Software Abstract   Thomas J. Wolery   6-5-2013

1a. Software Acronym:

EQ3/6 version 8.0a

1b. Short Title:

EQ3/6, A Software Package for Geochemical Modeling, version 8.0a

2. Author Name(s) and Affiliations:

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3. Software Completion Date:

12/13/2010 (Windows PC part only)

4. Brief Description:

EQ3/6 is a software package for modeling geochemical interactions between aqueous solutions, solids, and gases, following principles of chemical thermodynamics and chemical kinetics. It is useful for interpreting aqueous solution chemical compositions and for calculating the consequences of reaction of such solutions with minerals, other solids, and gases. It is designed to run in a command line environment. EQPT is a thermodynamic data file preprocessor. EQ3NR is a speciation-solubility code. EQ6 is a reaction path code.

5. Method of Solution

This software utilizes the Newton-Raphson method and a Gear-like predictor-corrector method.

6. Computer(s) for which software is written:

Primarily for Windows PCs (source code and executables included). Secondly for Linux and Unix platforms (source code included but no executables).

7. Operating System:

Windows XP, Windows 7, Windows 8;
Various flavors of Linux and Unix (user must create executables)

8. Programming Language(s) Used:

Fortran 95 (100% in base case); some C-Shell scripts equivalent to a number of small auxiliary Fortran programs are included for alternative use on Linux and Unix systems

9. Software Limitations:

None on modern platforms

10. Unique Features of the Software:

The software is designed to run in a command line environment, using text-based input files that are suggestive of a GUI interface. A library of sample problems including input and matching output files is provided. A set of various supporting thermodynamic data files is provided; the user must choose the one that best matches a given problem. The EQ6 code produces both a text-based output file and a .csv (comma-separated-variable) output file.

11. Related and Auxiliary Software

The software package is self-contained. Three supporting libraries are included. Running the principal codes is facilitated by using small auxiliary codes, which are either small Fortran codes or equivalent C-Shell scripts. These have the names RUNEQPT, RUNEQ3, RUNEQ6, XCIF3, and XCIF6.

12. Other Programming or Operating Information or Restrictions:

EQ3NR output files created by running this code under the auxiliary software RUNEQ3 have the filename extension .3o. These are text files and on a Windows PC, it is helpful to associate the .3o extension with Wordpad. EQ6 output files created by running this code under the auxiliary software RUNEQ6 have the filename extensions .6o and .csv. On a Windows PC, it may be similarly helpful to associate the .6o extension with Wordpad. If Microsoft Excel or a similar spreadsheet tool is installed, the .csv extension will probably already be associated with that tool.

13. Hardware Requirements

There are no significant hardware requirements, assuming that the platform to be used is a desktop or laptop PC, an equivalent Linux or Unix box, or something more powerful. This software has not been tested on a tablet.

14. Time Requirements:

On a desktop PC, EQ3NR run times typically less than a few seconds. EQ6 run times may run to several minutes or more, depending on problem complexity.

15. References:

   See code manuals included as PDF files in the software distribution package.