SOFTWARE RELEASE NOTICE

1. SRN Number: 263

2. Project Title: Radionuclide Transport Key Technical Issue	Project No. 20.01402.871
3. SRN Title: PHREEQC, Version 2.4.2	
4. Originator/Requestor: David R. Turner	Date: 02/22/2002

5. Summary of Actions

X Release of new software ☐ Change of access software

☐ Release of modified software: ☐ Software Retirement

☐ Enhancements made

☐ Corrections made

6. Validation Status

☐ Validated

☐ Limited Validation

X Not Validated Explain: Scheduled for Validation in FY2003

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
David R. Turner	Read-Write	
F. Paul Bertetti	Read-Write	

8. Element Manager Approval: Date: 2/25/2002

9. Remarks:

NOTE: This acquired code was developed by the U.S. Geological Survey and supersedes/replaces PHREEQC, Version 1.6 currently under configuration management.

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 02/22/2002	02. Summary prepared by (Name and phone) David R. Turner (CNWRA): (201) 522-2139	03. Summary Action: REPLACEMENT (Replaces PHREEQC, Version 1.6)
04. Software Date: 06/2000	05. Short Title: PHREEQC, Version 2.4.2	
06. Software Title: PHREEQC, Version 4.02: A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System X Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch X Combination	10. Application Area a. General: X Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Acquired Geochemical Equilibrium Speciation Code. Developed by U.S. Geological Survey
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: David R. Turner (210) 522-2139

13. Software Application: PHREEQC, Version 2.4.2 is a DOS-based geochemical equilibrium speciation model for dilute aqueous species. Input uses keyword blocks to describe the geochemical system of interest. PHREEQC, Version 2.4.2 uses a thermodynamic database with that contains chemical reactions, equilibrium constants, and enthalpies of reaction to solve mass action and mass balance constraints in geochemical systems. The code is used to investigate geochemical processes such as aqueous speciation, precipitation/dissolution, gas partial pressures, redox behavior, sorption, ion exchange, and one-dimensional reactive transport.

14. Computer Platform PC/Pentium running at 100 Mhz or faster	15. Computer Operating System: Windows 9x/Me, Windows NT 4.0, or Windows 2000	16. Programming Language(s): ANSI C++	17. Number of Source Program Statements: Unknown
18. Computer Memory Requirements: 8 Mb RAM; 20 Mb free disk space	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements

23. Software Availability: X Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: X Available ☐ Preliminary ☐ In-House ONLY

25. Acquired Code developed by U.S. Geological Survey

Software Developer: David R. Turner Date: 02/22/2002

CNWRA Form TOP-4-1 (05/98)

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: PHREEQC
Version: 2.4.2
Demonstration workstation: Pentium II, Room A218
Operating System: Windows 9x/Me, Windows NT 4.0 or Windows 2000
User: David R. Turner

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system?
Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: IBM Workstation, Pentium II Room A218 Operating Systems: Windows NT 4.0

Location of Acceptance Test Results: QA Records Room

Comments:. Installation testing completed for IBM Workstation, Windows NT 4.0

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version?
Yes: ☐ No: ☑ N/A: ☐

Date and Time Displayed: None
Name/Version Displayed: None
Comments: Data base used is identified in the calculation. Data base is also identified in the input and output files.
NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?
Yes: ☑ No: ☐ N/A: ☐

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ACQUIRED SOFTWARE NOT TO BE MODIFIED←

User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date? Yes: ☑ No: ☐ N/A: ☐
300 plus page users manual is contained on the CD.

User's Manual Version and Date: 2.0 Dated 1999

Comments: CD also contains updated "readme" files.

Are there basic instructions for the *installation* and *use* of the software? Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: Users Manual

Comments: Located in a readme file.

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed? Yes: ☑ No: ☐ N/A: ☐

Date of Approval: 2/22/2002

Is the list of files attached to the Software Summary Form complete and accurate? Yes: ☑ No: ☐ N/A: ☐

Comments:

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)? Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: Located on the C.D.

