PHREEQC

Authors

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Homepage

The project homepage contains the sources, binaries (Windows, Linux, Mac OS X), documentation and lots of other useful stuff.
https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

Source

Source code is available in the project homepage.
https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

Reference

Parkhurst, D.L., and Appelo, C.A.J., 2013, Description of input and examples for PHREEQC version 3—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Techniques and Methods, book 6, chap. A43, 497 p.

Description & Use

PHREEQC is one of the major nowadays geochemical programs used for aqueous speciation modelling. For more information about the program and its usage in geochemistry and chemistry, please visit the project homepage, read the attached original manuals or check our attempts (Mobile Chemistry Portal).
https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/
http://www.jh-inst.cas.cz/~liska/PHREEQC2.htm
http://www.jh-inst.cas.cz/~liska/Phreeqc.htm

Quick start

Use in command line / shell:

`phreeqc` (then the user is prompted to type name of the input file, then output file and filnally the database file)
(in Windows command line)

or

`./phreeqc` (then the user is prompted to type name of the input file, then output file and filnally the database file)
(in Android shell).

The result will appear in the same location.

PHREEQC and chemistry

PHREEQC is one of the most favourite geochemical modelling software which is, however, generally still not known among chemists. PhreePlot is a charting & plotting extension of PHREEQC for creating commonly needed types of diagrams.
https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/
http://www.phreeplot.org/index.html

JH-CEBOCALE

The program package contains several database files, which differ in number of included species and related parameters. The newly presented database JH-CEBOCALE.dat is a composition of existing files llnl.dat, sit.dat, minteq.v4.dat, thermoddem.dat and PSINA.dat plus many other equilibrium data added either directly from literature (i.e. they are experimental-based), or as results of qualified predictions (mainly empirical). The main distinctions from the already existing databases are:

- constrained equilibrium concept based definitions of many species, especially organic and bioorganic building blocks. Their formulation was made with respect to the molecular structure and expected reactivity sites identification (valid for aqueous solutions). The concept was used for redox couples with no reliable thermodynamic connections to the parent element as well, e.g. $[Ru(CN)_6]^{3-}$/$[Ru(CN)_6]^{4-}$.
- use of any available data (experimental, calculated or predicted on basis of qualified estimations) for better description of complex systems where huge number of species are employed. The data integrity was in this case preffered to critical selection in terms of unified experimental, evaluation and statistical methology. Therefore, the ambition of collecting as many elements, their valence states and individual species equilibrium data as possible was at least at zeroth level fulfilled.

The mentioned unique features of JH-CEBOCALE.dat are, however, connected with few risks, namely:

- problem with (re)definition of some species. It arises from the non-uniform denotation of the identical species in the literature. Typical examples of this category are couples as $HNbO_3$/$Nb(OH)_5$, AlO_2^-/$[Al(OH)_4]^-$ etc.
- difficulties related to standard state definition. They can result in either incorrect values of equilibrium constants or even in mismatch among particular species involved in the equilibrium. Such troubles sometimes occur in case of e.g. Rh(III), Ru(III), Pd(II), Ir(III), Os(III), Pt(II), Pt(IV), Au(III) complexes because the typical aquo ions (on whose basis the complex formation equilibria with other ligands are likely to be formulated) either do not exist at all or they are ill-defined.
- lack of internal data consistency from the point of view of additional properties. Each source database contains for each entry an unique set of tabulated data that enables advanced calculations, e.g. speciation temperature dependence, density of the solution etc.
- due to inconsistency of temperature dependence data it is highly recommended not to perform calculations on systems far away from 25 °C.

The experimental (at the moment very incomplete) kinetic version JH-CEBOCALE-k.dat enables modelling of systems where the rate laws and appropriate rate constants are known from the literature, with respect to PHREEQC limitation to aqueous solutions mainly of inorganic species. The RATES definition block is included in the database, the KINETICS block is available in the file JH-CEBOCALE-k_1.1_kinetics.phr. It can be used either whole as it is (e.g. Test.phr) or - better (not all of the reactions are tabulated for the same temperature) - by copying the desired reaction number with the input parameters to the user defined input file. Because the database contains intentionally disconnections between individual oxidation states of each element, it is also possible to use it only for equilibrium calculations in cases where redox processes are known not to proceed.

To get inspiration, for what PHREEQC calculations could be useful not in geology, geochemistry or hydrogeology but in chemistry, few typical application examples were prepared.

Program status

The current package contains PHREEQC binaries of version 3.4.8 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

IMPORTANT: Although we provide here our specific PHREEQC packages, they are strongly based on the Notepad++ distribution except the main executable, our database, example files and few remarks. Please note that the effort of our team is to bring PHREEQC also to platforms other than i686 and x86_64, however, we are not authors of PHREEQC and did no scientific work concerning the code itself. For this, we gratefully acknowledge D.L. Parkhurst and C.A.J. Appelo.

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PHREEQC

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For completeness, together with our newly proposed database and chemical examples, all other files from the standard PHREEQC distribution (incl. manual, geochemical sample files, default database files) are also packed. **Please note that some example files (which require plotting capabilities) will work only to produce the text output, not the graphs.**

MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime.
http://www.mingw.org/

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X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.
http://x11-basic.sourceforge.net/
https://www.libsdl.org/

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).
https://www.advancedinstaller.com/
https://www.advancedinstaller.com/top-freeware-features.html

Contact

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