Civilian Radioactive Waste Management System

Management & Operating Contractor

CSCI: LLYMP9602100

QA: L

EQ3/6 Software Installation and Testing Report for Pentium Based Personal Computers (PCs)

Author: Harlan W. Stockman

Responsible Manager: Peter Gottlieb

Approvals:

Preparer: Harlan W. Stockman Date 6-30-98

Reviewed by: Paul L. Cloke Date 6/30/98

Responsible Manager: Peter Gottlieb Date 6/30/98

1. OBJECTIVE

In accordance with Section 5.5 of the Computer Software Qualification Procedure, QAP-SI-03, this report provides a plan and checklists for installation and testing of a transferred computer software package, when this software is used without modification by M&O organizations.

2. SCOPE

This installation report covers the installation procedure, testing strategy, and establishes criteria to ensure the proper installation of the EQ3/6 Geochemical Modeling software package on a Pentium-based personal computer. Installation of this software package on systems not defined in section 3.2 does not meet the requirements of this plan.

For clarity, DOS commands and filenames are indicated below with **`bold courier`** font.

3. INSTALLATION PROCEDURE

3.0 PROCESS OUTLINE

3.1 SOFTWARE PACKAGE

The EQ3/6 Software Package for Geochemical Modeling was developed by Thomas Wolery at Lawrence Livermore National Laboratory. The codes in the EQ3/6 software package are written in FORTRAN 77 and have been developed to run under the UNIX operating system. The software package can be ported to various platforms including PCs with Windows or DOS operating systems. However, LLNL's certification of this software, for use in quality-affecting work on the Yucca Mountain Project, excludes VAXes (running either ULTRIX or VMS) and Crays. Included with the software package are detailed instructions as to the proper installation of this package on various platforms. The installation procedure defined in this report is predominantly taken from the original install instructions contained with the software package (in files **`install.txt`**, **`contents.txt`**, **`readme.txt`**, **`format.txt`**), with additional steps necessary for system-specific requirements.

The source code files in the EQ3/6 distribution contain all the platform-dependent coding for all supported platforms. In the UNIX distribution package, the UNIX platform-dependent coding is

active, while all others are inactive. The platform-dependent coding in the other distribution packages (e.g. PCs) is handled in the same manner with only the desired coding being active while all other platform-dependent coding commented out.

The PC executables used by the M&O are compiled from either the UNIX or PC source, depending on availability of source code revisions from LLNL. Before the PC executables are produced, all code sections entitled UNIX_DEPENDENT_CODE are commented out, and the corresponding sections entitled PC_DEPENDENT_CODE are uncommented. To use EQ3/6 for complex models of waste form degradation, it is necessary to make minor changes to the source, and to recompile the source. These changes do not "affect the calculational structure or flow, data flow, and logic and mathematical algorithms", and therefore are not classed as modifications, per QAP-SI-0 rev 3, section 3.34. In the source code, all changes are identified by comment lines that include the initials plc (for Paul L. Cloke) or hws (for Harlan W. Stockman). The specific changes are:

In file **eqlib.for**, subroutine **initim**, the data statement for the number of days in each month was corrected; as supplied this statement showed 31 days in November and 30 for December.

Globally, in both the **eq6.for** and **eqlib.for** files, the dimensions were increased for four arrays. The dimensions are changed though parameter statements; specifically the following parameters were changed.

(1) The parameter **nstpar** (maximum number of aqueous species) was increased from 800 to 2000. This change also required a change in format statement 2030 of subroutine **echoz** in **eq6.for**, to permit proper printing of the changed array dimension.
(2) The parameter **nxmdpa** (maximum number of species/reactions that can be affected by the suppress/alter options) was increased from 20 to 60.
(3) The parameter **nrctpa** (maximum number of specified reactant species) was increased from 25 to 50.
(4) The parameter **nsrtpa** (maximum number of special reactant species) was increased from 5 to 10.

After these changes were made, the source code was recompiled and linked with version 1.10e (or later) of the Lahey LF90 compiler. The compilation followed the procedure recommended in **install.txt**, with the addition of the **-pack** switch during linking, to reduce the size of the executables.

In addition to these minor code changes, a new database has been added to the EQ3/6 distribution. This database is named **data1.nR8**, and is derived from the **data0.alt** file

provided by LLNL. However, the `data0.nR8` file (which corresponds to `data0.nuc.R8` in the Unix package) was emended to include rare earth aqueous and solid species, to facilitate the modeling of waste packages with gadolinium and other rare earth neutron poisons. To reduce the calculation time and the size of output files, many organic species have been removed from this database.

The various files in each software distribution package are primarily in compressed form, and need to be extracted prior to installation of the software. Contained within the distribution package, there is a file named `contents.txt`, which is a listing of all the files in the original LLNL distribution. The file `contents.txt` should be reviewed to ensure that all the files were included in the distribution package and uncompressed successfully.

3.2 SYSTEM REQUIREMENTS

The installation procedures as described in Section 3.3 are specific to personal computers (PCs) based on the Intel Pentium processor line. The PC, on which EQ3/6 is installed, must have at least a 340 MB (megabyte) hard disk and 16 or more MB of RAM. For purposes of this document, the term "Pentium" includes the "Pentium Pro" and "Pentium II" microprocessors. The PC executables will run on any 32-bit Intel x86-compatible CPU, including 386 PCs with math co-processors, and 486DX PCs, and PCs based on equivalent CPUs, provided the system contains a math coprocessor (internal or external). However, `EQ6` performance is likely to be inadequate on 386- and 486-based systems. In addition, the executables supplied in the distribution have been compiled with Pentium-specific optimizations, which may actually degrade performance on older CPUs. For these reasons, the installation procedure described in Section 3.3 is for Pentium based PCs using DOS- or Windows 95-based operating systems.

While the EQ3/6 Geochemical Software Package is portable to many UNIX and non-UNIX based platforms, installation procedures as outlined below are specific to the platform used by the M&O PA organization. Revision of this report may be necessary if this software package is to be installed on platforms not covered in this plan.

3.3 INSTALLATION PROCESS

This section describes the installation procedure for the EQ3/6 Geochemical Software Package on Pentium based PCs. This installation procedure needs to be documented with the associated checklist (Attachment I). This attachment will be filed for every CPU on which the software is installed.

3.3.1 Installation on Pentium PCs

The PC distribution package is about 5 MB in size in compressed form, and about 30 MB uncompressed. The PC distribution is supplied in five self-extracting files, labeled **disk1.exe** through **disk5.exe**; in the following discussion we will assume each of these files is on a separate 1.44 MB floppy disk. However, the five files may be supplied on another medium, such as an Iomega 100 MB zip disk

To copy the distribution package to the computer, first obtain a DOS prompt, either by opening a MS-DOS window (under Windows 95), or by rebooting the system to DOS mode. All the commands discussed below (and indicated by bold **courier** font) will be entered in the DOS window. Next set up a directory structure to contain the software. This structure will include an uppermost directory, placed in the root directory of the hard drive (**C:** or **D:**); and three sub-directories to contain the binary executables, the data1 files, and the source code. In the following discussion, the name **eq3_6v7.2b** will be used for the uppermost directory, and the names **bin**, **database**, and **import** will be used to indicate the sub-directories. However, the actual directory names may differ from these suggestions, as long as the correct names are listed in the installation report (attachment I).

Create the uppermost directory **eq3_6v7.2b** within the root directory of the chosen hard drive. Within this **eq3_6v7.2b**, create three directories. The first directory in **eq3_6v7.2b** will be called **import**. The second directory will be the EQ3/6 code directory called **bin**; this is where executable files will be kept. The third directory will be called **database**, and will be the location for the **DATA1** files that are read by **EQ3NR** and **EQ6**.

3.3.2 Setup Procedure

On a Pentium PC, enter the following two commands into the **AUTOEXEC.BAT** file (Step 2, Installation Checklist):

```
set EQ36CO=c:\eq3_6v7.2b\bin
set EQ36DA=c:\eq3_6v7.2b\database
```

Once again, we note that the actual directory names may differ, as long as the correct names are indicated in the installation and test sheet (attachment I).

