Installing PHREEQC-COM and running PhreeqXcel

Downloading PHREEQC-COM
The Windows COM module for PHREEQC can be downloaded from:
http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

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-3.5.0-14000.msi [13M] - Executable, database files, examples, PDF documentation
- Windows 32-bit: Notepad + + interface - Appelo's Notepad + + interface to PHREEQC version 3
- Windows 32-bit: PHREEQC for windows - PHREEQC for windows home page

Batch Versions of PHREEQC
- Windows 64-bit: phreeqc-3.5.0-14000-x64.msi [15.5M] - 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-3.5.0-14000.zip [12M] - Source, CMake, database files, examples, PDF documentation
- Linux (any processor): phreeqc-3.5.0-14000.tar.gz [12M] - Source, configure, database files, examples, PDF documentation

PhreeqcRM Reaction Module for Transport Models
- Windows (any processor): phreeqcrm-3.5.0-14000.zip [2M] - Source, CMake, database files, examples, HTML documentation
- Any Platform (any processor): phreeqcrm-3.5.0-14000.tar.gz [2M] - Source, configure, database files, examples, HTML documentation

IPhreeqc Modules
- Windows (any processor): iphreeqc-3.5.0-14000.zip [7.5M] - Source with CMake, database files, examples, and documentation
- Linux (any processor): iphreeqc-3.5.0-14000.tar.gz [7.4M] - Source with configure, database files, examples, and documentation
- Windows COM 32-bit: IphreeqcCOM-3.5.0-14000-win32.msi [3.3M] - COM server, CHM documentation
- Windows COM 64-bit: IphreeqcCOM-3.5.0-14000-x64.msi [3.5M] - 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.
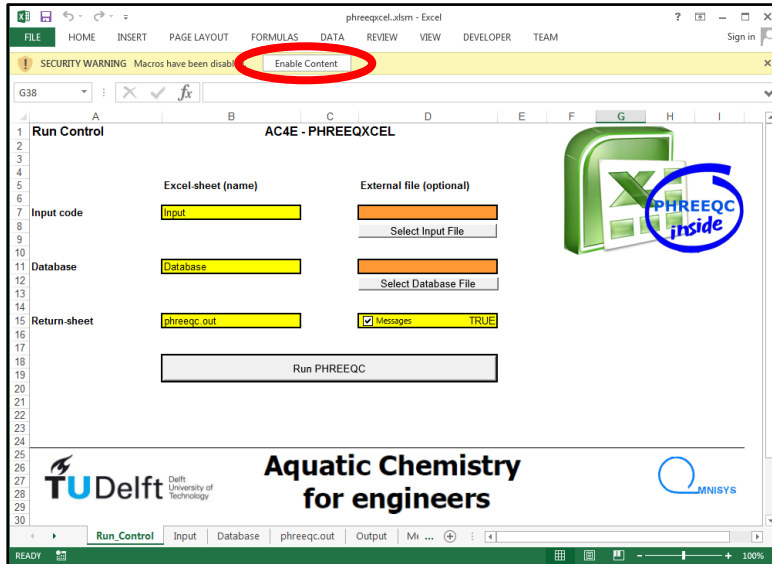
Testing PHREEQC-COM by running PhreeqXcel
The installed COM-module can be tested by running a PhreeqXcel application.
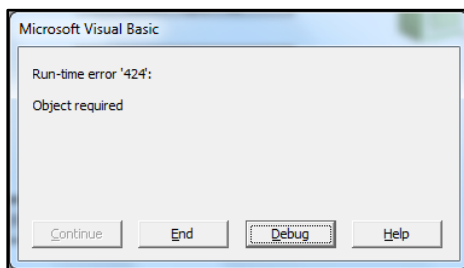PhreeqXcel can be downloaded from:
http://ac4e.omnisys.nl

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:
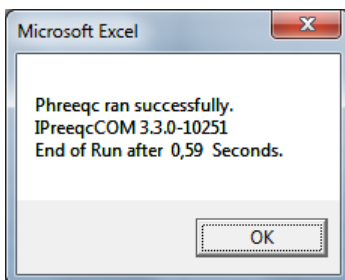

On opening a PhreeqXcel application the PHREEQC-code on sheet Input is executed, in 'silent' server-mode, as defined in the VBA-sub 'Workbook_Open'. This run includes the initial loading of the COM-module.
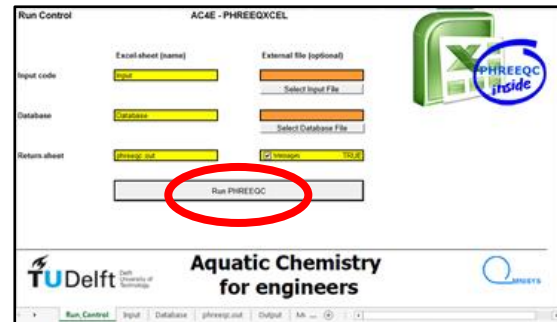In case the COM-module is not installed the VBA-code in Excel gives an error message:

Proper functioning of the COM-module might be tested again 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:

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.
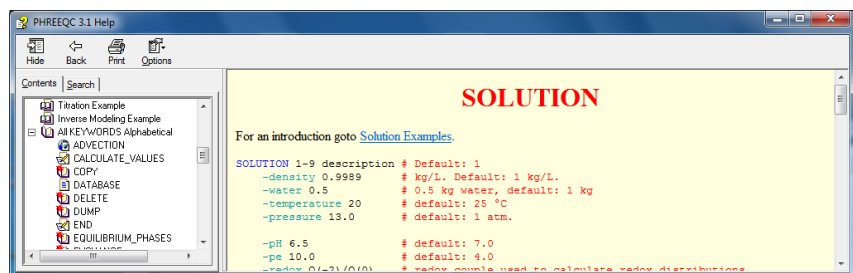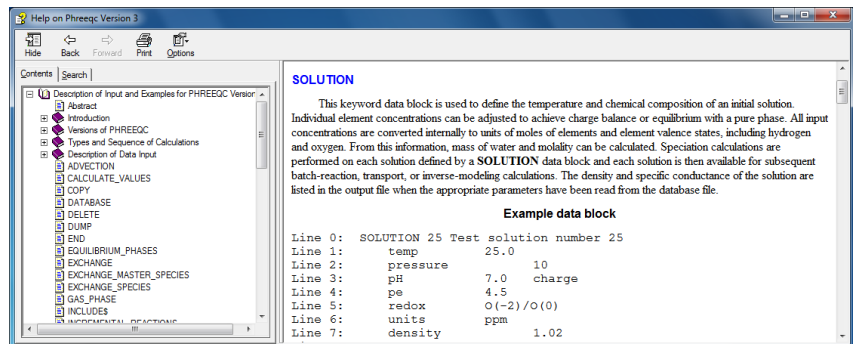
Creating PHREEQC-code

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.
These Compiled HTML Help files are modified after PHREEQC language modification (indicated by a two-digit version number as in version 3.1), but not for bug fix versions (indicated by an extended version number as in version 3.1.2). 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 and as an online version. These manuals are not modified after PHREEQC language modifications.

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: