Installing PHREEQC-COM for PhreeqXcel

Downloading PHREEQC-COM
The Windows COM module for PHREEQC can be downloaded from:
https://www.usgs.gov/software/phreeqc-version-3

In de section **Download Current Version of PHREEQC** the install files for Windows COM can be found:

Download Current Version of PHREEQC

Graphical User Interfaces

- Windows 32-bit: phreeqci-3.7.3-15968.msi [13M] – Executable, database files, examples, PDF documentation
- Windows 32-bit: Notepad + + interface – Appelo's Notepad + + interface to PHREEQC version 3

Batch Versions of PHREEQC

- Windows 64-bit: phreeqc-3.7.3-15968-x64.msi [16M] – Executable, database files, examples, PDF documentation
- MacOS (OS 10.7 - 10.12) 64bit: phreeqc-3.5.0-14000.dmg [12M] – Executable, database files, examples, and PDF documentation
- Windows (any processor): phreeqc-3.7.3-15968.zip [12M] – Source, CMake, database files, examples, PDF documentation
- Linux (any processor): phreeqc-3.7.3-15968.tar.gz [12M] – Source, configure, database files, examples, PDF documentation

PhreeqcRM Reaction Module for Transport Models

- Windows (any processor): phreeqcrm-3.7.3-15968.zip [7M] – Source, CMake, database files, examples, HTML documentation
- Any Platform (any processor): phreeqcrm-3.7.3-15968.tar.gz [7M] – Source, configure, database files, examples, HTML documentation

IPhreeqc Modules

- Windows (any processor): iphreeqc-3.7.3-15968.zip [13M] – Source with CMake, database files, examples, and documentation
- Linux (any processor): iphreeqc-3.7.3-15968.tar.gz [13M] – Source with configure, database files, examples, and documentation
- Windows COM 32-bit: IPhreeqcCOM-3.7.3-15968-win32.msi [4M] – COM server, CHM documentation
- Windows COM 64-bit: IPhreeqcCOM-3.7.3-15968-x64.msi [4M] – COM server, CHM documentation (Both 32-bit and 64-bit COM versions should be installed on 64-bit versions of Windows)

The install file names are changed for succeeding releases.
It is recommended to use the latest release, since this will include resolved bugs, updated databases etc.

The Windows COM module for PHREEQC requires one install file on a 32-bits Windows system and two install files on a 64-bits Windows system:

Platform	Processor	File name
Windows COM	32-bit	IPhreeqcCOM-[*version*]-win32.msi
	64-bit *	IPhreeqcCOM-[*version*]-x64.msi

Both 32-bit and 64-bit COM versions should be installed on 64-bit versions of Windows

Installing PHREEQC-COM

Installing the downloaded .msi files will (by default) create the following maps:
- on 32 bits Windows: C:\Program Files\USGS\ IPhreeqcCOM [*version*]
- on 64 bits Windows: C:\Program Files\USGS\ IPhreeqcCOM [*version*]
                                       C:\Program Files (x86)\USGS\ IPhreeqcCOM [*version*]

The following sub maps will be created:
- bin   IPhreeqcCOM dynamic link library (DLL) and type library (TLB) files
- database   10 chemistry database files in PHREEQC format, including phreeqc.dat
- doc   documentation files (pdf, chm), release notes
- examples   in sub map ./com/excel: 4 runphreeqc example files and phreeqc.dat,
                              including runphreeqc_3.xlsm (= PhreeqXcel 3.1.7).
Updating an installed COM module results in the removal of the old version, including its folders.

After installing the .msi-files, you might check whether these maps and files exist at your computer.