Next add **\eq3_6v7.2b\bin** to the **PATH** statement in **AUTOEXEC.BAT** (Step 3, Installation Checklist). If the software will be installed on drive **D**, substitute "**D:**" for "**C:**". The system must be rebooted in order for these changes to take effect.

3.3.3 Installation Procedure

Copy the files from each floppy disk onto the hard drive. For purposes of discussion, we will assume that the **A:** drive is a 3.5-inch floppy drive (it could be the **B:** drive). First change to the **import** directory (e.g., **cd \eq3_6v7.2b\import**) on the hard drive. Place disk 1 in the **A:** drive and enter:

```
A:\DISK1.EXE
```

Then place disk 2 in the floppy drive and enter:

```
A:\DISK2.EXE
```

These commands execute the single file on each disk, extracting its contents into the current working directory on the hard drive. Next change to the code directory defined in the **EQ36CO** variable (e.g., **\eq3_6v7.2b\bin** in the following example). Use the commands

```
A:\DISK3.EXE
A:\DISK4.EXE
```

To copy the 3rd and 4th disks into the **\eq3_6v7.2b\bin** directory. (Step 5, Installation Checklist). This step will place the executable files and DATA1 files in the EQ3/6 code directory. For disk 5, change to the directory defined by the **EQ36DA** variable (e.g., **\eq3_6v7.2b\database** in the following example). Execute the command **A:\DISK5.EXE** (Step 6a, Installation Checklist). Then, move the DATA1 files from the **import** directory to the data file directory (**database**) by entering the following commands (Step 6b, Installation Checklist):

```
cd \eq3_6v7.2b\database
move ..\import\data*.* .
```

(note the last "period" above is part of the move command). Make sure that all of the ***.exe** files are in the **bin** directory; if not, move them there. Check the package contents against the list of files given in the file **CONTENTS.TXT**.

The installation steps are now complete. The Installation Checklist should be signed by the Installer and by a technically qualified Verifier. Section 3 describes the running of test cases supplied with the software to ensure and document the proper installation and operation of the software package on the Pentium-PC.

4. TESTING STRATEGY

4.1 Setup Procedure

A suite of input and output files for **EQ3NR** and **EQ6** is included in the distribution package and should now be in the **import** directory. Eight of these files will be used to verify proper installation of the software. First, create a directory in **eq3_6v7.2b** called **test** and enter with the following commands at the DOS prompt (Step 1, Test Case Checklist):

```
cd \eq3_6v7.2b
md test
cd test
```

To copy the **EQ3NR** input files in **import** into this directory, enter (Step 2, Test Case Checklist):

```
copy ..\import\*.3i
```

To copy the **EQ6** input files from the **import** directory to the **test** directory, enter (Step 3, Test Case Checklist):

```
copy ..\import\*.6i
```

4.2 Running the Test Cases

All the "**.3i**" input files, compatible with the "**com**" data file, can be run together by entering (from the **test** directory) (Step 4, Test Case Checklist):

```
runeq3 com *.3i
```

The input files that require a Pitzer database will not run with the **com** database; **runeq6** will identify and print these cases to the DOS screen. To run all the input files that use Pitzer's equations, enter (Step 5, Test Case Checklist):

```
runeq3 hmw *.3i
```

Note that **runeq3** renames files created by **eq3nr** after the input file. For example, in the case of the input file **swmaj.3i**, the output file will be named **swmaj.3o**, and the pickup file will be named **swmaj.3p**.

To run **EQ6**, simply enter a command of the form (Step 6 and Step 7, Test Case Checklist):

```
runeq6 com *.6i
```

then,

```
runeq6 hmw *.6i
```

Note that **runeq6** renames the files created by **EQ6** after the input file. In the case of the input file **micro.6i**, the output file is **micro.6o**, the pickup file is **micro.6p**, the tab file **is micro.6t**, and the tabx file is **micro.6tx**.

