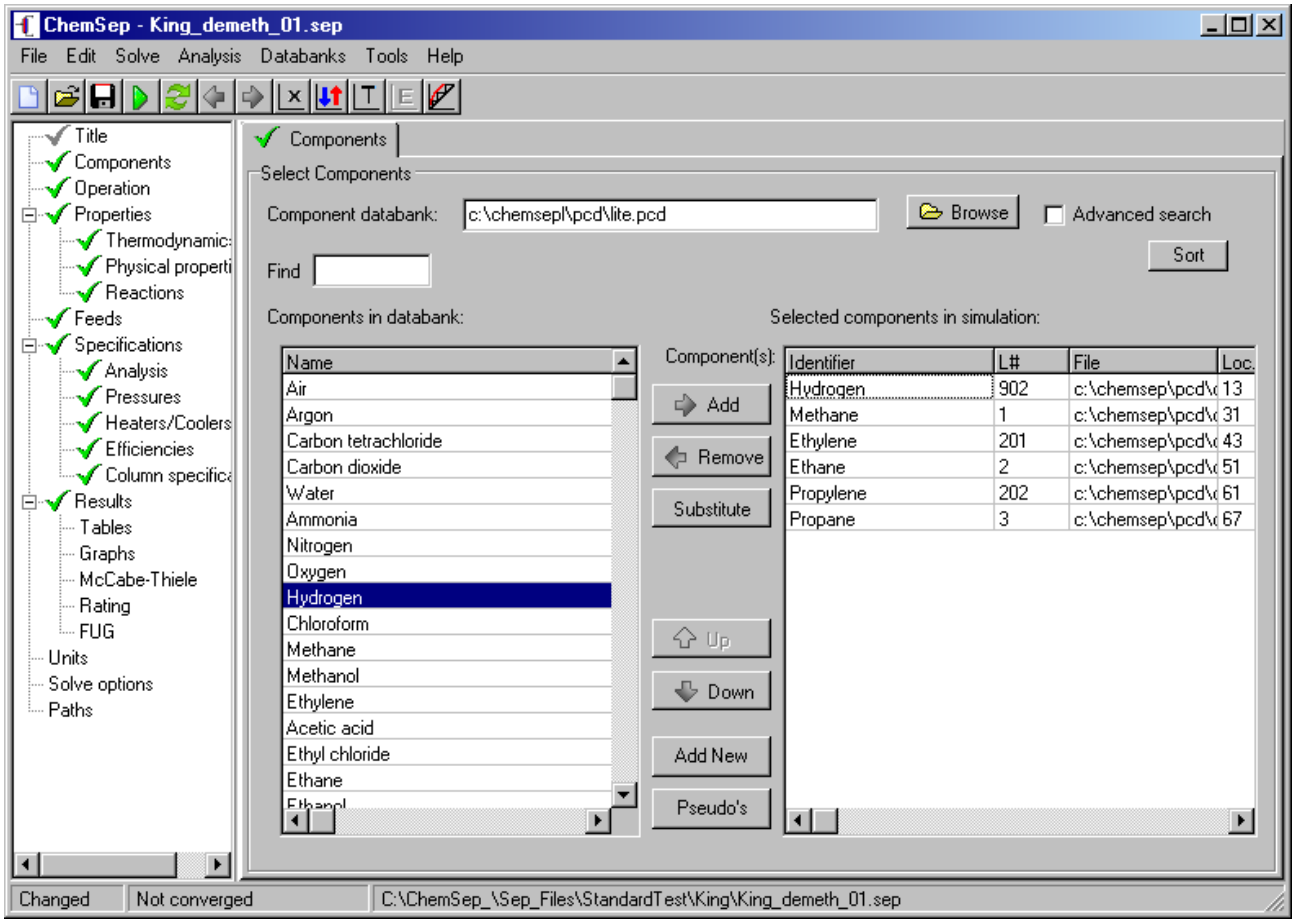
ChemSep Tutorial: Selecting Components

Ross Taylor and Harry Kooijman

This short tutorial is devoted to the one step common to every *ChemSep* simulation: The selection of components.

If we click on *Components* in the list on the left of the ChemSep window we will see a screen that might look something like this one:



This is the part of *ChemSep* where we add and subtract components to be used in the simulation. In what follows we describe how to use this panel.

