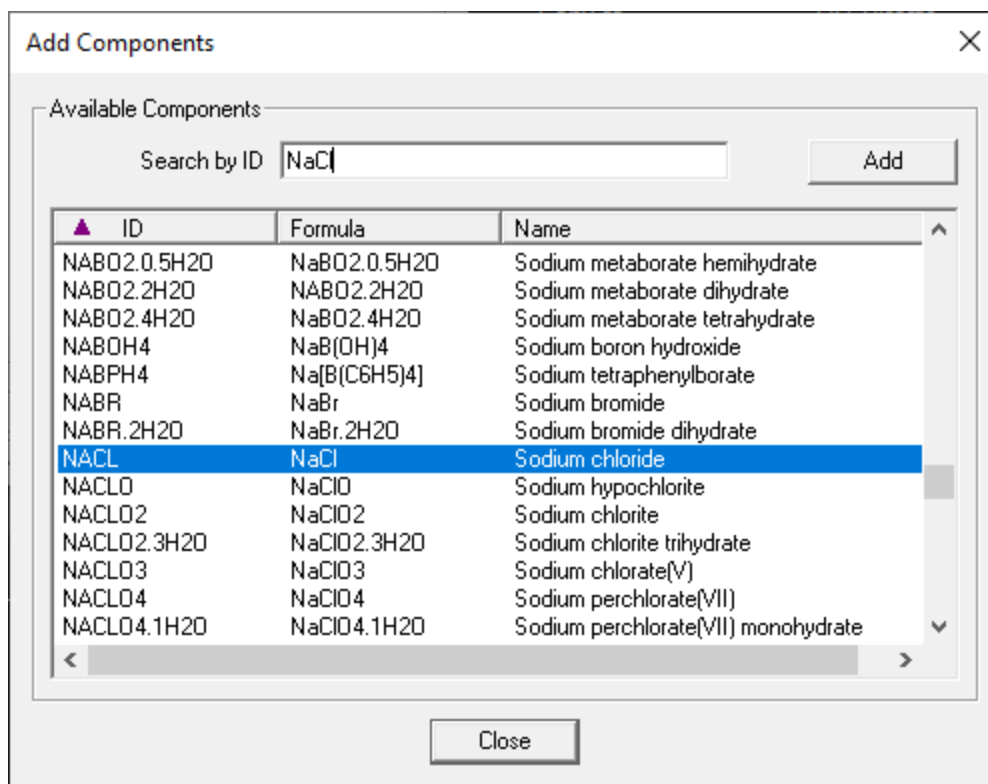


Figure 5 Searching components

The **Add Component** dialog lets you scroll or search for components in the OLI databanks by ID, Formula or Name. The column being searched has a plum colored arrow pointing up (ascending sort order) or down (descending sort order). To find and highlight NaCl, type “NaCl” in the **Search by ID** field. If you press ENTER or click the **Add** button, the highlighted component will be added to your list of selected components.

Do not close this dialog yet. Type “CO2” and press ENTER. Type “H2S” and press ENTER. Now, close the dialog by clicking the “Close” button.

Your “Selected Components” page should now look like this:

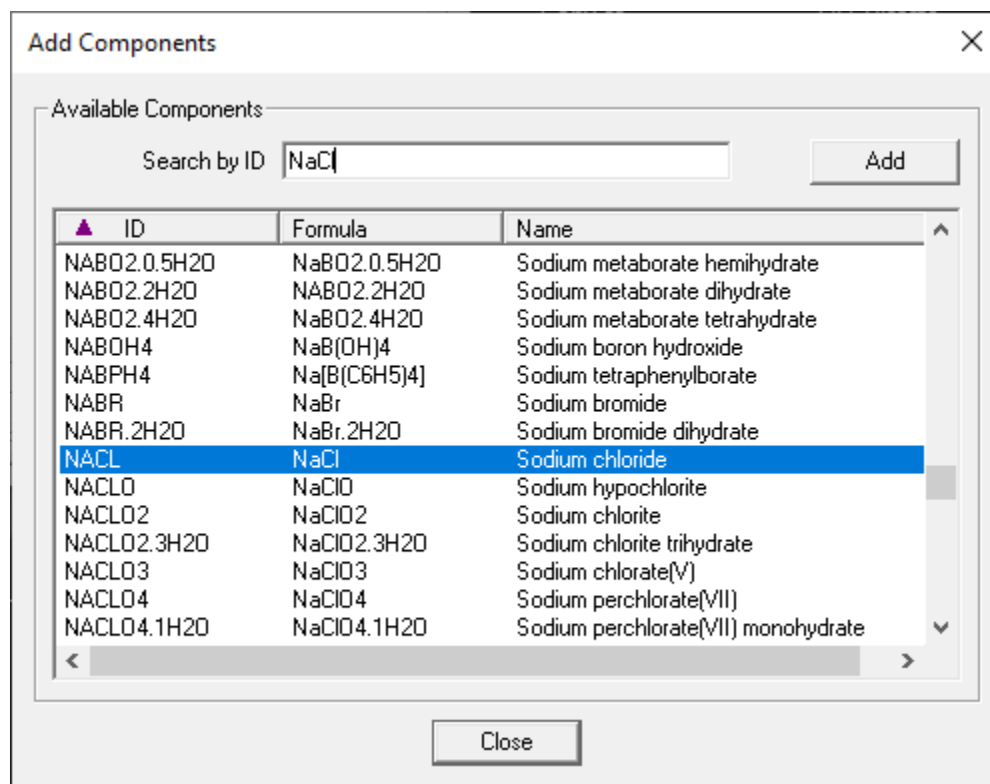


Figure 6 Selected Components

Notice that you can sort selected components by **ID**, **Formula** or **Name**.

Click **Next** to proceed.

