



**Department of Energy**  
 Yucca Mountain Site Characterization  
 Project Office  
 P. O. Box 98608  
 Las Vegas, NV 89193-8608

WBS 1.2.5.2  
 QA: N/A

FEB 21 1991

B. Joe Youngblood, Director  
 Repository Licensing Project Directorate  
 Division of Waste Management  
 U. S. Nuclear Regulatory Commission  
 4-H-3  
 Washington, DC 20555

CLOSURE OF U.S. NUCLEAR REGULATORY COMMISSION (NRC) REQUEST FOR COMPUTER CODE EQ3/6

Reference: Ltr, Linehan to Stein, dtd 8/28/89

In the referenced letter, the NRC requested that the U.S. Department of Energy provide copies of Computer Code EQ3/6 and its associated documentation.

On November 29, 1990, Lawrence Livermore National Laboratory, the Yucca Mountain Site Characterization Project participant responsible for the development and maintenance of the Computer Code EQ3/6, transferred Version 3245.1090 of the code and data base to Dr. William Murphy, Southwest Research Institute. Enclosed is a copy of a letter which documents the transfer. This action should fulfill the request made in the referenced NRC letter.

If you have any questions, please contact David C. Dobson at FTS 544-7940 or (702) 794-7940, or Ardyth M. Simmons at FTS 544-7998 or (702) 794-7998.

*for Maxwell Blanchard*  
 Carl P. Gertz  
 Project Manager

YMP:AMS-2180

Enclosure:  
 Ltr, 12/21/90, Jardine to Gertz w/encls.

- cc w/encl:
- C. J. Macaluso, HQ (RW-331) FORS
  - D. E. Shelor, HQ (RW-30) FORS
  - A. R. Jennetta, W, Las Vegas, NV, 517/T-27
  - L. J. Jardine, LLNL, Livermore, CA
  - M. A. Gloria, SAIC, Las Vegas, NV, 517/T-27
  - J. L. King, SAIC, Las Vegas, NV, 517/T-03



# Lawrence Livermore National Laboratory

LLYMP90012058  
December 21, 1990

WBS 1.2.1.4.5  
QA: N/A

NNA.910109.0119

Carl P. Gertz, Project Manager  
Yucca Mountain Site Characterization Project Office (YMPO)  
P. O. Box 98608  
Las Vegas, NV 89193-8608

REFERENCE: LLYMP8910055, Ltr from C. Gertz to L. Jardine, dated 10/3/89,  
YMP:DCD-6078 (NN1-1989-0111) which in turn references a  
letter from Linehan to Stein dated 8/28/89

SUBJECT: Release of EQ3/6, Version 3245.1090

Dear Carl:

On November 29, Version 3245.1090 of the EQ3/6 Code and database was released. Attached is a description of the code and database.

One copy was transmitted to Southwest Research Institute (SWRI), to Dr. William Murphy. SWRI is a major contractor to the U.S. Nuclear Regulatory Commission. The transfer was made over INTERNET using the ftp utility. This fulfills the request made by the referenced NRC letter.

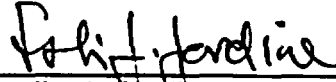
Another copy was transmitted to Los Alamos National Laboratory (LANL), to Dr. Michael Ebinger. The transfer was made via a nine-track magnetic tape reel written using the dd utility. Formal documentation of the transfer using AP5.19Q is underway.

Attached is the "Read-me" documentation that accompanied this transfer. This documentation includes a statement indicating the QA status of the code. Also included is a license/collaboration agreement which must be signed by users of the code/database outside the University of California system.

This release partially satisfies Milestone P333, "Revised EQ3/6 Code Release" of the PCSB milestone system. In transition to PACS, milestone P333 is being split into milestone 0L145BPH (Database verification report) and 0L145BPE (Revised Code Release). This release of the code and database satisfies milestone BPH. Ongoing revision of the user manuals will satisfy milestone BPE, currently scheduled for April 1991. As noted in the "Read-me" attachment, the code has not yet been fully approved for use in quality affecting activities. The PCSB and PACS milestone descriptions are being modified to reflect the QA status of the current code.

ENCLOSURE

If you need any further information, please contact Dwayne Chesnut of my staff at 415-423-5053 or FTS543-5053.



Leslie J. Jardine  
Technical Project Officer  
Yucca Mountain Project

LJ/JB/ec

**Attachments**

Code description  
Read-me file  
Collaboration agreement

cc:

M. Blanchard, YMPO  
T. Blejwas, SNL  
M. Cloninger, YMPO  
D. Dobson, YMPO  
L. Hayes, USGS  
R. Herbst, LANL  
D. Morissette, SAIC  
E. Petrie, YMPO

EQ3/6.3245.1090  
Summary of Improved Code and Database Capabilities

The most significant advance in the modeling capabilities of the EQ3/6 software package between releases 3245.0888 (August, 1988) and 3245.1090 (October, 1990) lies in the improved versatility and quality of the thermodynamic database that supports species distribution (EQ3) and mass transfer (EQ6) calculations. What follows is a summary of improvements in the thermodynamic database and their impact on EQ3/6 calculations.

To appreciate these improvements, however, one must first have a basic understanding of the database and associated software that facilitate its interface with EQ3/6. Relevant compositional and standard state thermodynamic data for over 1700 chemical species are maintained in the local INGRES relational database GEMBOCHS (Geologic & Engineering Materials: Bibliography of Chemical Species). The computer code D0OUT retrieves requisite species information from GEMBOCHS, calculates species dissociation constants at elevated temperatures and pressures using various equations of state and extrapolation algorithms, and writes these properties together with other relevant information to an output file DATA0. The DATA0 file is then piped through the filter program EQPT which strips comment lines, replaces dissociation constants with regression-polynomial coefficients, and writes the modified dataset to the unformatted output file DATA1. The DATA1 file is subsequently input to EQ3/6 together with user-generated files that define the specific speciation/mass transfer problem to be addressed.

Improvement: A suite of five distinct DATA0 files, each particularly suited to modeling certain chemical systems and geochemical problems, has superseded the single "composite" database (referred to as R43 below) issued with release 3245.0888.

This improvement required major restructuring of GEMBOCHS together with incorporation of many new species and updated parameter values taken from the revised SUPCRT91 database and recent NEA-TDB compilations.

The SUPCRT91 software and database comprise a well-known package which has recently been extensively revised and improved by LLNL-YMP in collaboration with H. C. Helgeson and co-workers at the University of California, Berkeley.

Impact: EQ3/6 users can now select an appropriate thermodynamic database with which to attack specific geochemical problems; decision criteria include compositional complexity of the problem, acceptable level of internal consistency among the data, and choice of activity coefficient formalism.

**Improvement:** Reaction properties reported within the new suite of databases are calculated from the improved equations of state for H<sub>2</sub>O and aqueous solutes encoded in the SUPCRT91 software package; R54 was based on now-obsolete predecessors to these formulations.

Relevant SUPCRT91 routines were successfully interfaced with D0OUT, resulting in full calculational compatibility between the two codes.

**Impact:** These improved equation-of-state formulations facilitate closer representation of geochemical reality than was possible with their predecessors.

**Improvement:** All reference data reported in the database suite have been cross-checked with their literature counterparts to ensure accuracy; such was not the case for R54.

This year-long activity (completed August, 1990) involved verification of data for over 1700 chemical species, taken from approximately 300 literature sources; it was performed in the context of TIP-GM-[10,12,13]. This verification effort revealed over 300 discrepancies - several of which led to significant errors in EQ3/6 calculations - which were then resolved, also as part of this activity.

**Impact:** Improved accuracy in the transfer of data from literature source to the EQ3/6 database suite necessarily leads to an improvement in the quality of EQ3/6 calculations.

**Improvement:** Several errors in D0OUT routines that implement extrapolation algorithms used to calculate the thermodynamic properties of minerals and aqueous species at elevated temperatures and pressures have been resolved; some of these errors appear to have infiltrated R54.

This informal - in the sense of TIPs and milestones - but nevertheless critical verification activity involved hand validation of calculational accuracy and extensive debugging of D0OUT.

**Impact:** Resolution of these D0OUT errors has resulted in improved accuracy of EQ3/6 calculations at elevated temperatures and pressures.

**Improvement:** The new database suite contains standard molal volumes for all included minerals; in R54, many minerals lacked volume data.

Addition of mineral volumes to the database suite followed a massive literature search/compilation activity, undertaken and completed during the past year.

**Impact:** Inclusion of a comprehensive set of mineral volume data permits improved accuracy of solubility calculations at elevated pressures.

**Improvement:** The data formats of individual species blocks have been significantly modified to expand the scope as well as improve its readability; the new formats provide additional data with superior clarity relative to those of R54.

Extensive modification of D0OUT was required to achieve the desired results.

**Impact:** The expanded and modified species-block formats in the new database suite give the EQ3/6 user a more complete and easier-to-decipher summary of relevant information.

**Improvement:** Each member of the new database suite is entirely self-contained; i.e., all compositional, reaction, and activity-coefficient data required for a given EQ3/6 run is isolated in a single datafile; in R54, one was forced to specify an additional file if certain activity coefficient formalisms were to be invoked by EQ3/6.

This improvement involved major restructuring of both GEMBOCHS and EQPT.

**Impact:** Achievement of this streamlined, single-pipe data flow through the EQ3/6 package makes operation more straightforward and decreases the likelihood of user errors.

**Improvement:** The EQ3/6 codes now permit the user to employ a new form of input file, which is menu-like in form.

**Impact:** The menu-like input is more straightforward and decreases the likelihood of user errors.

**Improvement:** The kinetics mode in the EQ6 code now allows specification of activation energies, allowing the temperature dependence of rate constants to be handled automatically.

**Impact:** External hand calculations are reduced, decreasing the likelihood of user errors.

**Improvement:** The EQ3/6 codes now also incorporate a methodology for dealing with pH in brine solutions, which was developed at LLNL for the WIPP project.

**Impact:** A large scope of problems can be run, increasing the number of users and the likelihood of detecting code bugs.

**Improvement:** Feedback from the outside user community, which consists of about 200 users from all over the world, has resulted in the elimination of a number of code and data base bugs. The new release has been tested with a newly developed library of 68 test problems (42 for EQ3NR, 26 for EQ6). About half of these problems are taken from sources describing other codes or code comparison studies, and thus represent code-to-code verification. About a dozen and a half deal with systems that are directly tied to precise measurements, and thus represent validation. Most of these deal with brine mineral equilibria, and they overlap strongly with the set representing code-to-code verification. About a half dozen problems represent internal verification in which the input/output status of certain parameters is reversed from one problem to another. Other problems utilize capabilities not present in other codes or deal with systems or scenarios lacking precise measurements (e.g., any process occurring over long time periods).

**Impact:** Verification and validation activities increase confidence in the calculations conducted with the code and database.

90/12/06  
08:26:25

wolery  
README.txt

1

README.txt last revised 10/31/90

EQ3/6, A Software Package for Geochemical Modeling  
Version 3245.1090

Copyright (c) 1987, 1990 The Regents of the University of California,  
Lawrence Livermore National Laboratory. All rights reserved.

This work was produced at the University of California,  
Lawrence Livermore National Laboratory (UC LLNL) under  
contract no. W-7405-ENG-48 between the U. S. Department of  
Energy (DOE) and The Regents of the University of California  
(University) for the operation of UC LLNL. Copyright is  
reserved to the University for purposes of controlled  
dissemination, commercialization through formal licensing,  
or other disposition under terms of Contract 48; DOE  
policies, regulations, and orders; and U. S. statutes.

DISCLAIMER

This computer code was prepared as an account of work  
sponsored by an agency of the United States Government.  
Neither the United States Government nor the University of  
California nor any of their employees, makes any warranty,  
express or implied, or assumes any liability or responsibility  
for the accuracy, completeness, or usefulness of any  
information, apparatus, product, or process disclosed, or  
represents that its use would not infringe privately-owned  
rights. Reference herein to any specific commercial products,  
process, or service by trade name, trademark, manufacturer,  
or otherwise, does not necessarily constitute or imply its  
endorsement, recommendation, or favoring by the United States  
Government or the University of California. The views and  
opinions of authors expressed herein do not necessarily state  
or reflect those of the United States government or the  
University of California, and shall not be used for  
advertising or product endorsement purposes.

LLNL YUCCA MOUNTAIN PROJECT DISCLAIMER

The Lawrence Livermore National Laboratory, a participant in  
the Yucca Mountain Project, has not determined that this  
software constitutes "approved code" for the conduct of  
"quality affecting work" for the Yucca Mountain Project.

-----  
\*\*\* WARNING REGARDING PACKAGE MAINTENANCE AT LLNL \*\*\*

The above paragraph on copyright following the copyright notice ending  
in "All rights reserved" as well as the above LLNL and LLNL-YMP  
disclaimers are written to both the output file (if any) and to the  
screen whenever any of the codes in the EQ3/6 package is run. They are  
written by the EQLIB routine prcndi.f (copies are directly incorporated  
in the source codes of the input file conversion routines). Any changes  
in the above standard language must be made in all versions of this  
routine, as well as in the present file. In the EQPT, EQ3NR, and EQ6  
codes, prcndi.f is called by the fellow EQLIB routine eqlib.f. In the  
input file conversion routines, calls are made by the main programs.

-----  
This is an update of the 3245.0888 version. A summary of changes may  
be found in the file WHATSNEW.txt: a list of package contents in



90/12/06  
08:26:25

wolery  
README.txt

2

CONTENTS.txt; description of export medium formats, in FORMATS.txt; comments regarding installation in INSTALL.txt; and a list of pertinent documents in DOCS.txt. Any known bugs are described in a file called BUGS.txt. Any post-release fixes to the present version may be found in files called FIXES1.txt, FIXES2.txt, etc.

-----

The EQ3/6 computer codes and associated data base files are now maintained and developed by separate tasks. Correspondence by E-mail is highly encouraged.

Address correspondence regarding the computer codes or the software package in general to:

Dr. Thomas J. Wolery, L-219  
Lawrence Livermore National Laboratory  
P.O. Box 808  
Livermore, CA 94550

Telephone: (415) 422-5789      FTS 532-5789  
E-mail: wolery@s45.es.llnl.gov      FAX: (415) 422-1002  
Secretary: (415) 423-2970      FTS 534-2970

Address correspondence regarding the data files and their contents to:

Dr. James W. Johnson, L-219  
Lawrence Livermore National Laboratory  
P.O. Box 808  
Livermore, CA 94550

Telephone: (415) 423-7352      FTS 534-7352  
E-mail: johnson@s05.es.llnl.gov      FAX: (415) 422-1002  
Secretary: (415) 423-2970      FTS 534-2970

If you are a Yucca Mountain Project participant, please be aware that development and maintenance of the data files is scheduled to continue as part the the Yucca Mountain Project at Lawrence Livermore National Laboratory. At the present time, no development or maintenance activities for the EQ3/6 modeling codes are scheduled as part of this program. Thus, if you report a bug in the data files, you may be able to initiate QA-qualified action resulting in a fix. If you report a bug in the modeling codes, your report may be informally filed by Dr. Wolery for future reference, but no QA-qualified action can be taken.

In any correspondence, please be prepared to specify the exact version of the codes and data files that you have. In addition to the version identification of the package you are working with (3245.1090), you may be asked the "stage numbers" of individual source code files or data files. These are generally of the form "RXXX", where XXX is a one-to-three digit number, and terminate the root part of the file names (e.g., the "R124" in "eq3nrR124.fsc"). Some stage numbers may terminate with a literal "X", which indicates that post-release fixes have been made.

-----

end of the README.txt file