Comments:

Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted. Yes: ☑ No: ☐ N/A: ☐

Location of executable files: QA Records Room

Comments:

(04/01)

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: 263

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTP: N/A

Date Reviewed and Approved via QAP-002: N/A

Comments: To be validated in FY-2003

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTR: ____

Date Reviewed and Approved via QAP-002: ____

Comments.: See above

Additional Comments:

David R. Wynn 03/07/2002
Software Evaluator/User/Date

Bruce Mabrito 3/7/2002
~~David R. Wynn 03/07/2002~~
Software Custodian/Date

```
Directory PATH listing for volume
020222_1732
Volume serial number is 00[illegible]C94
FDBE:A2D9
F:\
+---PHREEQC_Configuration
    |   phreeqc.bat
    |
    +---doc
    |       manual.pdf
    |       Notice.txt
    |       Phreeqc.txt
    |       README.TXT
    |       RELEASE.TXT
    |       USGS_website.txt
    |
    +---Download_File
    |       phrqc242.exe
    |
    +---examples_as_received
    |       ex1
    |       ex1.out
    |       ex10
    |       ex10.out
    |       ex10.sel
    |       ex11
    |       ex11.out
    |       ex11adv.sel
    |       ex11trn.sel
    |       ex12
    |       ex12.out
    |       ex12.sel
    |       ex13a
    |       ex13a.out
    |       ex13a.sel
    |       ex13b
    |       ex13b.out
    |       ex13b.sel
    |       ex13c
    |       ex13c.out
    |       ex13c.sel
    |       ex14
    |       ex14.out
    |       ex14.sel
    |       ex15
    |       ex15.dat
    |       ex15.out
    |       ex15.sel
    |       ex16
    |       ex16.out
    |       ex17
    |       ex17.out
    |       ex18
    |       ex18.out
    |       ex2
    |       ex2.out
    |       ex2.sel
    |       ex3
    |       ex3.out
    |       ex4
    |       ex4.out
    |       ex5
    |       ex5.out
    |       ex5.sel
    |       ex6
    |       ex6.out
    |       ex6A-B.sel
    |       ex6C.sel
    |       ex7
    |       ex7.out
    |       ex7.sel
    |       ex8
    |       ex8.out
    |       ex8.sel
    |       ex9
    |       ex9.out
    |       ex9.sel
    |
    +---Installation_test
    |       check.bat
    |       check.log
    |       clean.bat
    |       ex1.out
    |       ex10.out
    |       ex10.sel
    |       ex11[illegible]t
    |       ex11[illegible].sel
    |       ex11trn.sel
    |       ex12.out
    |       ex12.sel
    |       ex13a.out
    |       ex13a.sel
    |       ex13b.out
    |       ex13b.sel
    |       ex13c.out
    |       ex13c.sel
    |       ex14.out
    |       ex14.sel
    |       ex15.out
    |       ex15.sel
    |       ex16.out
    |       ex17.out
    |       ex18.out
    |       ex2.out
    |       ex2.sel
    |       ex3.out
    |       ex4.out
    |       ex5.out
    |       ex5.sel
    |       ex6.out
    |       ex6A-B.sel
    |       ex6C.sel
    |       ex7.out
    |       ex7.sel
    |       ex8.out
    |       ex8.sel
    |       ex9.out
    |       ex9.sel
    |       phreeqc.log
    |       test.bat
    |
    +---src
    |   |   advection.c
    |   |   basic.c
    |   |   cl1.c
    |   |   global.h
    |   |   integrate.c
    |   |   inverse.c
    |   |   kinetics.c
    |   |   main.c
    |   |   mainsubs.c
    |   |   Makefile
    |   |   model.c
    |   |   p2c.h
    |   |   p2clib.c
    |   |   parse.c
    |   |   phqalloc.c
    |   |   phqalloc.h
    |   |   phreeqc.rev
    |   |   prep.c
    |   |   print.c
    |   |   read.c
    |   |   readtr.c
    |   |   spread.c
    |   |   step.c
    |   |   structures.c
    |   |   phqalloc.h
    |   |   phreeqc.rev
    |   |   prep.c
    |   |   print.c
    |   |   read.c
    |   |   readtr.c
    |   |   spread.c
    |   |   step.c
    |   |   structures.c
    |   |   tidy.c
    |   |   transport.c
    |   |   utilities.c
    |   |
    |   +---Release
    |           phreeqc.exe
    |
    +---ThermoData
            llnl.dat
            minteq.dat
            phreeqc.dat
            wateq4f.dat
```