2.5 Redox, Assay and Pseudo component Selection

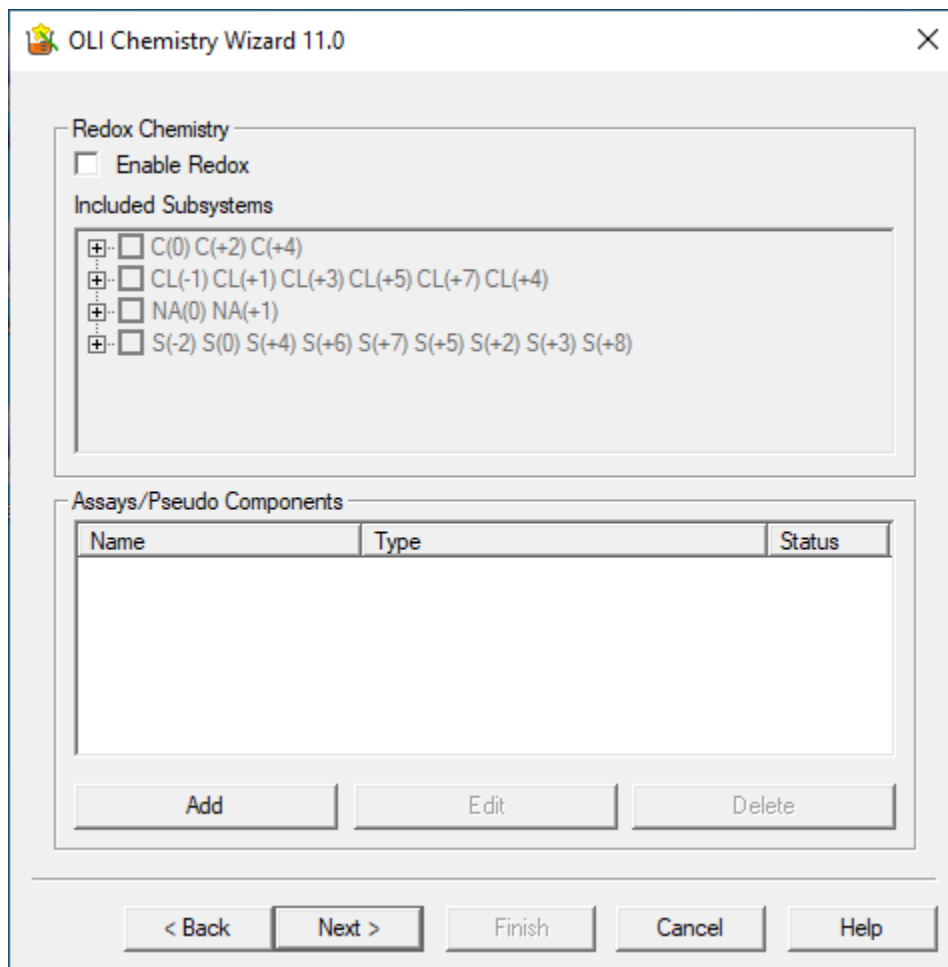


Figure 7 Redox Selection (off by default)

This dialog allows inclusion of reduction/oxidation chemistry as well as assays and pseudocomponents in the chemistry model. For this tutorial, we will ignore redox, assays and pseudocomponents. If you would like to consider these components in your models, please refer to Sections 3.2 and 3.3 for a detailed description.

For now, click **Next** to proceed.

2.6 Phase Selection

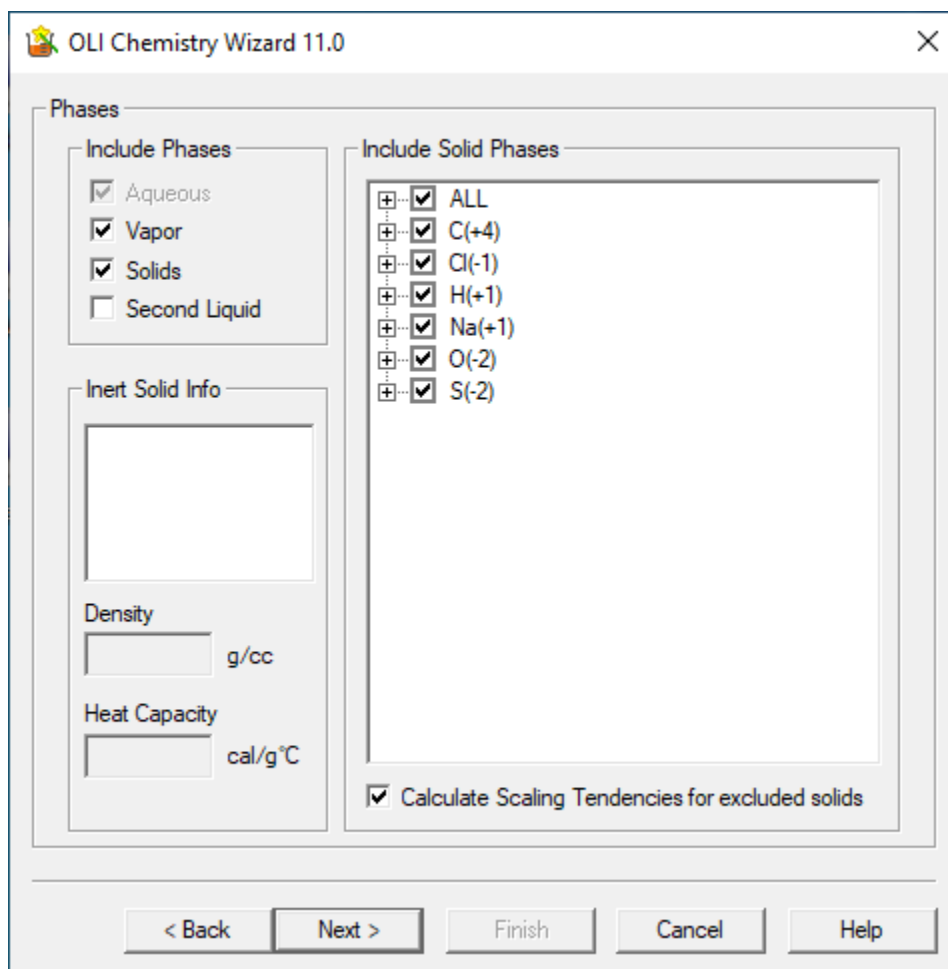


Figure 8 Phases

This page shows the **Phases** that will be included in all equilibrium calculations. By default, the aqueous, vapor and all solid phases are considered. If your problem includes organic species, then you may wish to enable the **Second Liquid** phase.