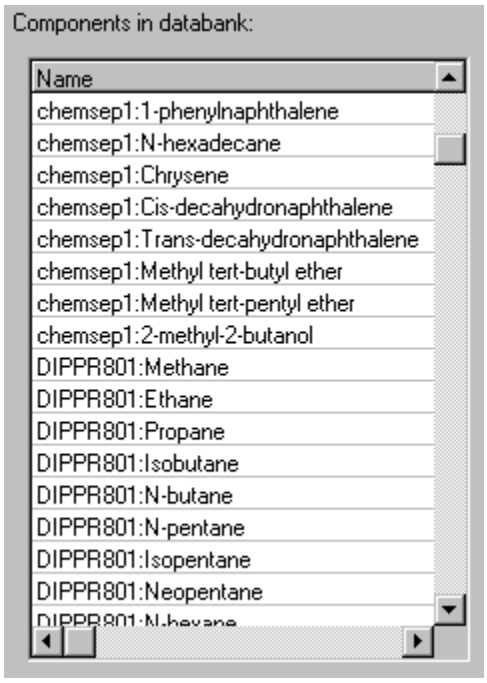
Near the top of the panel is the name of databank:

To search for alternative databanks from which to load compounds click on the **Browse** button that appears to the right. *ChemSep* databanks have the pcd (for Pure Component Date) file extension and the databank that comes with *ChemSep* is installed in the pcd subdirectory under the main *ChemSep* directory.

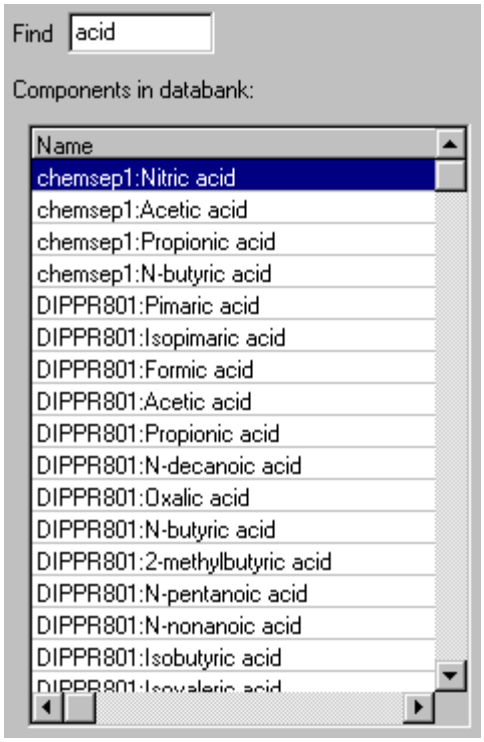
Once a databank has been selected a list of chemical names will appear in the white space on the left of the Components panel as can be seen in the full screen shot above.

For many readers the databank that comes with *ChemSep* will not contain all the compounds of interest, and you may have created your own additional databanks. In the event that there is more than one databank in the current pcd directory. In the event that there are multiple databanks in the same directory then typing *.pcd in the databank space:

will allow *ChemSep* to display the names of all of the chemicals in all of the databanks as shown below where compounds from the standard *ChemSep* databank (chemsep1.pcd) appear before those in another databank called DIPPR801.pcd (*ChemSep*'s version of the databank available from DIPPR). In this case we see that the name of the databank is included in the list so that the user will know from where the compound has been selected.



Selecting components by scrolling up and down this list can be rather a chore (the file chemsep1.pcd has nearly 200 compounds included, but DIPPR801.pcd has nearly 2000 compounds. If we type (any part of) the name of the compound(s) of interest *ChemSep* will list only those chemicals whose name includes the (partial) name. For example, if we type “acid” the list collapses to show:



The white space that fills the lower right “quarter” of the components panel lists just those compounds that have been selected to be included in the simulation. Between the lists of available compounds and selected compounds is a column of buttons. The purpose of these buttons is explained below.

Adds compound selected on the left to the list on the right.

Removes compound from list of previously selected compounds on right.

Replaces compound selected on right with compound selected at left.

Moves compound selected at right up one place in the list.

Moves compound selected at right down on place in the list.

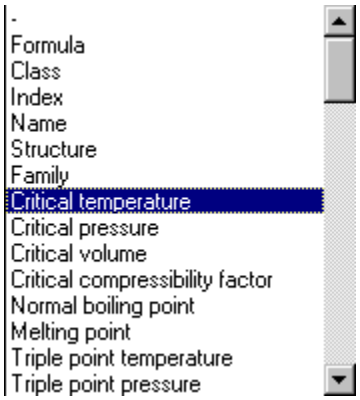
Initiates web search for additional compounds and launches database manager.