4.3 Testing Critera

The **import** directory contains sample **.3o** and **.6o** output files, from **EQ3NR** and **EQ6** runs performed by LLNL:

EQ3NR Sample Output Files

```
fo2mineq.3o
j13wa.3o
swmajp.3o
swtst.3o
```

EQ6 Sample Output Files

```
fwbrmix.6o
heatqf.6o
micro.6o
pptqtza.6o
```

Verify the correct installation by comparing these output files (in the **import** directory) with corresponding outputs obtained by running the input files in the **test** directory of the computer (Attachment II, Test Case Checklist, Steps 8 and 9a or 9b). For important geochemical quantities (such as the molar mineral amounts, or the molality of aqueous species), the results should agree to the first three to six significant figures. However, the results need not be identical to be considered satisfactory. Exact results may vary from platform to platform, and may vary on a single platform with changes in the compiler or the compiler switches.

These test runs must be documented and recorded according to the Checklist in attachment II.

4.3.1 Testing within a Revision

If the output files have the same revision numbers as the EQ3/6 executables (cf. Attachment II, Step 8), a simple file comparison is adequate to verify the installation, using the command "`FC`" in DOS or in an MSDOS window under Windows95. To compare the files, enter the `test` directory (e.g., `cd \eq3_6v7.2b\test`), then enter commands of the form:

```
fc \eq3_6v7.2b\import\filename.3o filename.3o > filename.txt
```

For example,

```
fc \eq3_6v7.2b\import\j13wa.3o j13wa.3o  > j13wa.txt
```

It is important to recognize that there may be minor differences between the `.3o` and `.6o` files supplied by LLNL (in the `eq3_6v7.2b\import` directory) and the `.3o` and `.6o` files created in the `test` directory. These differences can result from (e.g.) compiler upgrades, and slight differences in the library algorithms for transcendental functions.

If the simple `fc` method is used (attachment II, step 9a), the Test Case Checklist for that procedure will be signed by the Test Performer and by a technically qualified Reviewer.

It is up to the responsible manager to ensure that the test runs are compared and checked against the reference output files distributed with the software package.

4.3.2 Alternate Testing Criteria: Between Revisions

If the reference outputs in the `import` directory were created with a different revision than the executables, the `fc` method described in section 4.3.1 may not provide a useful installation test. Thus, an alternate installation test has been developed and is described in attachment II, step 9b.

The revisions are patches to the EQ3/6 source code and/or executables, provided by the LLNL custodians of the EQ3/6 package. Revisions are minor bug fixes, often to prevent the iteration step size from stalling at small value. For this very reason, different revisions can yield quite different convergence paths, and different step sizes, given the same input file (e.g. `micro.6i`). However, among different revisions, the final calculated aqueous species concentrations, and the mineral saturation states in the output files, should agree to the most significant 3 to 6 digits, even when the convergence paths are very different. Some of the revisions are made to fix bugs found by NRC contractors (e.g. the Southwest Research Institute in San Antonio), and it is generally a good idea to apply such revisions as they are made available, since the regulatory

agency expects us to use the most capable version of the code.

When a revision to EQ3/6 is received, the installation and test report must be performed on the new revision. However, revisions are generally not supplied with a new set of sample outputs, so one must compare against sample outputs created with a prior revision. When `fc` is used to compare files created with different revisions, many differences will be found for the affinities, `zvclgl` parameter (log master iteration variables), electrical imbalance, and step sizes calculated by EQ3/6 during convergence tests. When EQ3/6 reports the iteration progress (between data printouts), it reports only the `zvclgl` values that are changing most rapidly along the search path; therefore these values are inherently likely to vary between revisions, as different revisions will take different paths to minimize the residuals. It is important to realize this convergence information is principally provided for diagnostics purposes, should the program stall; the affinities and `zvclgl` are not quantities that are used for geochemical modeling of waste systems. Hence the comparison file created by `fc` will overemphasize unimportant differences in the convergence paths, and will make it extremely difficult for the reviewer to determine how the important quantities compare (quantities such as aqueous species concentrations, saturation states, and mineral amounts).

Because of the weaknesses of the `fc` approach, an alternate installation testing procedure is provided in attachment II (step 9b). If the alternative installation test is chosen, the Test Case Checklist for that procedure will be signed by the Test Performer and by a technically qualified Reviewer.

It is up to the responsible manager to ensure that the test runs are compared and checked against the reference output files distributed with the software package.

5. REFERENCES

5.1 Wolery, T.J., *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems: Package Overview and Installation Guide (Version 7.0) Spetember 14, 1992.* Lawrence Livermore National Laboratory.

5.2 QAP-SI-0 *Computer Software Qualification*, Rev. 3, December 8, 1997.

5.3 QAP-SI-03 *Software Configuration Management*, Rev. 2, December 8, 1997.

6. ATTACHMENTS

Attachment I: **Pentium-PC Installation Checklist**
Attachment II: **Pentium-PC Test Case Checklist**

Attachment I: Installation Checklist

EQ3/6 Geochemical Modeling Software Code
Pentium PC Installation Checklist for CPU# _____
Date _____

Directory names
Enter below the actual directory names used for this installation. As noted in section 3.3.1, the actual directory names need not match those in the examples.

Uppermost EQ3/6 directory name (default is **eq3_6v7.2b**) : _____

For executables: (default is **eq3_6v7.2b\bin**): _____

For databases: (default is **eq3_6v7.2b\database**): _____

For source: (default is **eq3_6v7.2b\import**): _____

For testing: (default is **eq3_6v7.2b\test**): _____

Listed below are the steps required for the installation of the EQ3/6 distribution on a Pentium PC in accordance with the EQ3/6 Installation Plan, Document # CSCI: LLYMP0902100

Operation	GO	NOGO

A. Set-Up Procedures

1. **Create** EQ3/6 directories on either `C:` or `D:` Drive:

```
cd\                                    ____  ____
md eq3_6v7.2b                          ____  ____
cd eq3_6v7.2b                          ____  ____
md import                              ____  ____
md bin                                 ____  ____
md database                            ____  ____
```

2. **Create** the following commands by editing the **`AUTOEXEC.BAT`**:

```
set EQ36CO=c:\eq3_6v7.2b\bin           ____  ____
set EQ36DA=c:\eq3_6v7.2b\database      ____  ____
```

3. **Add** the binary file directory, to the search path; e.g. add the following statement, then reboot the system to make changes take effect:

```
\eq3_6v7.2b\bin                        ____  ____
```

Note: on some networked systems, the path statement may be implicit, and it may be necessary to add a statement of the form:

```
PATH= \eq3_6v7.2b\bin;%path%
```

This statement adds to an existing path.

4. **Install** Disk 1 & Disk 2 by entering: (from the **`import`** directory)

```
A:\DISK1.EXE                           ____  ____
A:\DISK2.EXE                           ____  ____
```

5. **Install** Disk 3 & Disk 4 by entering: (from the **`bin`** directory)

```
A:\DISK3.EXE                                    ____  ____
A:\DISK4.EXE                                    ____  ____
```

6. a) **Install** Disk 5 by entering: (from the **database** directory)

```
A:\DISK5.EXE                                    ____  ____
```

b) **Move** **DATA1** from **import** directory to the data files directory **database** by entering: (from the **import** directory)

```
move data*.* \eq3_6v7.2b\database               ____  ____
```

7. **Make sure** all the ***.exe** files are in the **bin** directory, if not move them from the **import** directory to the **bin** directory by entering the following: (from the **import** directory)

```
move *.exe \eq3_6v7.2b\bin                      ____  ____
```

NOTE: For a successful installation test all test points must receive a "GO". Any "NO GO" steps shall be rerun successfully, with a test discrepancy report completed, indicating the failure description, reason and corrective action.

Installer _____ Date _____

Attachment II: Test Case Checklist

EQ3/6 Geochemical Modeling Software Code Package Pentium PC Test Case Checklist CPU#_____ Date_____

A suite of input and output files for **EQ3NR** and **EQ6** is included in the distribution package and should now be in the **import** directory. Eight of these files will be used to verify proper installation of the software.

GO NOGO

1. Create a directory in **eq3_6v7.2b** called **test** and enter it by entering:

```
cd \eq3_6v7.2b
md test
cd test
```

___ ___

2. Copy the **EQ3NR** input files in **import** into the **test** directory; enter:

```
copy ..\import\*.3i
```

___ ___

3. Copy the **EQ6** input files in **import** into the **test** directory; enter:

```
copy ..\import\*.6i
```

___ ___

4. Run all of the "**.3i**" input files compatible with the "**com**" data file by entering:

```
runeq3 com *.3i
```

___ ___

5. Run all of the "**.3i**" input files compatible with the "**hmw**" data file by entering:

```
runeq3 hmw *.3i
```

___ ___

Note that **runeq3** creates several files with the same root name as the input files. For example, in the case of the input file **swmaj.3i**, **runeq3** creates an output file named **swmaj.3o**, and a pickup file named **swmaj.3p**.

6. Run all of the "**.6i**" input files compatible with the "**com**" data file by entering:

```
runeq6 com *.6i
```

7. **Run** all of the "`.6i`" input files compatible with the "`hmw`" data file by entering:

```
runeq6 hmw *.6i
```

Note that `runeq6` renames the files, created by `eq6`, based on the input file name. In the case of the input file `micro.6i`, the output file is `micro.6o`, the pickup file is `micro.6p`, the tab file is `micro.6t`, and the tabx file is `micro.6tx`.

8. **Obtain and write down the revision numbers** for `EQ6`, `EQ3NR`, and `EQLIB`, for both the LLNL "`.6o`" and "`.3o`" distribution (in the `import` directory) and the "`.6o`" and "`.3o`" files generated in the `test` directory. The revision numbers will be found in text lines at the top of the output files; the lines will resemble (example for `.6o`):

```
EQ6 Reaction-Path Code (EQ3/6-V7-EQ6-EXE-R136-P5)
Supported by the EQLIB library (EQ3/6-V7-EQLIB-LIB-R168-P5)
```

In this case, `R136-P5` is the revision number for `EQ6`, and `R168-P5` is the revision number for `EQLIB`. To find the revision numbers for `EQ3NR`, examine the `.3o` files.

Write the revision numbers for the installation below:

	LLNL-supplied files in `import` directory:	Files generated in `test` directory:
`EQ6:`	_____	_____
`EQ3NR:`	_____	_____
`EQLIB:`	_____	_____

If all the revision numbers match between the left and right columns above, use procedure 9a to verify correct installation. If any of the revision numbers do not match between the left and right columns above, the installation can be verified by choosing either one of procedures 9a or 9b below.

The verification procedure used in this installation is (choose either 9a or 9b): _____

9a. **Use the DOS `fc` command** to compare the output files (created in the `test` directory via step7), with the reference output files from the distribution package (in the `import` directory).

The **import** and **test** directories should each contain the following files:

EQ3NR Sample Output Files		EQ6 Sample Output Files	
fo2mineq.3o	___	fwbrmix.6o	___
j13wa.3o	___	heatqf.6o	___
swmajp.3o	___	micro.6o	___
swtst.3o	___	pptqtza.6o	___

To compare the files, first enter the **test** directory, then use the DOS **fc** command as in the example below (example for **j13wa.3o**):

```
fc \eq3_6v7.2b\import\j13wa.3o j13wa.3o  > j13wa.txt
```

Repeat this process for each of the reference output files listed above.

Note: The results should be very close (to the first three to six significant figures), but need not be identical to be considered satisfactory. Exact results may vary from platform to platform, and may vary on a single platform with changes in compiler options or change of compiler or version of compiler. Each reference file listed above should be checked off to indicate successful results. It is up to the responsible manager to ensure that the test runs are compared and checked against the reference output files distributed with the software package. Skip step 9b and go directly to the signature block in step 10.

9b. Use an Excel spreadsheet to verify the correct installation by comparing the output files (created in the **test** directory via step 7), with the reference output files from the distribution package (in the **import** directory). The **import** and **test** directories should each contain the following files:

EQ3NR Sample Output Files		EQ6 Sample Output Files	
fo2mineq.3o	___	fwbrmix.6o	___
j13wa.3o	___	heatqf.6o	___
swmajp.3o	___	micro.6o	___
swtst.3o	___	pptqtza.6o	___

Eight of the test files in the **test** and **import** directories must now be compared. In overview,

the process is as follows. Find the last "species molality" and "summary of pure mineral saturation states" blocks in each file; extract and save these blocks as **ascii** text files, with names: **name_import_QK.txt** and **name_import_Mol.txt** for files in the **import** directory, and **name_test_QK.txt** and **name_test_Mol.txt** for files in the **test** directory, where **name** represents the corresponding output filename, before the extension (e.g., **j13wa** or **micro** above). Note that "Q/K" is a common notation for the saturation state.

Check off to verify that each file was created:

fo2mineq_import_Mol.txt	___	fwbrmix_import_Mol.txt	___
j13wa_import_Mol.txt	___	heatqf_import_Mol.txt	___
swmajp_import_Mol.txt	___	micro_import_Mol.txt	___
swtst_import_Mol.txt	___	pptqtza_import_Mol.txt	___
fo2mineq_import_QK.txt	___	fwbrmix_import_QK.txt	___
j13wa_import_QK.txt	___	heatqf_import_QK.txt	___
swmajp_import_QK.txt	___	micro_import_QK.txt	___
swtst_import_QK.txt	___	pptqtza_import_QK.txt	___
fo2mineq_test_Mol.txt	___	fwbrmix_test_Mol.txt	___
j13wa_test_Mol.txt	___	heatqf_test_Mol.txt	___
swmajp_test_Mol.txt	___	micro_test_Mol.txt	___
swtst_test_Mol.txt	___	pptqtza_test_Mol.txt	___
fo2mineq_test_QK.txt	___	fwbrmix_test_QK.txt	___
j13wa_test_QK.txt	___	heatqf_test_QK.txt	___
swmajp_test_QK.txt	___	micro_test_QK.txt	___
swtst_test_QK.txt	___	pptqtza_test_QK.txt	___

Next, create a blank Excel workbook named **name_comp.xls**. Within this workbook, create 5 sheets, named **import_Mol**, **import_QK**, **test_Mol**, **test_QK**, and **compare**.

Now select the **import_Mol** sheet, and open the **name_import_Mol.txt** file, as "fixed width" columns, in this sheet. Then select the **test_Mol** sheet, and open the **name_test_Mol.txt** file in this sheet, again as "fixed width" columns. Then select the **import_QK** sheet, and open the **name_import_QK.txt** file, as "fixed width" columns, in this sheet. Then select the **test_QK** sheet, and open the **name_test_QK.txt** file in this sheet, again as "fixed width" columns.

Next, select the **compare** sheet. In the **A1** cell, type "Mol. Frac. Err", and in the **B1** cell, type "QK Frac. Err." In cell **A2**, type the following formula, either manually or by pointing and clicking the appropriate sheets:

```
=('import_Mol'!B1 - 'test_Mol'!B1)*2/('import_Mol'!B1 + 'test_Mol'!B1).
```

Similarly, in the **B2** cell of **compare**, type the formula:

```
=('import_QK'!B1 - 'test_QK'!B1)*2/('import_QK'!B1 + 'test_QK'!B1),
```

then copy these formulae throughout the **A** and **B** columns, and format the columns to show 5 digits of precision. These formulae calculate the fractional difference between the **test** and **import** values for the final aqueous species molalities, and the final saturation states. The absolute values of the differences should be less than 0.001. Note that when both the test and import values for a parameter are identically zero, the result will be undefined, and Excel will report "#DIV/0!" for that cell.

Check below that each file was created, and that the values in the **A** and **B** columns of the **compare** sheet all have absolute values < 0.001:

fo2mineq_comp.xls	___	fwbrmix_comp.xls	___
j13wa_comp.xls	___	heatqf_comp.xls	___
swmajp_comp.xls	___	micro_comp.xls	___
swtst_comp.xls	___	pptqtza_comp.xls	___

10. Sign below that the verification test has been completed.

Test Performer _____ Date _____