You can exclude individual solid phases. This helps to limit the size of your chemistry model and improves equilibrium calculation performance. We suggest that you include all solids until you are sure that you can safely ignore one or more solids in the temperature, pressure, and concentration region of interest.

The **Insert Solid Info** section allows you to specify the density and heat capacity of non-reactive components which are included in the model. Non-reactive components include ash, carbon, coal, and coke.

Click **Next** to proceed.

2.7 Summary

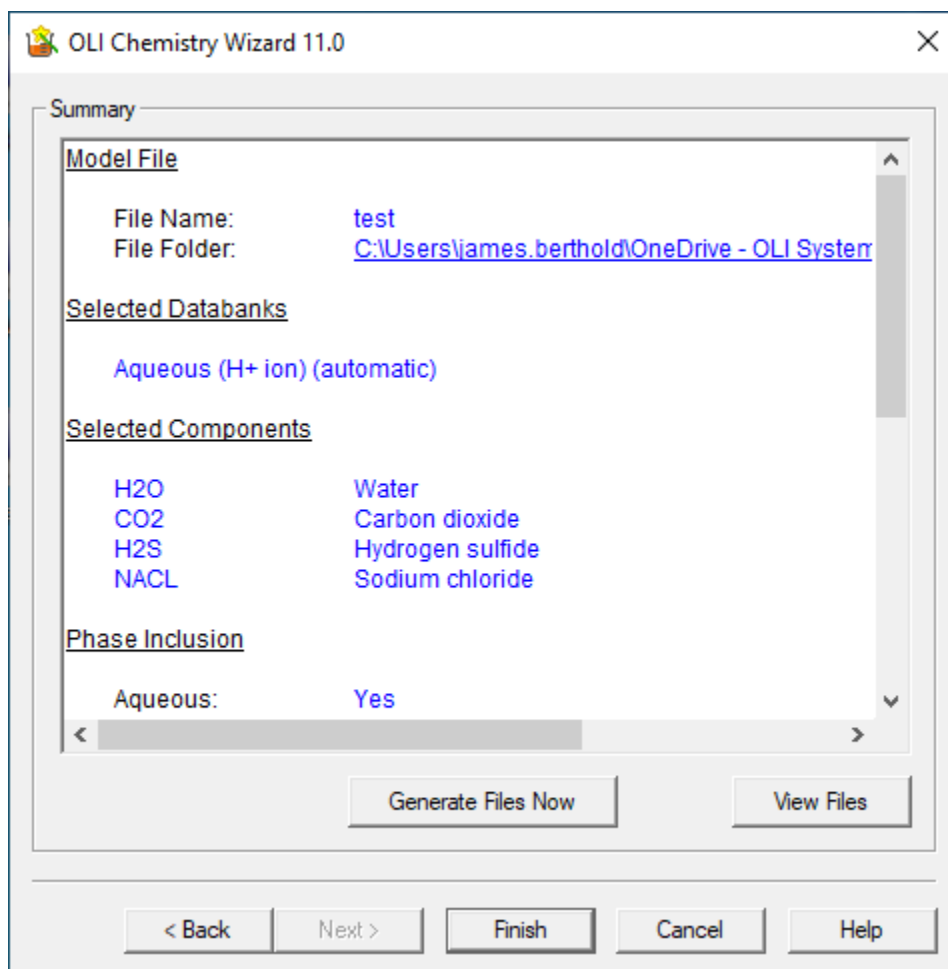


Figure 9 Generating files

Finally, you will end up at the **Summary** page that shows you all the selections that you have made.

If you click the **Generate Files Now**, then all chemistry model files will be generated without leaving the application. It is possible to go back to previous pages, make changes and then regenerate model files.

If you click the **Finish** button, then the files will be generated, and the application will exit.

Click **Finish** to proceed.

2.8 Generating Model Files

If your model files are generated successfully, then the following dialog will appear:

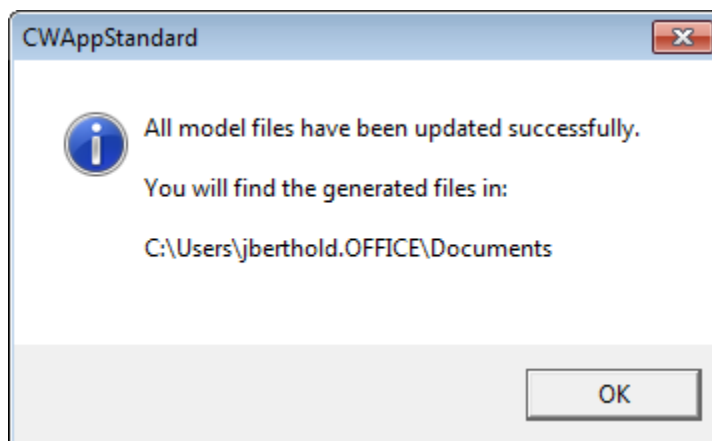







Figure 10 Generated file location

This dialog tells you where the files were written. Click **OK** to close the application.

You should have these files in your Working Directory:

 DocDemo.cws	8/17/2017 12:44 PM	CWS File	3 KB
 DocDemo.dbs	8/17/2017 12:44 PM	DBS File	129 KB
 DocDemo.mdl	8/17/2017 12:44 PM	MDL File	1 KB
 DocDemo.mod	8/17/2017 12:44 PM	MOD File	4 KB
 DocDemo_1.CSV	8/17/2017 12:44 PM	Microsoft Ex...	3 KB

All these files are ASCII files that can be inspected using an editor like Notepad.

In Windows Explorer, if you double-click on the “DocDemo.cws” file then you will start the Chemistry Wizard with the case already loaded.

3 Details

3.1 Location of Databanks

The Chemistry Wizard program has a preference that allows you to control where it searches for OLI databanks. By default, this preference is the directory where the “OLI Chemistry Wizard 11.0 installation program copied the OLI databanks.