Launches window for creation of pseudo-components.

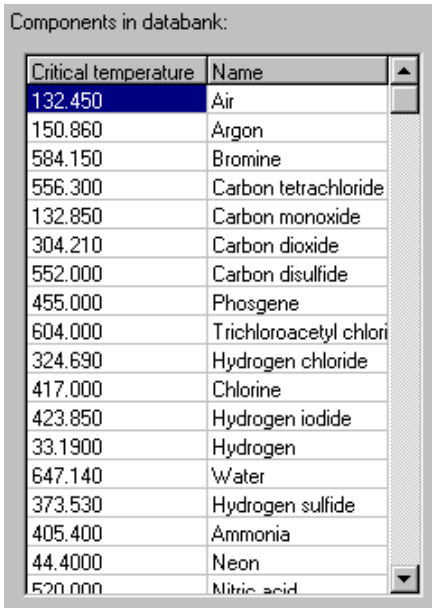
Advanced Search

There is one more feature of the *Components* panel that deserves discussion (even though we admit that we hardly ever use it ourselves). That is the *Advanced search* check box. Click in this box and the upper section of the panel changes appearance:

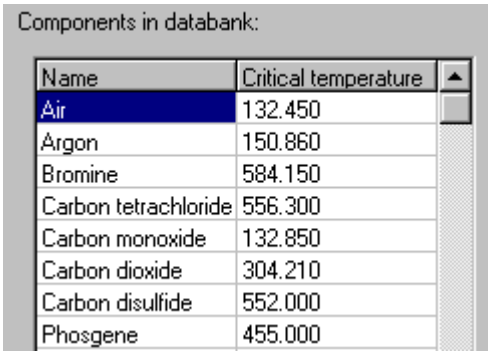
This feature allows us to search the databank for compounds based on criteria other than their name. Click on the drop down list by *Filter* to bring up a long list:



The illustration above shows just a small portion of the entire list of properties that can be used as a basis for selecting compounds. In all, there are more than 50 properties that can be used as a basis for selecting compounds. For example, if we select Critical temperature as shown above then the list of compounds on the left appears as follows:

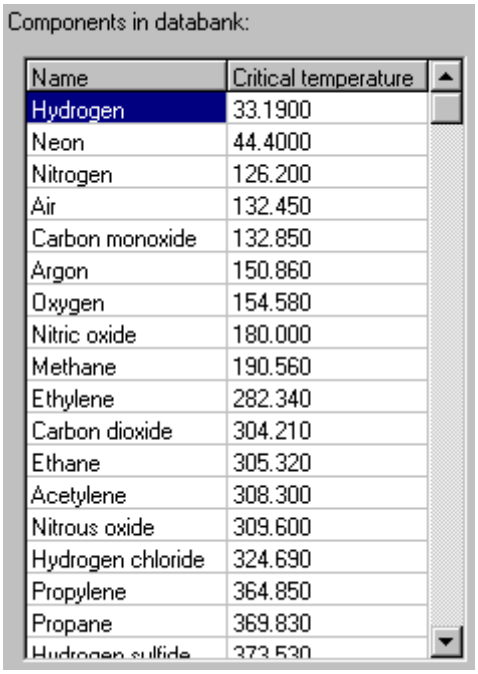


Click on the **Normal** button (upper far right) to switch the order of the columns:



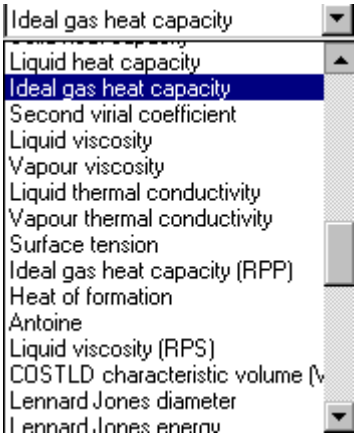
Note that the **Normal** button now says **Reverse**. Click on this button again to show the list in its original form.