Testing PHREEQC-COM by running PhreeqXcel

The installed COM-module can be tested by running a PhreeqXcel application.
PhreeqXcel can be downloaded from:
https://ac4e.omnisys.nl

Open AC4E-phreeqxcel-[*version*].xlsm.
Click 'Enable Content' whenever Excel gives the Security Warning 'Macros have been disabled'. Excel security warnings depends on user's security settings:
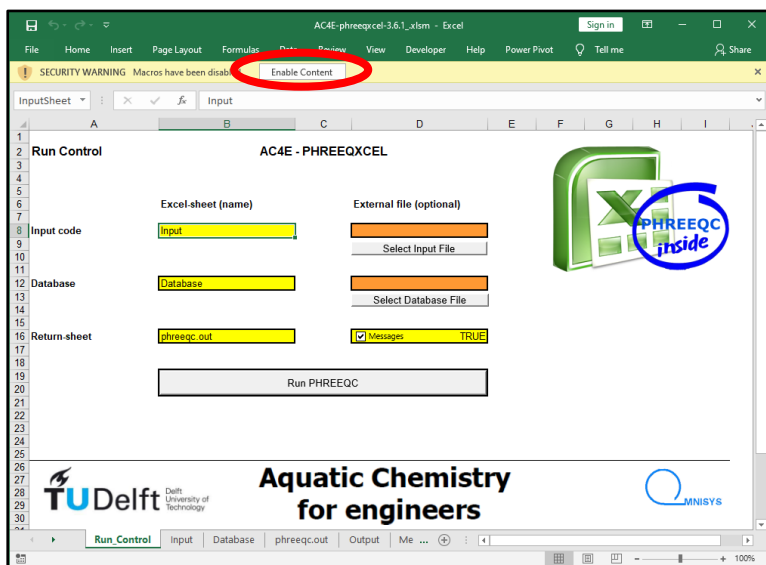

On opening a PhreeqXcel application the PHREEQC-code on sheet Input might be executed, in 'silent' server-mode, if defined so in the VBA-sub 'Workbook_Open', or the 'Run PHREEQC' button should be pushed to run Phreeqc. Such run includes loading of the COM-module.
In case the COM-module is not installed the VBA-code in Excel gives an error message:
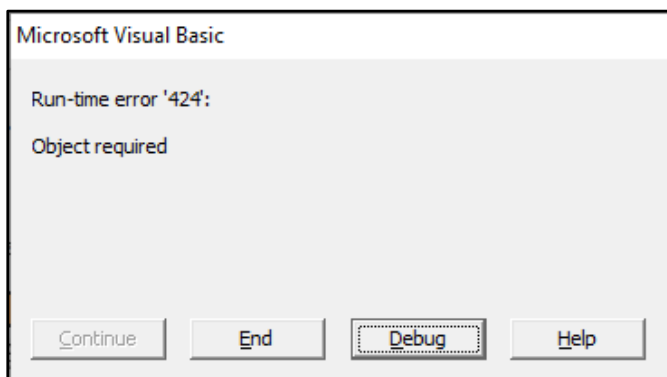
The same error will appear in case the Microsoft .NET Framework 3.5 is not installed, or not turned on (within Control panel – Program and features – Turn Windows features on and off).

Proper functioning of the COM-module might be tested by pushing the 'Run PHREEQC' button.
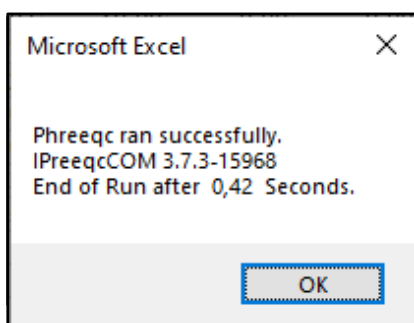
Now a message box confirms a successful run, and shows the version of the installed PHREEQC-COM-module, as well as the duration of the run. This requires Messages set as True on the Run_Control sheet of PhreeqXcel).

Controlling PhreeqXcel

The basic control functions of PhreeqXcel are presented and defined on sheet 'Run_Control'.
This sheet also contains a 'Run PHREEQC' button to start the Run.

Starting the PhreeqXcel application runs the simulations defined in the user input code on sheet 'Input' using the PHREEQC database on sheet 'Database'. The results are presented on the sheets 'Output' and 'phreeqc.out'.

Users might modify the names of these sheets, might use alternative sheets, or might use external files for Input and/or Database. External files are imported in related sheets, in order to fulfil the 'single file' container concept.
Users might unselect the message after running PhreeqXcel.
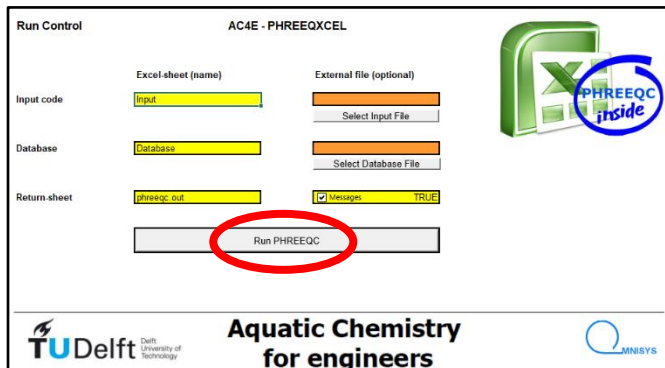
Creating PHREEQC-code

The PHREEQC versions 'Phreeqc Interactive' (USGS) and 'PHREEQC in adapted Notepad++' (Tony Appelo) include on their websites extended support for creating PHREEQC code.
'Phreeqc Interactive' (USGS) has been developed for the novice PHREEQC user. 'PHREEQC in adapted Notepad++' is focussed on users with a basic understanding of the PHREEQC concept.

PhreeqXcel does not include such support for code generation. PhreeqXcel users might use one of these container systems for code generation and import the code lines in the PhreeqXcel sheet 'Input'. Alternatively, users may directly create their own code in the PhreeqXcel sheet 'Input' using the extended help files and manuals for PHREEQC as reference systems.

The Compiled HTML Help files from both PHREEQC versions are included as part of the documentation files for PhreeqXcel.

The USGS Help file is not always updated after PHREEQC language modifications (indicated by a two-digit version number as in version 3.7), in contrary to the Appelo Help file.

The USGS Help file gives the full explanation of syntax options for all keywords. The Appelo Help file gives only examples of syntax options with minor comments.

Suggestion: Try out both PHREEQC Help files to find your most appropriate version.
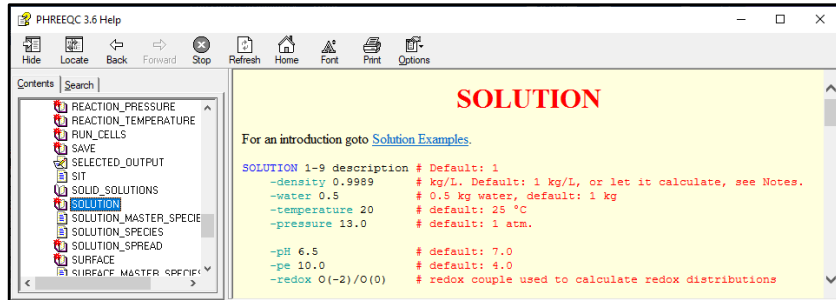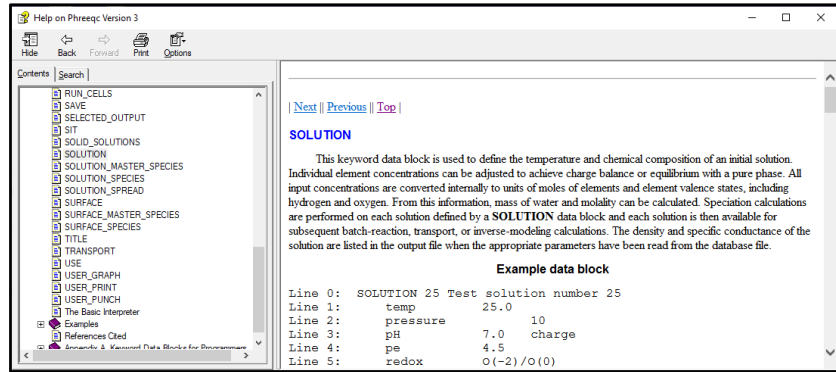
An extended PHREEQC manual for PHREEQC Version 3 can be found on the USGS website, as a pdf version. This manual is not modified after PHREEQC language modifications (3.1 etc).
However, the Online Version 3 User's Guide is updated after each modification.

Running PhreeqXcel apps

Within PhreeqXcel the imported code lines and the directly created code lines might be extended with the specific pre-processing options of Excel, for creating PhreeqXcel apps. These apps might also include post-processing of the results in Excel which will improve the presentation and interpretation of the calculated results.

PhreeqXcel apps might be used by its developer but also by users without any knowledge of PHREEQC. Running PhreeqXcel apps includes the following 3 steps:
-       input of user specific data
-       running the PHREEQC simulations
-       presenting the results.
This 3 steps concept within Excel is visualized in this figure:
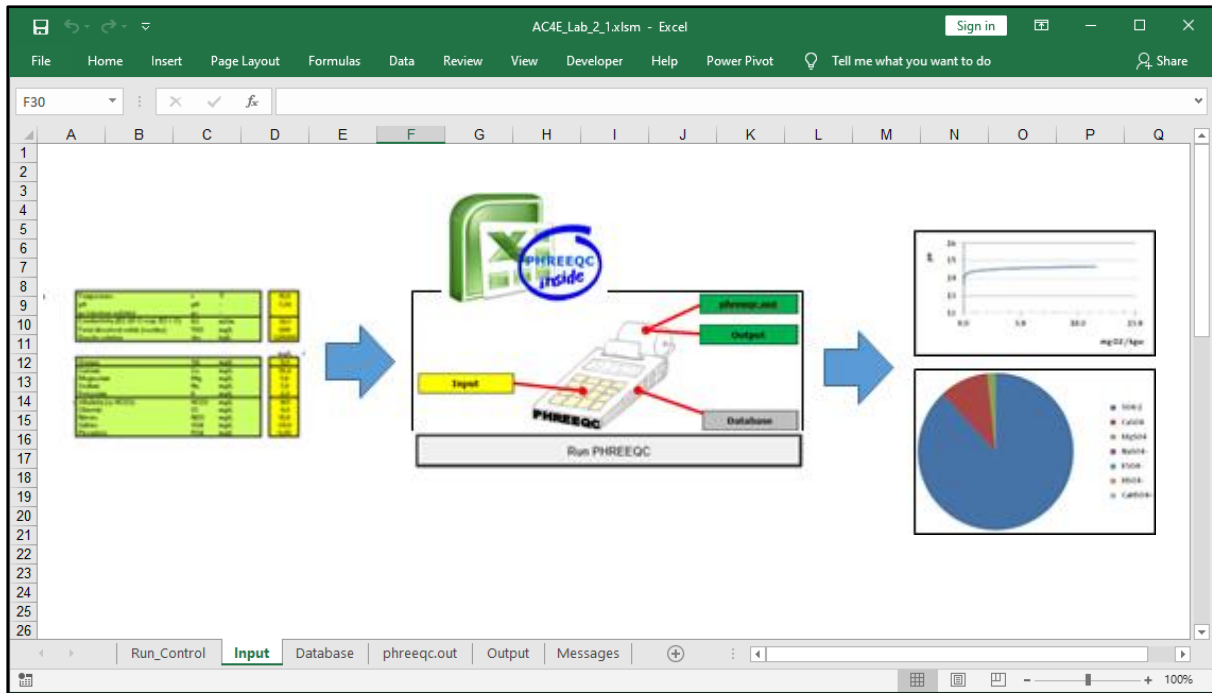
The user specific data is placed a specific sheet.
The content of this sheet modifies the code on sheet Input.
Running this Input will result in lined output on sheet phreeqc_out and tabulated output on sheet Output.
Data of the tabulated output can be used to create any table or graph in Excel, either on the sheet with specific user data or on anu other Excel sheet.

Further information
Further information on using PhreeqXcel can be found in the manual 'PHREEQC for Water Treatment', which includes Labs for explanation and examples for several applications in Water treatment.