If you would like to use databanks installed by another OLI product, then you can change the databank directory using a dialog accessed from the Databank selection page:

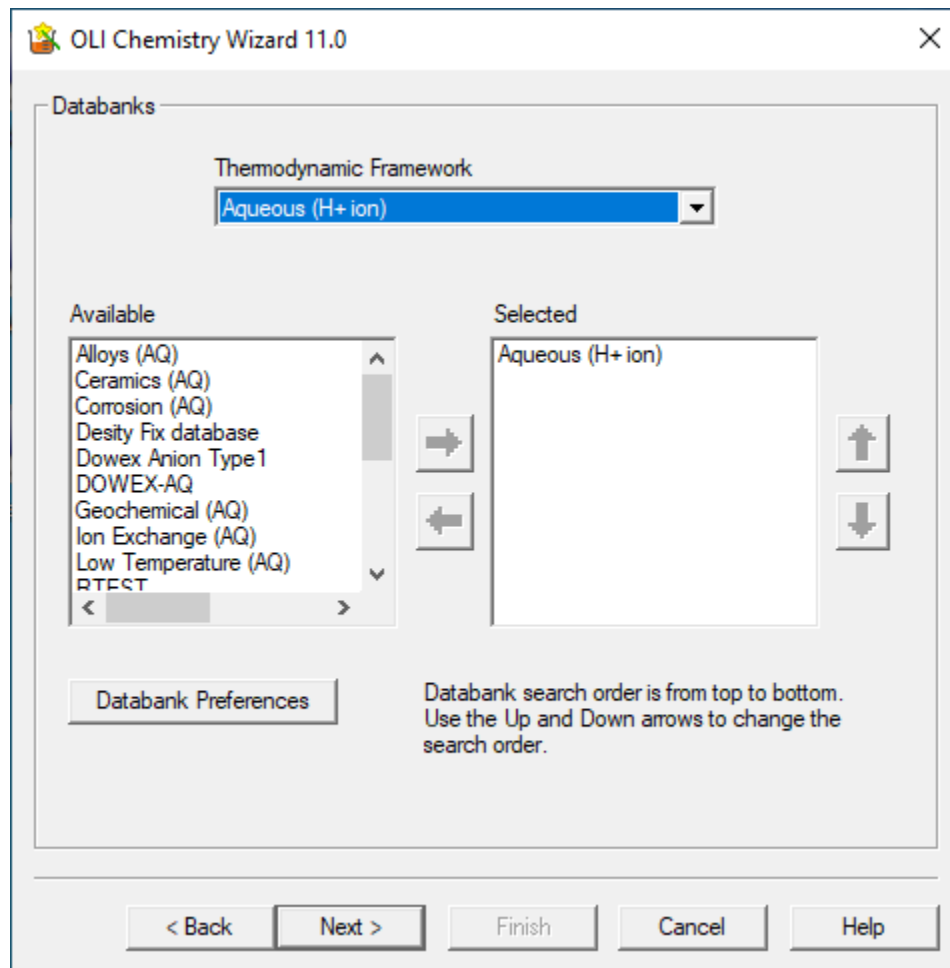


Figure 11 Databank Preferences

Notice the “Databank Preferences” button. Click on it to access the “Databank Preferences” dialog:

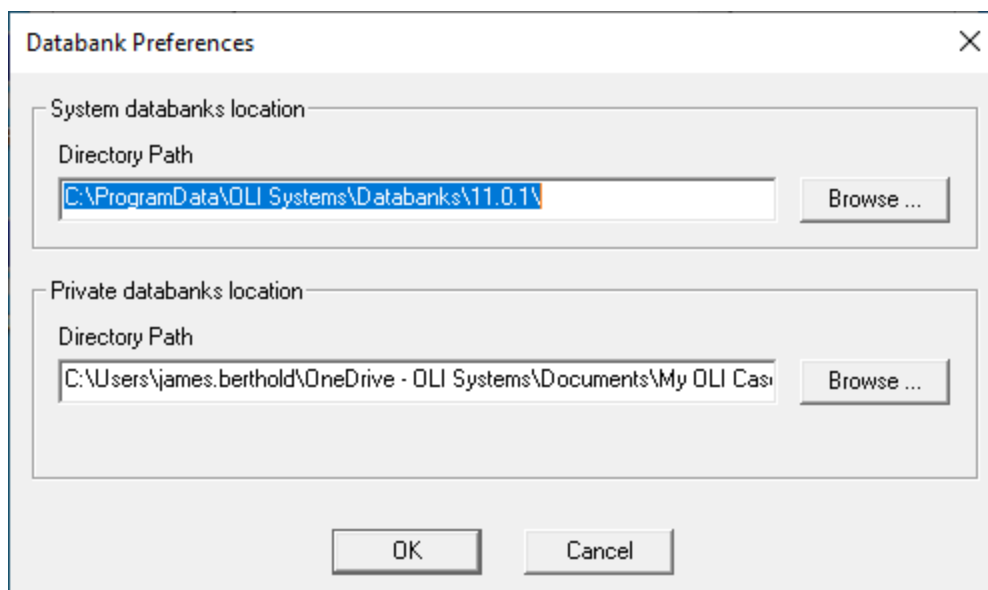


Figure 12 Selecting Path

Update the “Directory Path” to point to the directory where your other OLI system databanks are located.

3.2 Redox Selection

If you would like to consider reduction/oxidation chemistry in your simulation model, then you will need to enable the **Enable Redox Chemistry** checkbox:

The **Included Subsystems** list will update with all the Redox subsystems that are associated with the species that you have selected so far. Click on those subsystems that you would like to consider:

