Managing Chemicals and Chemical Databanks

SuperChems™ Technical Notes

An ioMosaic Special Technical Note

Georges A. Melhem, Ph.D.

melhem@iomosaic.com

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Managing Chemical Databanks

SuperChems v8.49 (release 12-22-2018 or later) introduces better tools for managing chemicals and chemicals databanks. These new tools enable the user to quickly select new databanks and/or create project specific databanks that can be included with the project file for complete portability. These new tools automatically update the chemicals mixtures and warn the user if there are potential mismatches or missing chemicals with databank selection. Databanks are no longer required when sharing project files that have embedded project specific databanks.

These tools can be found under the new main menu Tools option "Manage files":
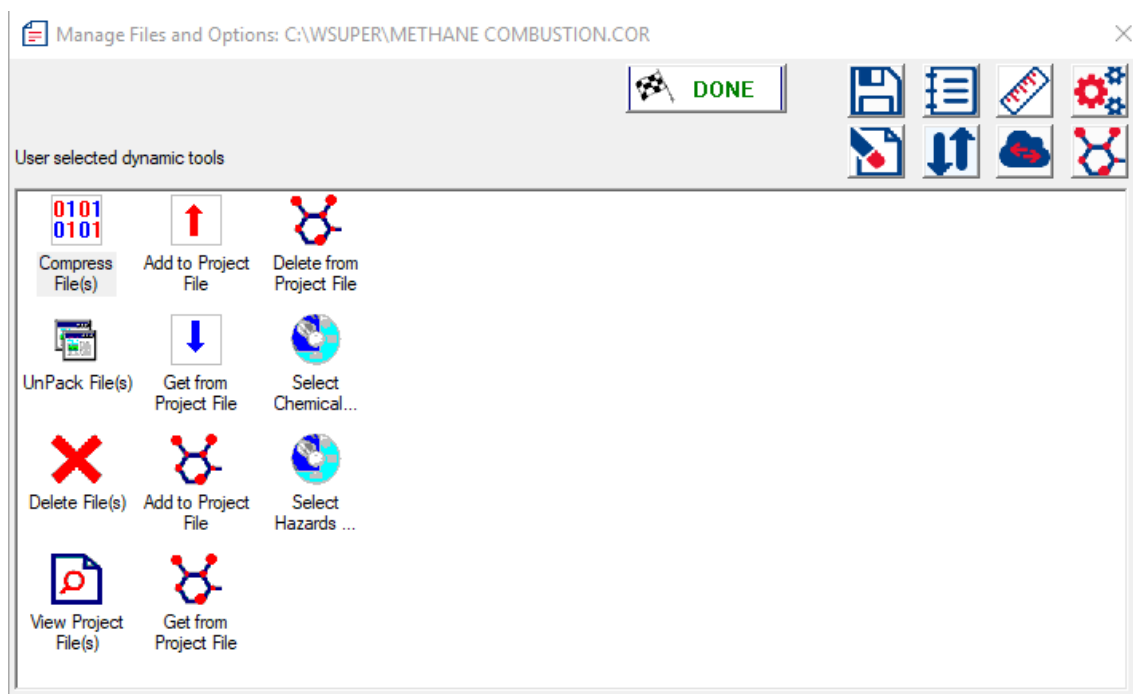
Creating Recovery Chemicals Databanks

Once your project file is completed or finalized, it is always recommended that project specific databanks are created and used.

First click on the Add to project file option

Then click on the Get from project file option:

The databanks are now project specific and a copy is placed in the project file. If this project is used by others, SuperChems™ will automatically recover the project specific databanks and place them in the ..\SUPERCHEMS\BANKS\ directory.

If you did not use the Get from Project file option to make your project file portable but manually loaded your own databanks into the project file, other users can still recover the databanks on their computer as shown in the next section (recovering chemicals databanks).

You can always revert to the original full databanks at any time if you wish by using the select chemicals databanks option from the main menu or the manage files tool.

