Software Release Notice
Acquired Software

1. Software Name: PHREEQCI Software Version: Version 2.15.0
   Project Number: 20.14002.01.357/359

2. Software Function: A computer program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations

3. Summary of Actions:
❑ New Software ✗ Update to Existing Software ❑ Software Retirement

4. Software Installation

4a. Computer Platform(s): PC/100 mHz or faster
4b. Operating System(s): Windows 95, 98, NT4.0,m ME, 2000, or XP
4c. Programming Language(s): ANSI C

4d. Installation Testing:
✗ Passed Performed by: D. Turner Testing Performed On: PC-Windows XP

Description of Testing Performed: Performed using the 18 installation tests that are described in the Software Validation Report for PHREEQC, Version 2.6 (2003)

4e. Archive Copy:
✗ Enclosed ❑ Not Available, Why:

Installation Performed by: J. Perkins/D. Turner	Date: 11/20/2008

Remarks: None

5. Software Assessment

Validation Status:
❑ Full Validation ✗ Limited Validation Date of Validation: 12/11/2008
❑ Not Validated, Explain:
[NOTE: See attached sheet for short summary of validation using SVTP for PHREEQC, Version 2.6 (February 2003)]

Software User: F.P. Bertetti, M. Juckett, J. McMurry, J. Myers, D. Turner	Date: 12/11/2008

Remarks:

6. Approval

Manager: D. C. Sevougian	Date: 12/11/2008

Remarks:

7. QA Verification

SRN Number: 457

Verified by: RO Grant	Date: 12/11/08

Remarks:

PHREEQCI, Version 2.15 Attachment

11 December 2008

Description of Acceptance Tests/Testers/Dates:

Repeated installation and validation tests from PHREEQC, v. 2.6 validation (February 2003 by D. Turner) using PHREEQCI, v. 2.15. In addition, the results were compared to the most recent validation of PHREEQCI, v. 2.12.5 (February 2006 by L. Sabido). Output files compared for discrepancies. Files with no unexplainable discrepancies considered successful tests. The comparison files for old and new results are contained in the attached CD.

Version 2.6 to Version 2.12.5

L. Sabido previously evaluated changes from PHREEQC, Version 2.6 to PHREEQCI, Version 2.12.5 in February 2006. She noted several types of acceptable discrepancies:

1) Changes in Ion Activity Product (IAP) and Log KT values. These values have changed in some cases, but the Saturation Index (SI) remains the same (e.g., ex1_out_compare.doc). The difference result from code changes fixed with Version 2.12.5: Saturation index phases that included water had wrong value if distribution of species, exchange, or surface not written also. Changed SI print out to use reaction and log K defined in PHASES definition. Previously, reaction could be rewritten to predominant redox species.

2) Small, yet insignificant changes in value as a result of rounding differences, e.g. 5.907 changed to 5.898. Some files contained differences of this type, possibly a result of different operating system. A multiple precision version of routine cl1, cl1mp, was included in version 2.12.5 for inverse modeling, with calculations carried out to about 30 significant digits, with associated rounding. (For example, see np_phrq2_new_2.6dat_compare.doc)

3) Changes in format such as spaces, tabs, minor text differences, etc. that do not affect the final output are considered insignificant. (Stumm96_new_out_compare.doc)

4) Changes in values such as iteration numbers, electrical balances, etc. that do not affect the final output are considered insignificant. (seawater_new_out_compare.doc)

Version 2.12.5 to Version 2.15

Comparison of PHREEQCI, Version 2.15 with the validation tests for PHREEQCI, Version 2.12.5 show no significant differences (see attached files). Note that according to the file RELEASE.2697.TXT (dated 5Feb2008, attached), most of the updates and revisions in going from Version 2.12.5 to 2.15 focus on implementing the multi-site sorption model (CD MUSIC), the PITZER activity formulation, diffusion, writing files from PHREEQCI to NETPATH, identifiers related to the KINETICS data block.