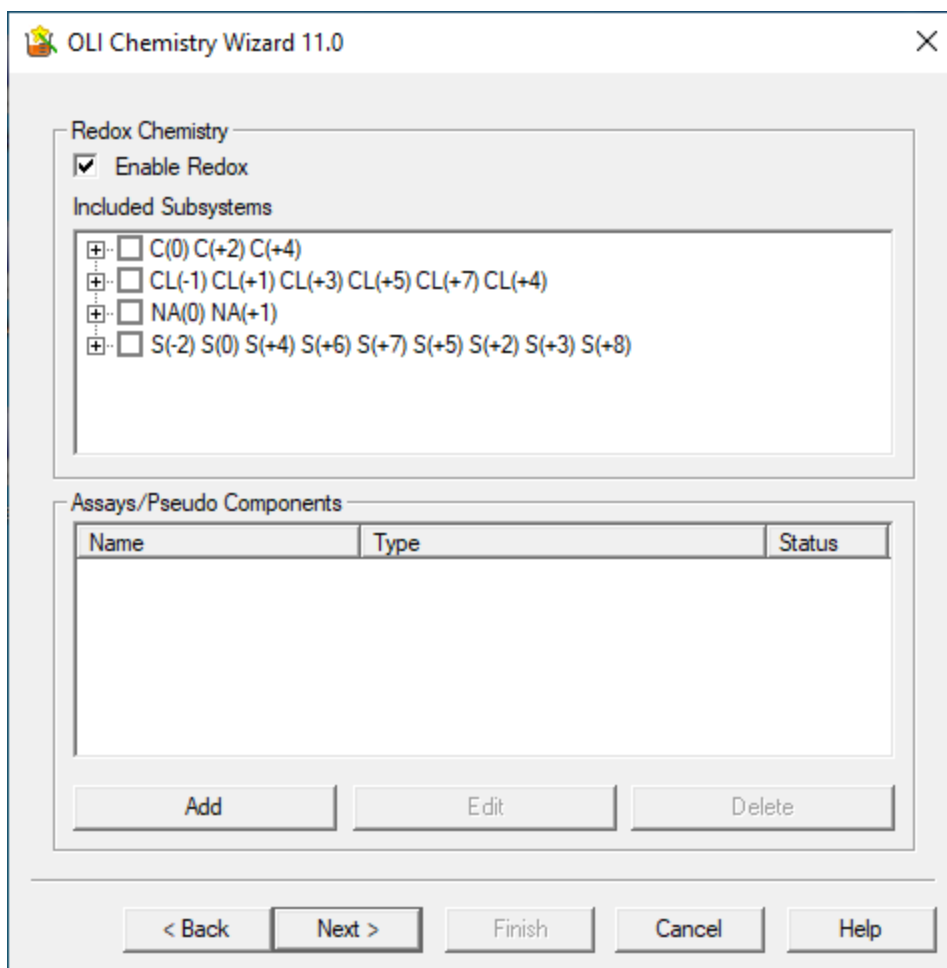


Figure 13 Enabling REDOX

In this example, we will consider all oxidation states for sulfur.

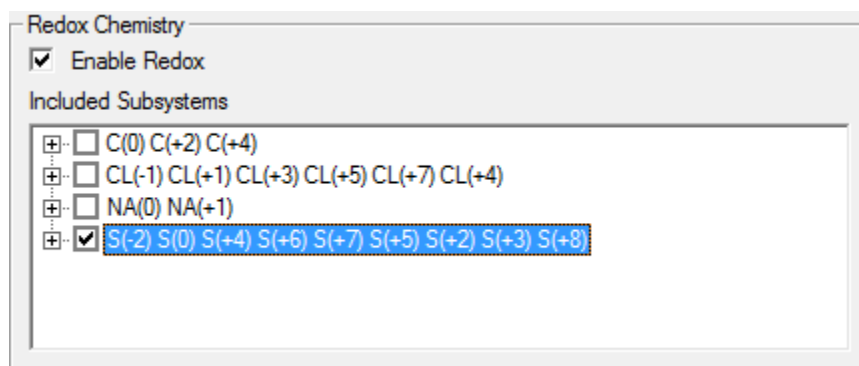


Figure 14 Enabling just Sulfur REDOX

This will dramatically increase the number of components involved in your simulation and will have an impact on calculation times.

If you are going to include redox chemistry, then make sure that you only pick those subsystems that are of most interest. The more redox subsystems you select, the more components you will have, and your calculations will take more time.

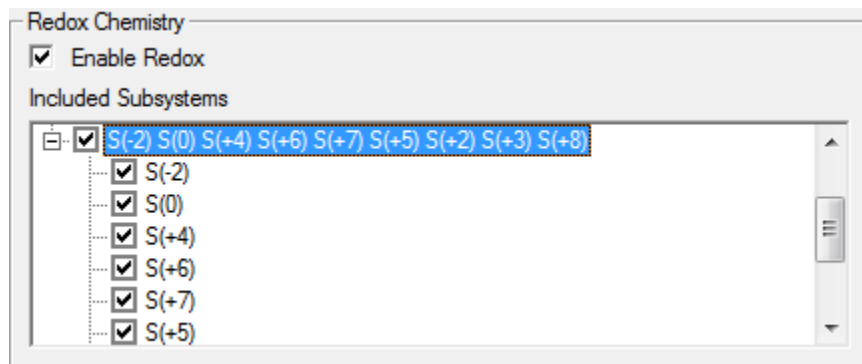


Figure 15 Expanded Sulfur Redox

3.3 Assays and Pseudocomponents

Chemistry Wizard V11 supports assays and pseudocomponents. These can be added by clicking on the **Add** button in the dialog. To add an assay, select **Assay** from the popup menu.

Selecting the **Assay** option will bring up the **Assay Entry** dialog.