Manual Recovery of Chemicals Databanks

If you load a project into SuperChems™ and you get the following message,
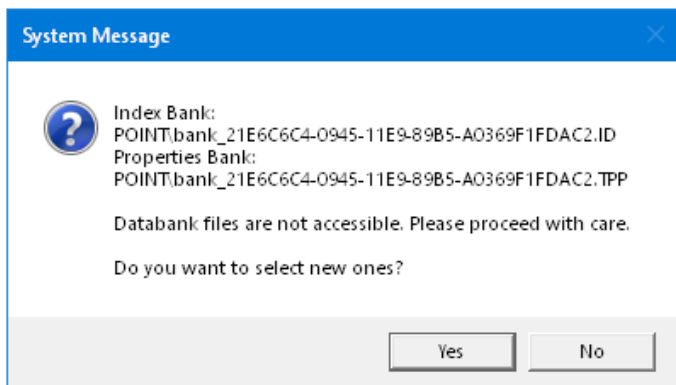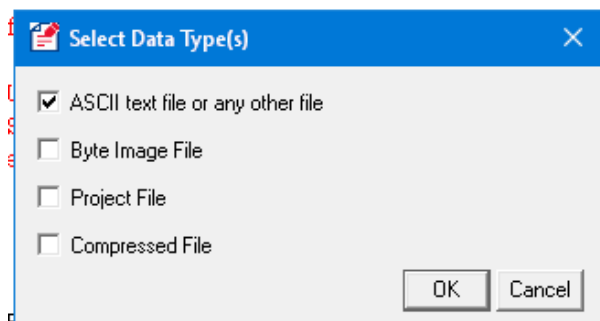

Click No

Go to the "Manage files" options.

Click on the option

Select ASCII text file or any other file

Select the two "bank_XXXXXX…" files. If you don't see the bank_XXXXXX files listed, the project specific databanks were not included in the project file and no recovery is possible without the original databanks used to create the project file.
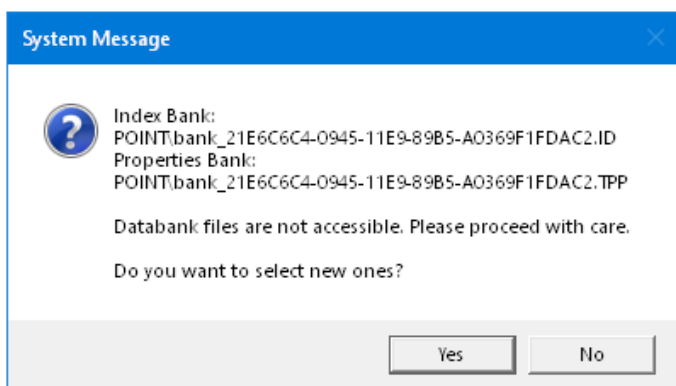
Select a folder to which to save the files

You should see a message that says "Extracted 2 files"

Click on the select chemical databanks option

You will get the same message as before:

This time clock Yes and select from the folder where you saved the files. You will see the following message (with the folder name you specified instead of \ZTEMP\):

```
Current databanks:
C:\ZTEMP\BANK_21E6C6C4-0945-11E9-89B5-A0369F1FDAC2.ID
C:\ZTEMP\BANK_21E6C6C4-0945-11E9-89B5-A0369F1FDAC2.TPP
Located and accessible
```

Then you will be asked to select the banks as the new databanks. Select the same files again. Once selected, you will see the following message:
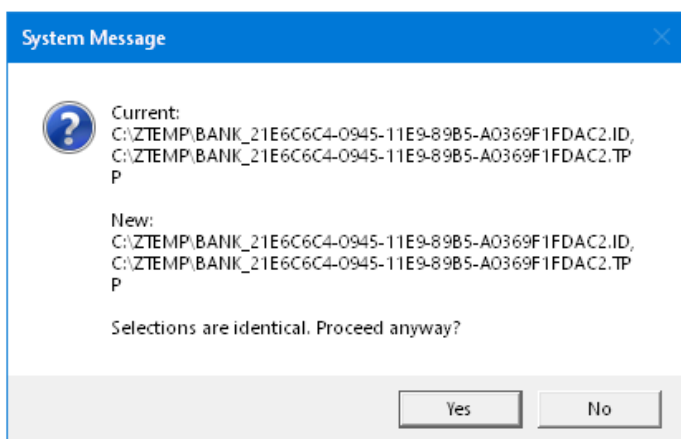
Click Yes, and the databanks are now recovered and the mixtures in the project file updated to reflect the databanks with the folder path you saved them in.

## Additional Options and Features

Compress Files

This option enables the user to select files/documents and to compress them using SuperChems™ compression tools. The compressed files will have the original file names with the extension ".PKD". Files can be added to the project file itself for better portability and documentation control. They can be extracted or viewed using SuperChems™ "unpack" and/or data exchange tools. Although adding files and documents can increase the project file size, it can help with version control, portability, and data integrity. One can also create a "documentation only" project file that can be used to store project files and other types of data as well.