CONFIGURATION MANAGEMENT: PHREEQC, Version 2.4.2

Prepared by

David R. Turner

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

1 TECHNICAL DESCRIPTION OF PHREEQC, Version 2.4.2

PHREEQC, Version 2.4.2 (June 2001 release) is an acquired geochemical speciation code, originally developed by the U.S. Geological Survey (USGS). The software is used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) to provide technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program. An earlier version, PHREEQC, Version 1.6 is currently under configuration control in accordance with Technical Operating Procedure (TOP) 018.

PHREEQC, Version 2.4.2 (released June 2001) is a geochemical equilibrium speciation code developed in ANSI C++ by the USGS to model dilute aqueous systems. The code as received was compiled using Microsoft Visual C++ 6.0. The code is PC-compatible, and is run in batch mode in the DOS-operating system. Since the original development, PHREEQC has become one of the more common codes used to simulate geochemical equilibria.

As described on the USGS website (http://water.usgs.gov/cgi-bin/man_wrdapp?phreeqc) PHREEQC, Version 2.4.2 is:

"designed to perform a wide variety of low-temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modeling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits."

1.1 Code Description

The documentation provided with the self-extracting PHREEQC, Version 2.4.2 file (downloaded from the U.S. Geological Survey website at http://water.usgs.gov/software/phreeqc.html) includes a user's manual that describes the features and their implementation of the code (Parkhurst and Appelo, 1999) in the PHREEQC geochemical speciation codes. Electronic and hard copies of these documents are included in this configuration control package for PHREEQC, Version 2.4.2. In addition, the download from the EPA website includes ASCII files that describe the installation and system requirements of the code (README.TXT) and provide a listing of specific updates to the PHREEQC, Version 2.4.2 code (RELEASE.TXT). A hard copy of README.TXT is included in Appendix A. Hard copy of RELEASE.TXT is included in Appendix B.

The entire self-extracting compressed download file as is included in this configuration management file.

1.1.1 Input

A PHREEQC, Version 2.4.2 user typically has a problem relevant to a natural chemical system. This system is described in terms of the physical conditions such as temperature, and the

concentrations of chemical components, species, solids and gases that are present. PHREEQC uses a free-format input file divided into keyword data blocks to identify the components of interest, read the concentrations, construct the chemical equilibrium model and solve for aqueous speciation and the distribution of species between the solid, gas, and liquid phases. Input flags can be set to determine the level of output. For speciation modeling, analytical data for a solution composition (SOLUTION keyword) are needed. For batch-reaction modeling, the initial solution composition is required (SOLUTION or MIX data block). Other equilibrium reactants may be defined with EQUILIBRIUM_PHASES, EXCHANGE, SURFACE, GAS_PHASE, and SOLID_SOLUTION data blocks. Nonequilibrium reactions may be defined with KINETICS and RATES, REACTION, and REACTION_TEMPERATURE data blocks. Input files are constructed by the user an ASCII text editor. During execution of a geochemical problem, the input file is read and the databases searched for the relevant component species and aqueous, gas, solid phases.

For 1D transport modeling, the modeled system requires the information necessary to establish the geochemistry in each cell. There is also physical information needed for each cell to describe the cell dimensions, time steps, and the boundary conditions used in the 1D model. For inverse modeling, the solution composition of the final solution and one or more initial solutions are needed (SOLUTION data block). Uncertainty limits can be defined explicitly or by default for each element and element redox state in the solutions.

Thermodynamic data are contained in a separate database that includes definition of aqueous species, exchange species, surface species, and mineral and phases for a set of elements. Additional elements, species, or phases can be added to the database if information on chemical reactions, log K, and data for the temperature dependence of log K are available for each added species and/or phase

1.1.2 Output

The results from the equilibrium geochemical speciation calculation are written to an output file specified by the user. PHREEQC, Version 2.4.2 will overwrite previously existing files with the same name. The output includes an echo of the input to verify that the input file was read correctly. PHREEQC, Version 2.4.2 does not provide a time stamp in the output file to verify the time of the run. The level of output varies and is set by the user in the input files. The equilibrium concentration of the element(s) of interest are reported in molality (moles aqueous component or species/kg H_2O) as distributed between the dissolved, sorbed, and precipitated phases.