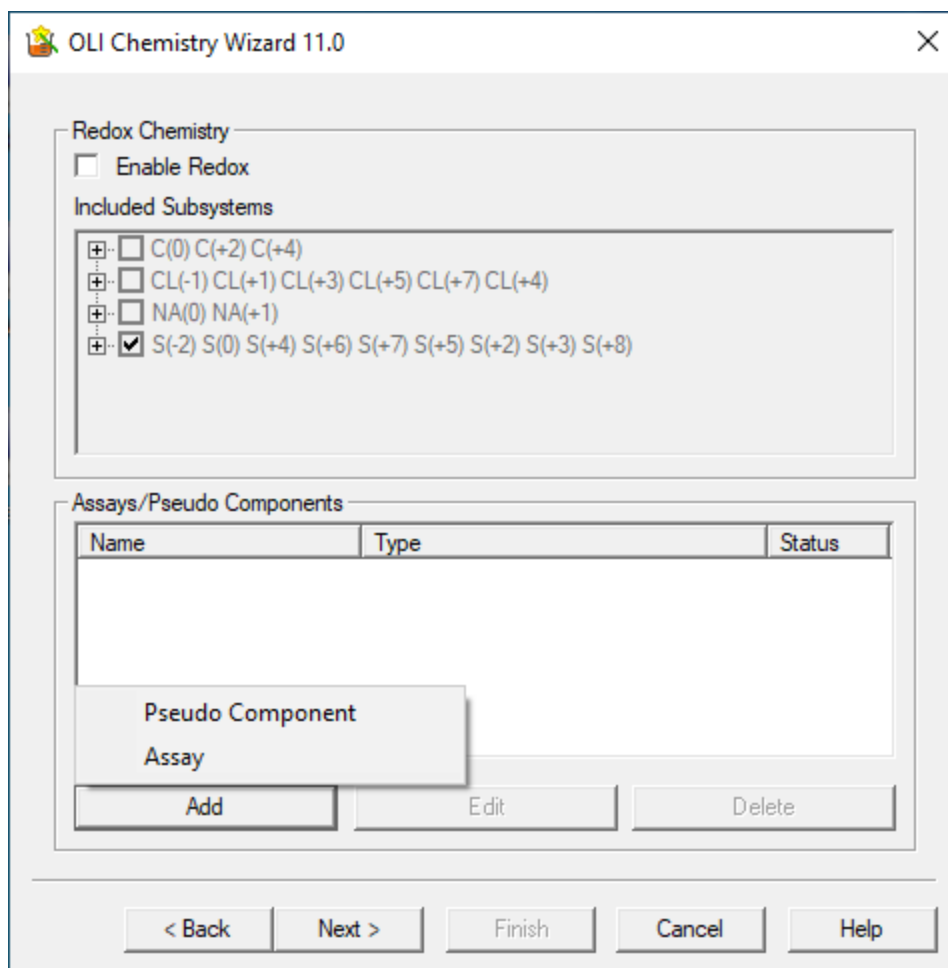
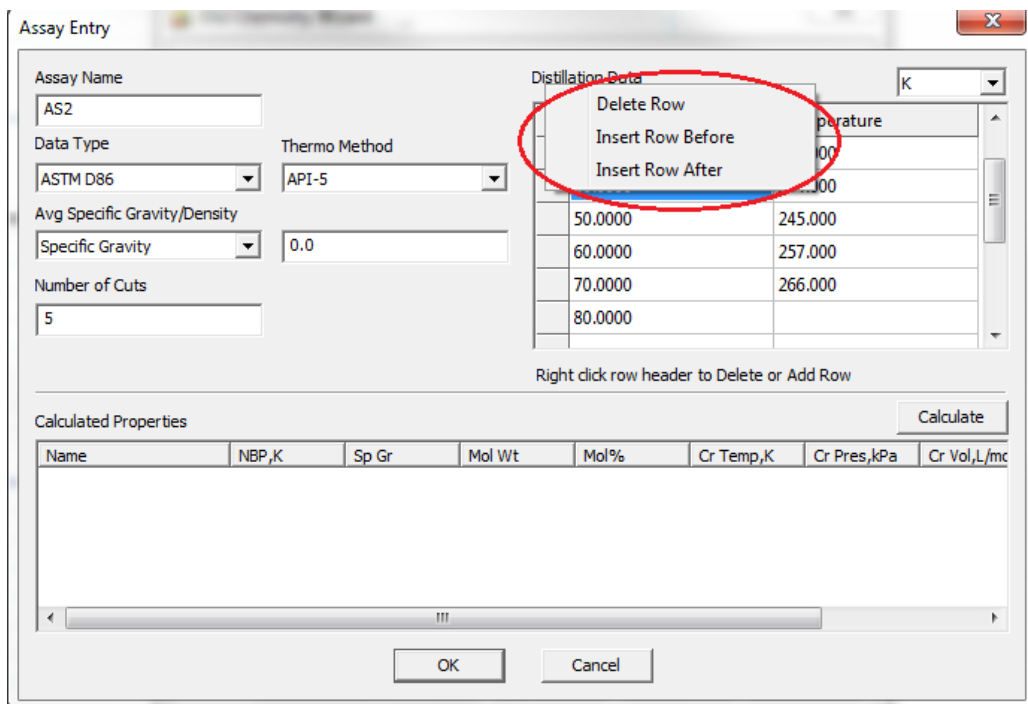
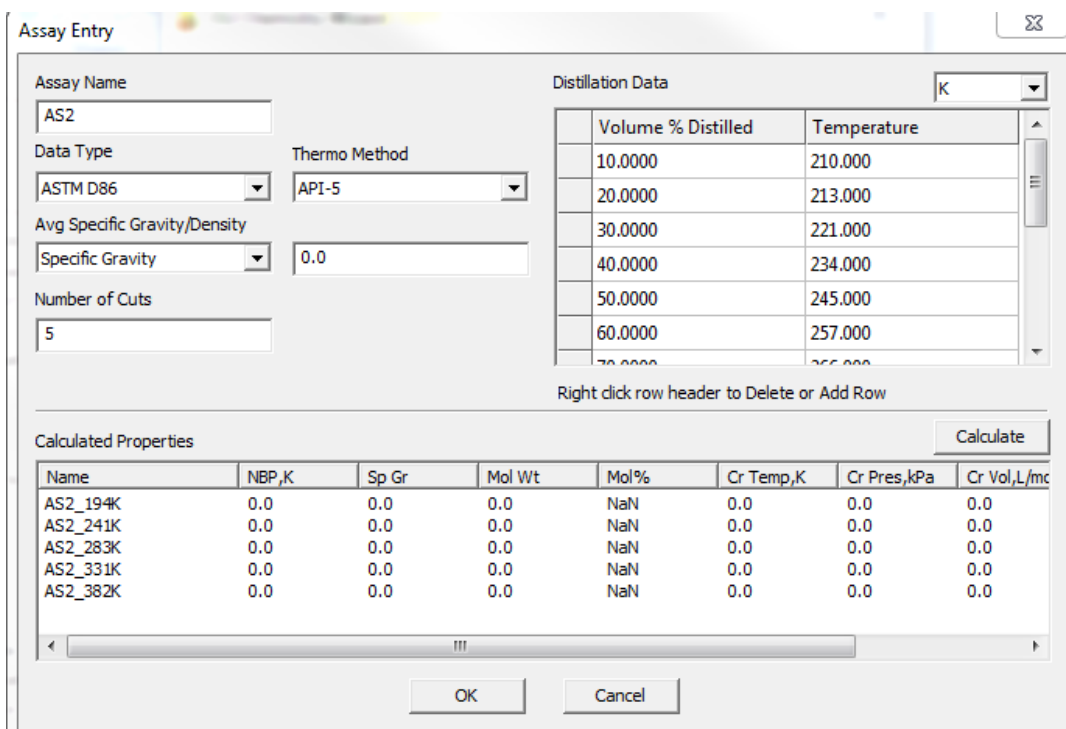


Figure 16 Adding Assays and Pseudo Components

This dialog allows you to define the assay by specifying the distillation data along with other physical parameters including average bulk density and the number of cuts. The **Distillation Data** grid allows you to enter ordered pairs of distillation volume and temperature values. Rows can be inserted or deleted by right-clicking on the row header in the grid.



Once all data has been entered, you can click on the **Calculate** button to view the list of components and their physical properties generated by Chemistry Wizard.



Click **OK** to save the assay definition and exit from the dialog.

Similarly, pseudocomponents can be added by selecting the **Pseudocomponent** option after clicking on the **Add** button. Chemistry Wizard displays a **Pseudocomponent Entry** dialog that can be used to enter

the parameters that define the Pseudo Component such as normal boiling point, specific gravity and molecular weight.

Pseudo Component Entry

Pseudo Component Name: PC1

Thermo Method: API-5

Enter Values for 2 of the 3 properties:

Normal Boiling Point: [] K

Specific Gravity/Density: Specific Gravity 0.920000

Molecular Weight: 32.0000

Calculated Properties

Property	Value
Mol Wt	32.0000
Sp Gravity	0.804980
Boiling Pt, K	232.893
Crit Temp, K	403.005
Crit Pres, kPa	11071.3
Crit Volume, L/mol	0.148095
App Factor	0.101264

OK Cancel

Click on the **Calculate** button to view the generated properties of the pseudo component. Click **OK** to save the Pseudo Component definition and exit from the dialog.

4 Aspen Plus Users

4.1 OLI systems for Aspen Plus

To load Chemistry Wizard for Aspen Plus, please go to programs and OLI Systems

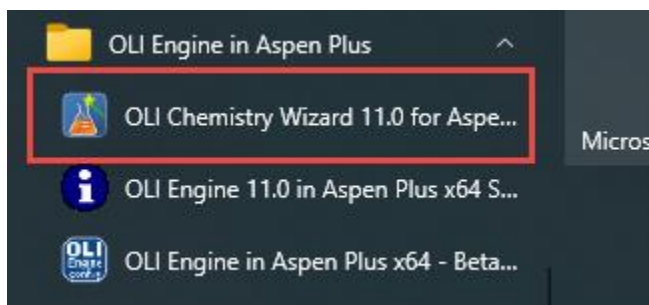


Figure 17 Locating the OLI Chemistry Wizard for Aspen Plus

You will see a similar welcome screen as in Figure 2. It will say OLI Chemistry Wizard for Aspen Plus instead.



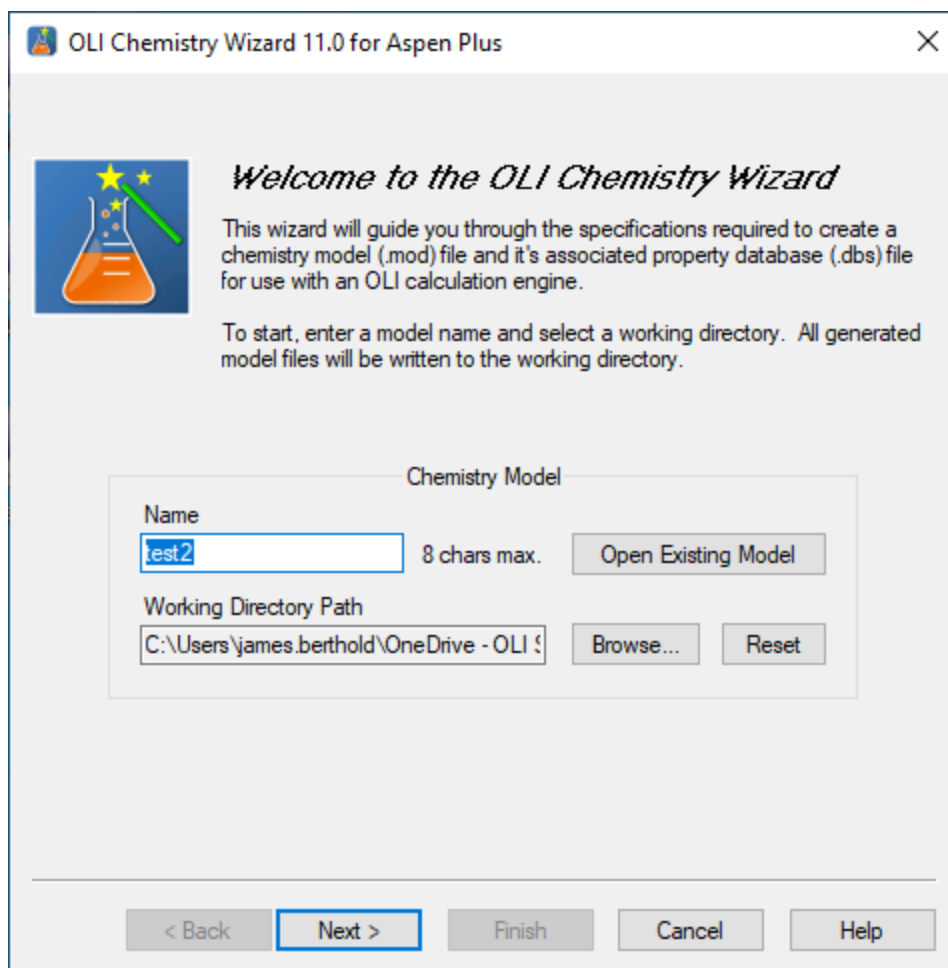


Figure 18 Chemistry Wizard for Aspen Plus (all versions)

The only screen you are going to see different is the Aspen Plus Component ID & Alias. This is before generating the .bkp file. *

* : Chemistry Wizard for Aspen Plus generates a bkp file which can be directly opened using Aspen Plus

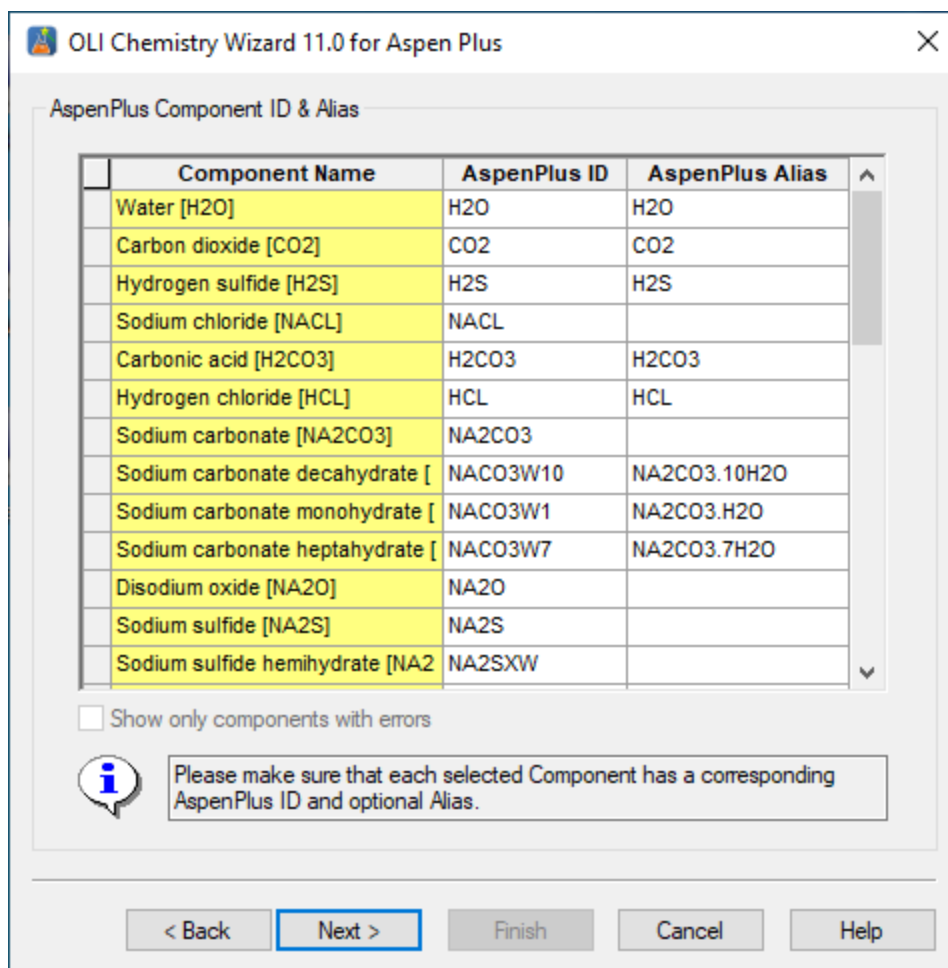


Figure 19 OLI Chemistry Wizard for Aspen Plus screen

Please make sure that you type in the Aspen Plus alias names in the third column as shown above. To import the right chemistry into Aspen Plus, this field is very important.

You might see the following screen when you click "Next".

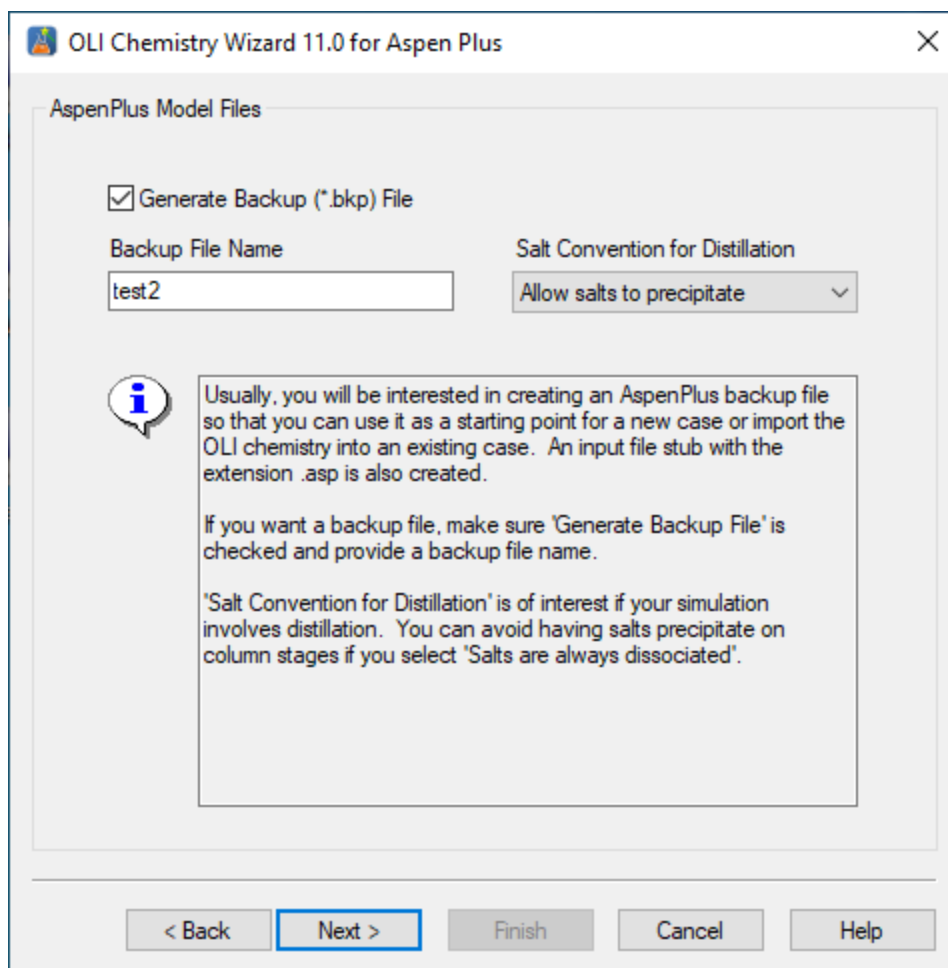


Figure 20 Generating a bkp file

"Next" will take you to the generating files screen. You can click on "Finish" as shown in figure 8, after generating the files.