

PACKAGE ID - 000324IB38602 EQ3/6 V7.2B

KWIC TITLE - Geochemical Modeling Of Aqueous Systems

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LIMITATION CODE -COPY **AUDIENCE CODE** - LIM

COMPLETION DATE - 08/18/1995 **PUBLICATION DATE** - 07/30/1993

DESCRIPTION - EQ3/6 is a software package for geochemical modeling of aqueous systems. This description pertains to version 7.2b. It addresses aqueous speciation, thermodynamic equilibrium, disequilibrium, and chemical kinetics. The major components of the package are EQ3NR, a speciation-solubility code, and EQ6 a reaction path code. EQ3NR is useful for analyzing groundwater chemistry data, calculating solubility limits, and determining whether certain reactions are in states of equilibrium or disequilibrium. It also initializes EQ6 calculations. EQ6 models the consequences of reacting an aqueous solution with a specified set of reactants (e.g., minerals or waste forms). It can also model fluid mixing and the effects of changes in temperature. Each of five supporting data files contain both standard state and activity coefficient-related data. Three support the use of the Davies or B-dot equations for the activity coefficients; the other two support the use of Pitzer's equations. The temperature range of the thermodynamic data on the data files varies from 25 degrees C only to 0-300 degrees C.

PACKAGE CONTENTS - Summary of Differences Between 7.2A and 7.2B; Zlist for PC Version (Media Directory and Installation Instructions 2 pages); Software Abstract; UCRL-MA-110662 Parts 1-4; Media Includes Source Code, Text Library, Executable Modules, Auxiliary Material, Compilation Instructions, Linking Instructions, Control Information, Sample Problem Input and Output;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 5 3.5 Diskettes

METHOD OF SOLUTION - EQ3NR and EQ6 use a hybrid Newton-Raphson technique to make thermodynamic calculations. This is supported by a set of algorithms which create and optimize starting values. The hybrid Newton-Raphson technique algorithm was recently modified to improve convergance behavior in dealing with systems containing concentrated salt solutions. EQ6 uses a Gear-like ODE integration algorithm to integrate rate equations when solving problems which have a time frame.

COMPUTER - IBM PC 386

OPERATING SYSTEMS - DOS 6.2 or later with MicroSoft Windows 3.1 or later. A Windows interface is not provided; the essential feature

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OPERATING SYSTEMS - (CONT) of Windows 3.1 is its memory manager.

PROGRAMMING LANGUAGES - Lahey extended Fortran (F77L-EM/32, v. 5.11)
with DOS system calls

SOFTWARE LIMITATIONS - Limitations pertain mainly to the range of physics/chemistry embedded in the current version (7.2A). Pressure is currently restricted to 1.013 bar up to 100 degrees C and the steam-liquid water curve from 100 degrees C to 300 degrees C. The EQ6 code does not allow treatment of redox disequilibrium or the kinetics among aqueous components. Neither EQ3NR or EQ6 contain any capabilities for modeling mineral surface chemistries. Apart from a pseudo-1D fluid centered flow-through model, the EQ6 code only models the chemical interactions taking place in a single box. The ODE integration method currently employed in EQ6 is fairly primitive and has trouble with stiff ODE systems.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - The software offers the user a wide spectrum of options. Calculations can be made over a broad range of temperature. The EQ3NR code allows speciation-solubility problems to be defined using nearly every conceivable combination of types of input. The pH in brine solutions can be constrained by the input of measured pHCl(pH+pCl). The EQ6 code allows the use of rate laws to constrain irreversible reactions. It allows calculations of models pertaining to closed systems, systems open to an external gas reservoir (such as the atmosphere), and a pseudo-1D fluid-centered flow-through system. The supporting thermodynamic data files are sufficient to support a wide range of applications. They are particularly well-adapted for applications pertaining to the geochemistry of a geologic repository for high-level nuclear waste.

RELATED SOFTWARE - Supersedes Version 7.2A. Auxiliary codes XCON3 and XCON6 allow users to update input files for EQ3NR and EQ6, respectively, that match older versions of EQ3/6 (e.g., v 6.0-6.1 and v. 7.0-7.1). These codes also convert input files from the more compact 'W' format to the menu-like 'D' format, and vice versa. Interface software is provided. For example, RUNEQ3 allows the user to run the EQ3NR code, specifying the data file to use and the input file(s) to run. This program is a non-standard Fortran program. Similar software is provided to run EQ6, EQPT, XCON3, and XCON6. An EQ6 graphics postprocessor is not yet available in any of the distribution packages.

OTHER PROG/OPER SYS INFO - EQ3NR input files end in .3i, EQ6 input files end in .6i. This is a recommended convention, and it is required in order to run these codes using the PC interface software. The data file names have the form exemplified by data0.com. Here com is one of the five data file descriptors. This

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OTHER PROG/OPER SYS INFO - (CONT) general form is required to run the RUNEQPT script. The main code FORTRAN source files end in .fsc. The PC interface software source codes end in .for. The EPCLIB library supports the PC interface codes. This library is included in the distribution package.

HARDWARE REQS - RAM of at least 16 megabytes; hard disk space of at least 30 megabytes.

REFERENCES - T.J. Wolery, EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems: Package Overview and Installation Guide, (Version 7.0), UCRL-MA-110662 PT I, September 14, 1992; S.A. Daveler, and T.J. Wolery, EQPT, A Data File Preprocessor for the EQ3/6 Software package: User's Guide and Related Documentation, (Version 7.0), UCRL-MA-110662 PT II, December 17, 1992; T.J. Wolery, EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0), UCRL-MA-110662 PT III, September 14, 1992; T.J. Wolery, and S.A. Daveler, EQ6, A Computer Program for Reaction Path Modeling of Aqueous Geochemical Systems: Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0), UCRL-MA-110662 PT IV, October 9, 1992; T.J. Wolery, Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: The EQ3/6 Software Package, UCRL-52658, February 1979; Thomas J. Wolery, EQ3NR A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: User's Guide and Documentation, UCRL-53414, April 18, 1983; T.J. Wolery and L.J. Walters, Jr., Calculation of Equilibrium Distributions of Chemical Species by Means of Monotone Sequences, Mathematical Geology, Vol. 7, pp. 99-115, 1975; H. C. Helgeson, Evaluation of Irreversible Reactions in Geochemical Processes Involving Minerals and Aqueous Solutions I. Thermodynamic Relations, Geochimica et Cosmochimica Acta, Vol. 32, pp. 853-877, 1968; Joan M. Delany, Reaction of Topopah Spring Tuff with J-13 Water: A Geochemical Modeling Approach Using the EQ3/6 Reaction Path Code, UCRL-53631, November 25, 1985.

ABSTRACT STATUS - Abstract first distributed August 1980. IBM 386 version submitted September 1993. Readied screened September 28, 1993. IBM 386 version 7.2A submitted February 1994. Version 7.2B released AS-IS 9/14/95.

SUBJECT CLASS CODE - R

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
E CODES
GEOCHEMISTRY
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MATHEMATICAL MODELS
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CHEMICAL REACTIONS
GEOTHERMAL SYSTEMS
GROUND WATER
HYDROTHERMAL SYSTEMS
RADIOACTIVE WASTE DISPOSAL
REDOX POTENTIAL
ROCK-FLUID INTERACTIONS
SIMULATION
THERMODYNAMICS
UNDERGROUND DISPOSAL
WASTE-ROCK INTERACTIONS
WATER CHEMISTRY

EDB SUBJECT CATEGORIES -

990200 052002 540220 580000 400201

SPONSOR - DOE/RW

PACKAGE TYPE - AS - IS