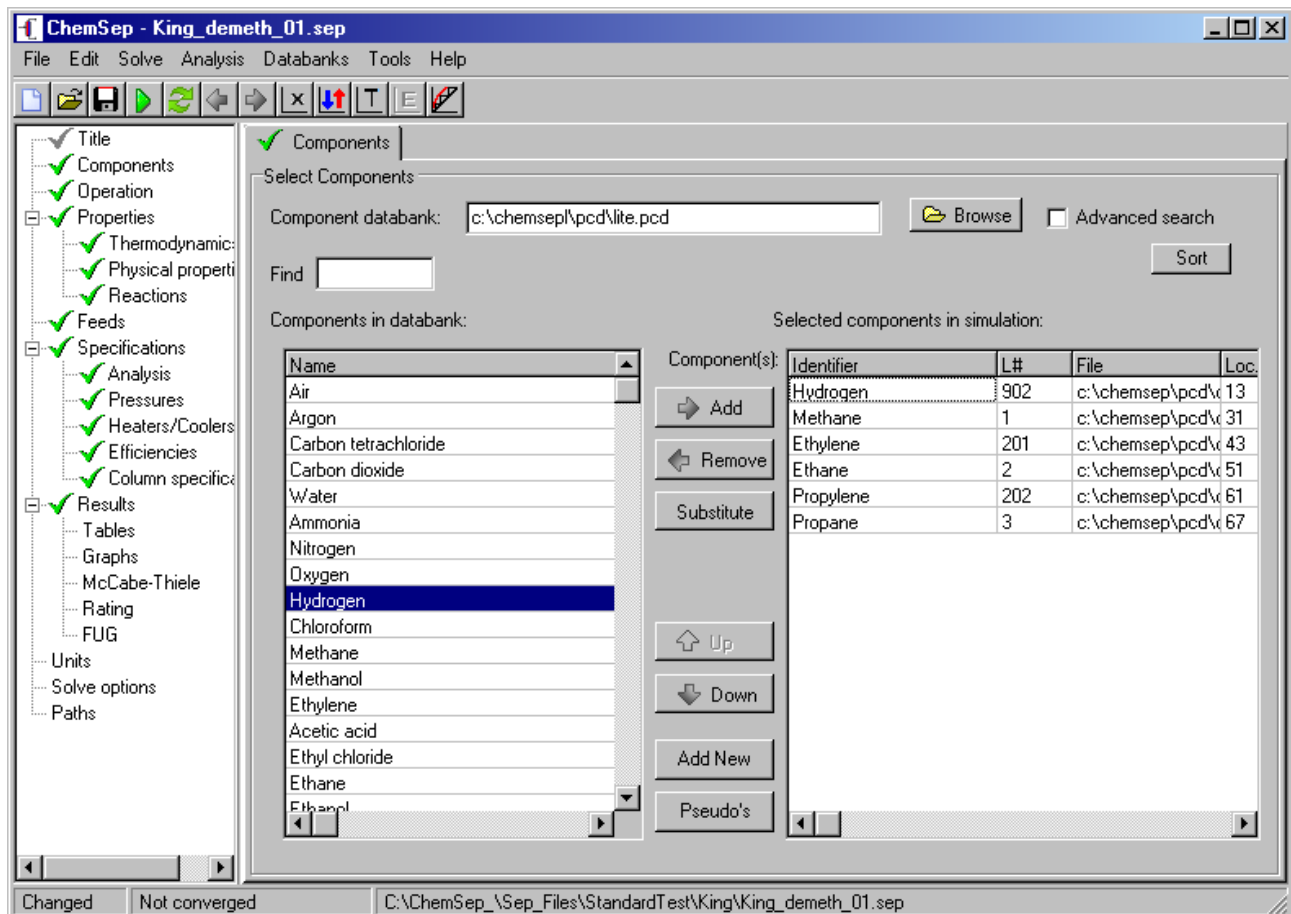


ChemSep Tutorial: Selecting Components

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.

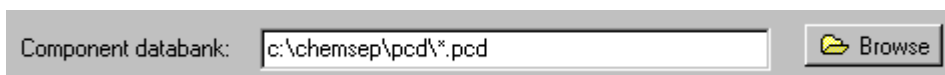
Near the top of the panel is the name of databank:



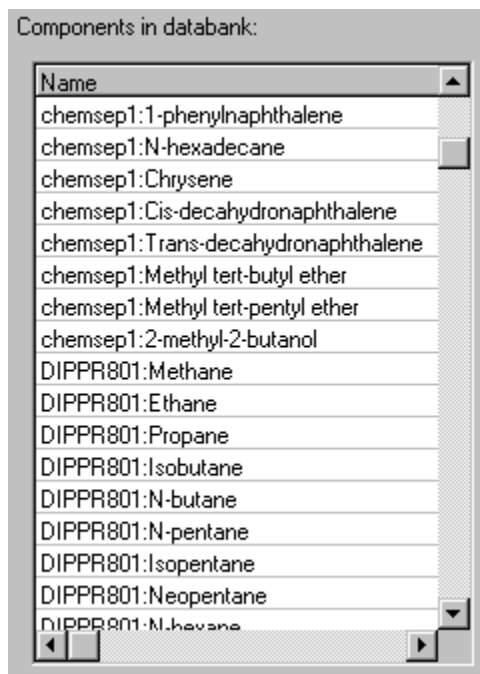
To search for alternative databanks from which to load compounds click on the **Browse** button that appears to the right. *ChemSep* databanks have the pcd (for Pure Component Date) file extension and the databank that comes with *ChemSep* is installed in the pcd subdirectory under the main *ChemSep*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

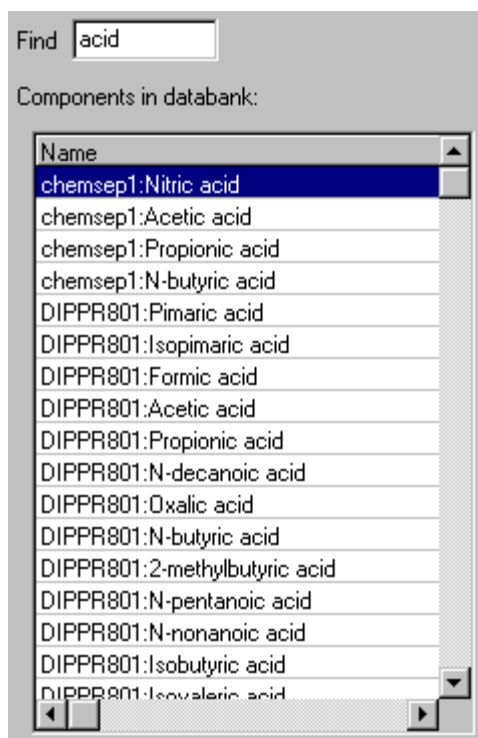
For many readers the databank that comes with *ChemSep* will not contain all the compounds of interest, and you may have created your own additional databanks. In the event that there is more than one databank in the current pcd directory. In the event that there are multiple databanks in the same directory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



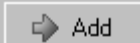



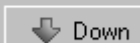
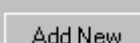

will allow *ChemSep* to display the names of all of the chemicals in all of the databanks as shown below where compounds from the standard *ChemSep* databank (chemsep1.pcd) appear before those in another databank called DIPPR801.pcd (*ChemSep's* version of the databank available from DIPPR). In this 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.

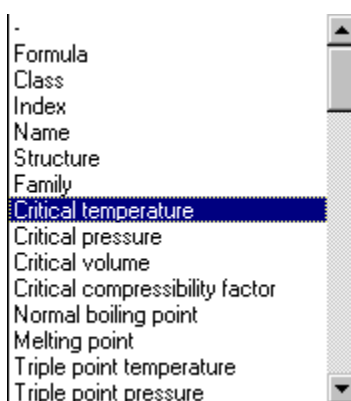
 Add	Adds compound selected on the left to the list on the right.
 Remove	Removes compound from list of previously selected compounds on right.
 Substitute	Replaces compound selected on right with compound selected at left.
 Up	Moves compound selected at right up one place in the list.
 Down	Moves compound selected at right down on place in the list.
 Add New	Initiates web search for additional compounds and launches database manager.
 Pseudo's	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:

Critical temperature	Name
132.450	Air
150.860	Argon
584.150	Bromine
556.300	Carbon tetrachloride
132.850	Carbon monoxide
304.210	Carbon dioxide
552.000	Carbon disulfide
455.000	Phosgene
604.000	Trichloroacetyl chlori
324.690	Hydrogen chloride
417.000	Chlorine
423.850	Hydrogen iodide
33.1900	Hydrogen
647.140	Water
373.530	Hydrogen sulfide
405.400	Ammonia
44.4000	Neon
520.000	Nitric acid

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

Components in databank:

Name	Critical temperature
Air	132.450
Argon	150.860
Bromine	584.150
Carbon tetrachloride	556.300
Carbon monoxide	132.850
Carbon dioxide	304.210
Carbon disulfide	552.000
Phosgene	455.000

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

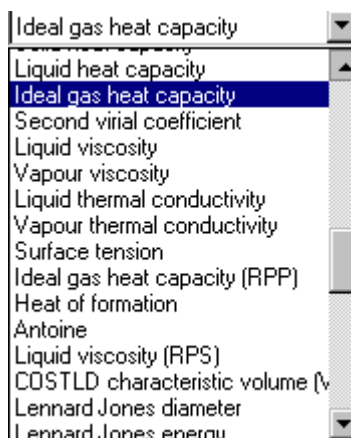
Click on **Sort** to sort the compound in order of their selected property value:

Components in databank:

Name	Critical temperature
Hydrogen	33.1900
Neon	44.4000
Nitrogen	126.200
Air	132.450
Carbon monoxide	132.850
Argon	150.860
Oxygen	154.580
Nitric oxide	180.000
Methane	190.560
Ethylene	282.340
Carbon dioxide	304.210
Ethane	305.320
Acetylene	308.300
Nitrous oxide	309.600
Hydrogen chloride	324.690
Propylene	364.850
Propane	369.830
Hydrogen sulfide	373.530

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)::



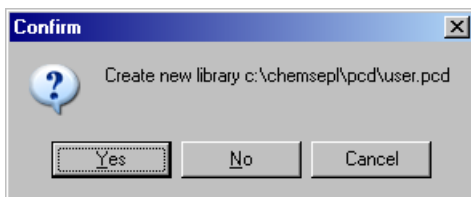
The list of available chemicals will now show their names along side the values of the selected properties

Components in databank:

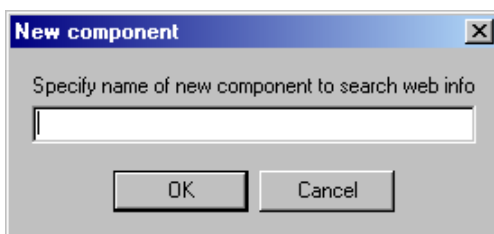
Name	Ideal gas heat capa
Argon	20784.9
Neon	20786.0
Hydrogen	28931.9
Hydrogen iodide	29142.9
Hydrogen chloride	29159.3
Air	29174.5
Nitrogen	29214.4
Carbon monoxide	29296.0
Oxygen	29793.3
Nitric oxide	30935.3
Water	33696.4
Chlorine	33934.0
Hydrogen sulfide	34288.2
Bromine	35707.5
Ammonia	35718.8
Hydrogen cyanide	35845.5
Formaldehyde	36277.6
Carbon dioxide	37056.3

Adding Compounds Not in the Databank

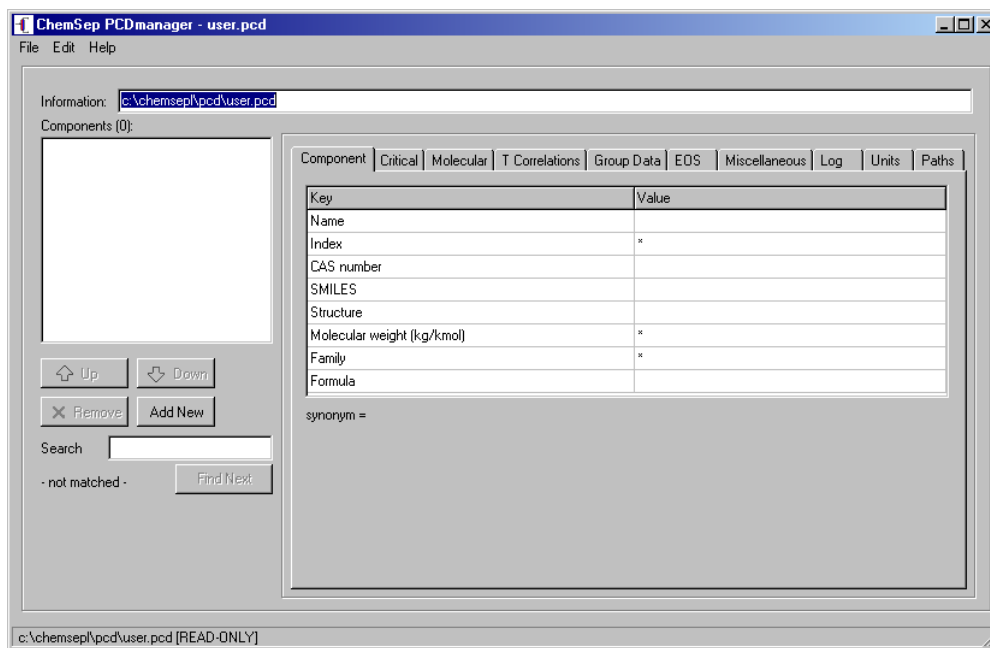
There will be many occasions when the available databanks do not contain all of the compounds needed for a simulation. It is times like that for which the **Add New** button was created. Click on this button (near the bottom of the central vertical row of buttons) and you will be asked if you wish to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