Add to Project Files

This option enables the selection of either compressed or regular files and documents for inclusion into the project file itself. Compressing the files first will reduce the project file size.

Unpack Files
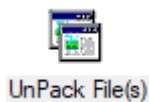
This option enables the unpacking or decompression of compressed files either stored on disk or in the actual project file. Files will first need to be selected from the project file and extracted to disk. Once on disk, files can be decompressed. Right clicking on a compressed file in the data exchange utility will decompress it on the fly and enable the user to open it automatically. It is recommended that large compressed files contained in the actual project file be extracted and decompressed before viewing.

Get from Project File

Use this option to select one or more files that are included in the project file for extraction to disk. One or more file types can be selected at a time. ASCII or any other files types include all file types that are not SuperChems™ byte images, SuperChems™ project files, or SuperChems™ compressed files. Extracting the files to disk does not delete them from the project file. To delete the data from the project file, use the data exchange tool or the delete from project file tool.
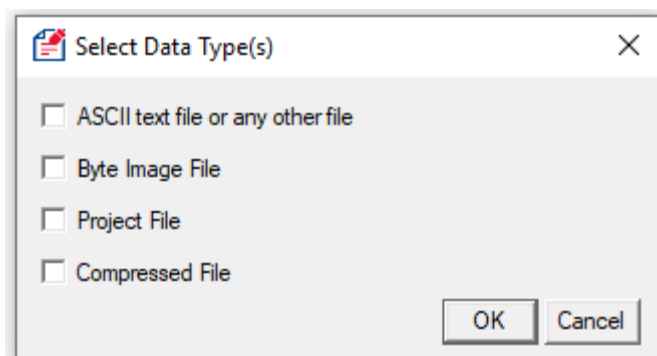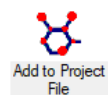
Delete Options

There are two delete options provided with the "manage files" tool. One allows for the selection and deletion of files from disk and the other one allows for the selection and deletion of files/data from the project file.

Add Chemicals Databanks to Project Files

This option enables the creation of a project specific chemicals databank that will be included in the project file. This tool will first identify all the chemicals used in the project file and then create chemical databanks for those specific chemicals plus 32 additional empty records. The databanks are included in the project file and will have a name that starts with "bank_..." as shown below:
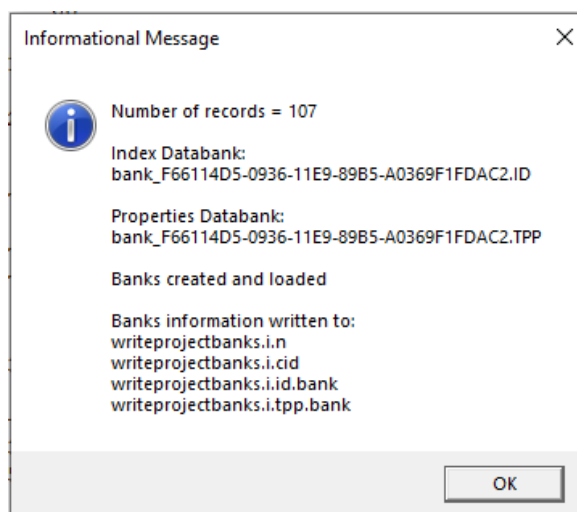
If this project file is used in the future by other users that don't have access to the chemical databanks used to create the project file in the first place, one can use the "Get from Project File" option to recover the databanks without needing access to the original databanks. This is a very useful option and it is highly recommended that all project files in final form should have this option actuated.

Get Chemicals Databanks from Project Files

This option enables the recovery of the project specific chemicals data. Once selected, the tool will ask for a folder location to extract the project specific databanks to. The tool will automatically re-index all the chemical mixture components to use the new databank records ids seamlessly.

Delete Chemicals Databanks from Project Files

This option will remove the project specific chemical databanks from the project file.

Select Chemicals Databanks

This option will allow the selection of new chemical databanks from disk. The tool will automatically re-index the project specific chemicals to the new databanks. If project files contain chemicals that are not in the new databanks to be selected, the utility will display the missing chemicals and the selection of new databanks is aborted.

Select Hazards Databanks

This option allows the user to select different hazards properties databanks. The latest available hazards databank is "hzdbanks_v8.5" and is provided in the banks directory of the SuperChems™ installation files.