1.2 Hardware/Software Requirements and Installation

PHREEQC, Version 2.4.2 is designed for IBM PC-compatible systems. For installation, 10 megabytes of free disk space is needed. Run requirements for PHREEQC, Version 2.4.2 include:

- Windows 9x/Me, Windows NT 4.0, or Windows 2000
- processor running at 100 megahertz or faster
- 8 megabytes RAM
- 20 megabytes free disk space

PHREEQC, Version 2.4.2 is installed by executing the self-extracting download file PHRQC242.EXE. The installation program included with the download file can optionally modify the PATH environment variable so that the PHREEQC program can be executed from any directory, without needing to type the full pathname of the program's location.

By default, the software is installed in the directory C:\Program Files\USGS\phreeqc2.4.2, but the author can specify an alternate directory. Using a customized installation option, the user can select only certain parts for the initial installation, but program components not installed initially can be installed later. The file PHRQC242.EXE also has a maintenance version of the installation program to reinstall any damaged or overwritten program files.

During installation, PHREEQC, Version 2.4.2 will create a directory structure:

phreeqc2.4.2	files NOTICE.TXT, RELEASE.TXT, and this README.TXT; a batch file to run PHREEQC, database files
'-----doc	documentation files
'-----examples	examples from user's guide--used in verification tests
'-----src	Makefile and source code
'-----release	compiled executable
'-----test	batch files to run verification tests

2 INSTALLATION CHECKS

The PHREEQC, Version 2.4.2 software has been checked to ensure that it was installed correctly on the CNWRA PC platform (Pentium-based PC, Windows NT 4.00 operating system). Part of self-extracting installation package for PHREEQC, Version 2.4.2 includes input and output for a set of 18 example problems developed to demonstrate the different capabilities of PHREEQC, Version 2.4.2. The test problems are described in the user's manual (Parkhurst and Appelo, 1999). To test the installation, in an MS-DOS Command Prompt window, the user changes to the phreeqc2.4.2\test directory:

```
c:
cd "program files"
cd usgs\phreeqc2.4.2\test
```

Execute the tests by typing the command:

```
test [start [stop]]
```

where: start = the number of the first test to perform, default = 1
stop = the number of the last test to perform, default = 18

After the tests are completed, the results are compared to the expected results included in PHREEQC examples directory. The file check.log is created to contain the comparison results. If the installation check matches the example files, there should be no differences.

The input files for these example problems were submitted in batch mode to PHREEQC, Version 2.4.2 as installed, and the output compared against the files provided in the installation package. Comparison results are included in the file check.log. **As installed, PHREEQC,**

Version 2.4.2 produced results identical to those provided by the code developers. Electronic versions of these installation checks are provided in this configuration management package.

3 CONTENTS OF THIS CONFIGURATION MANAGEMENT PACKAGE

This configuration management includes the following information

Self-extracting download file (PHRQC242.EXE) from the USGS website at http://water.usgs.gov/software/phreeqc.html (Electronic)

User's Manual for PHREEQC, Version 2.0 (Parkhurst and Appelo, 1999) (electronic copy in Acrobat Reader Portable Document Format (*.pdf)). Subsequent modifications are included in the ASCII file RELEASE.TXT included in Appendix B.

Software Summary Form TOP-4-1

Software Release Notice Form TOP-6

Installation check using 18 test problems with output as received, and output after installation on CNWRA PC platform (Electronic ASCII files)

Original databases as received (Electronic ASCII files)

Source code for PHREEQC, Version 2.4.2 (Electronic ASCII files)

4 REFERENCES

The following documents are referenced or used in this configuration package for PHREEQC, Version 2.4.2. Electronic copies of these documents are included in this configuration control package.

Parkhurst, D.L., and Appelo, C.A.J., 1999, User's guide to PHREEQC (Version 2)--a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Water-Resources Investigations Report 99-4259, 312 p.