Click on **Sort** to sort the compound in order of their selected property value:



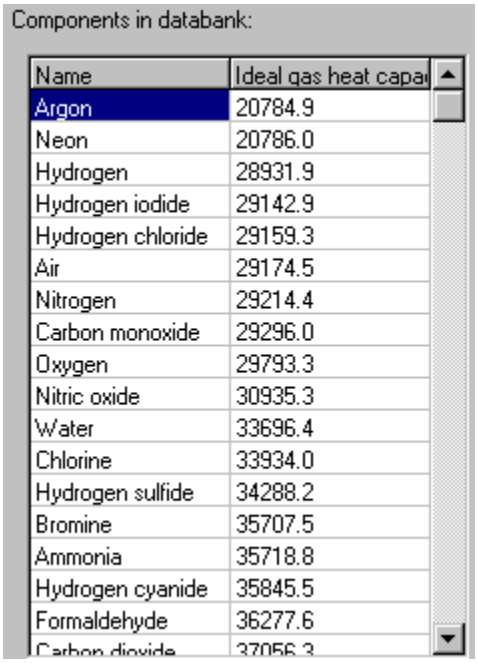
Sort now appears as **Unsort**; click on this button again to see the list in its prior order.

It is also possible to select compounds based on their values of temperature dependent properties. Select the desired property from the drop down list



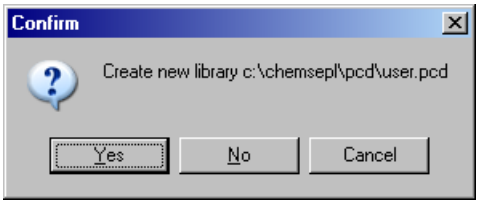
and fill in the temperature at which the property is to be evaluated in the box provided (the units displayed to the right of the box are the currently selected temperature units)::

The list of available chemicals will now show their names along side the values of the selected properties

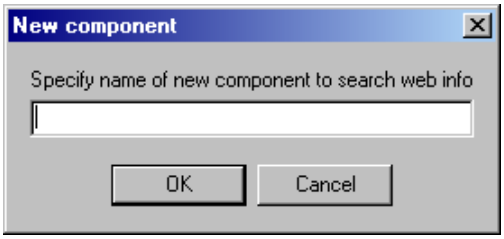


Adding Compounds Not in the Databank

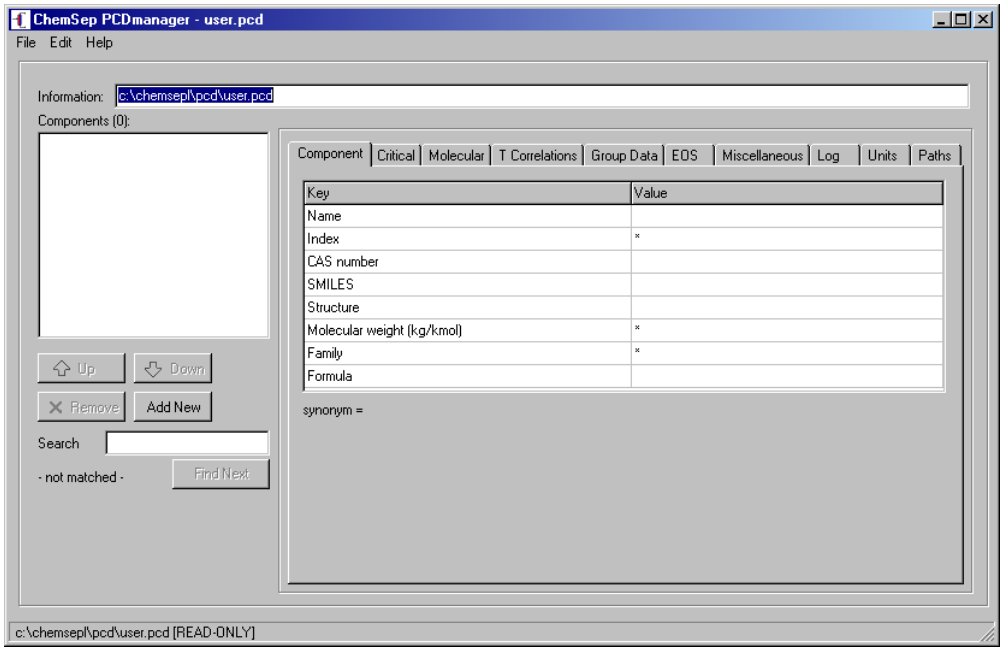
There will be many occasions when the available databanks do not contain all of the compounds needed for a simulation. It is times like that for which the **Add New** button was created. Click on this button (near the bottom of the central vertical row of buttons) and you will be asked if you wish to create a new library:



Click on yes and, if your computer is connected to the internet you will be asked another question:



Type in the name of the compound of interest and *ChemSep* will do two things, it will search the databank of NIST (National Institute of Science and Technology) for data and load what is available into a new data record. Simultaneously, it will start our own physical properties data management program:



However, using **ChemSep PCDmanager** is a story that we leave to its own tutorial.