SOFTWARE SUMMARY FORM

01. Summary Date: 02/22/2002	02. Summary prepared by (Name and phone) David R. Turner (CNWRA): (201) 522-2139	03. Summary Action: REPLACEMENT (Replaces PHREEQC, Version 1.6)
04. Software Date: 06/2000	05. Short Title: PHREEQC, Version 2.4.2	
06. Software Title: PHREEQC, Version 4.02: A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System X Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch X Combination	10. Application Area a. General: X Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Acquired Geochemical Equilibrium Speciation Code. Developed by U.S. Geological Survey
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: David R. Turner (210) 522-2139

13. Software Application: PHREEQC, Version 2.4.2 is a DOS-based geochemical equilibrium speciation model for dilute aqueous species. Input uses keyword blocks to describe the geochemical system of interest. PHREEQC, Version 2.4.2 uses a thermodynamic database with that contains chemical reactions, equilibrium constants, and enthalpies of reaction to solve mass action and mass balance constraints in geochemical systems. The code is used to investigate geochemical processes such as aqueous speciation, precipitation/dissolution, gas partial pressures, redox behavior, sorption, ion exchange, and one-dimensional reactive transport.

14. Computer Platform PC/Pentium running at 100 Mhz or faster	15. Computer Operating System: Windows 9x/Me, Windows NT 4.0, or Windows 2000	16. Programming Language(s): ANSI C++	17. Number of Source Program Statements: Unknown
18. Computer Memory Requirements: 8 Mb RAM; 20 Mb free disk space	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements

23. Software Availability: X Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: X Available ☐ Preliminary ☐ In-House ONLY

25. Acquired Code developed by U.S. Geological Survey

Software Developer: _____ Date: _____

CNWRA Form TOP-4-1 (05/98)

SOFTWARE RELEASE NOTICE

1. SRN Number:	
2. Project Title: Radionuclide Transport Key Technical Issue	Project No. 20.01402.871
3. SRN Title: PHREEQC, Version 2.4.2	
4. Originator/Requestor: David R. Turner	Date: 02/22/2002

5. Summary of Actions

X Release of new software ☐ Change of access software

☐ Release of modified software: ☐ Software Retirement

☐ Enhancements made

☐ Corrections made

6. Validation Status

☐ Validated

☐ Limited Validation

X Not Validated Explain: Scheduled for Validation in FY2003

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
David R. Turner F. Paul Bertetti	Read-Write Read-Write	

8. Element Manager Approval: Date:

9. Remarks:

NOTE: This acquired code was developed by the U.S. Geological Survey and supersedes/replaces PHREEQC, Version 1.6 currently under configuration management.

CNWRA Form TOP-6 (09/01)

APPENDIX A

PHREEQC

A program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations

PHREEQC - Version 2.4.2 2001/06/15

Instructions for installation, execution, and testing are provided below. After installation, see the file doc\phreeqc.txt in the PHREEQC installation directory for summary information on PHREEQC.

For assistance, enhancement requests, or to report bugs, contact the Hydrologic Analysis Software Support Program by sending e-mail to h2osoft@usgs.gov.

For all versions of Microsoft Windows, this Windows console version of PHREEQC must be run using an MS-DOS Command Prompt window.

TABLE OF CONTENTS

A. SYSTEM REQUIREMENTS
B. DISTRIBUTION FILE
C. DOCUMENTATION
D. INSTALLING
  o Installing PHREEQC
  o PHREEQC directory structure
E. COMPILING
F. RUNNING THE SOFTWARE
  o Out of environment space error
G. TESTING
H. CONTACTS

A. SYSTEM REQUIREMENTS

For installation of PHREEQC, 10 megabytes of free disk space is needed.

To run PHREEQC, the following are necessary:

- Windows 9x/Me, Windows NT 4.0, or Windows 2000
- processor running at 100 megahertz or faster
- 8 megabytes RAM
- 20 megabytes free disk space

B. DISTRIBUTION FILE

The following distribution file (containing the software, test data sets, and information files) is currently available.

phrqc242.exe - Compiled using Microsoft Visual C++ 6.0, includes source code

C. DOCUMENTATION

Parkhurst, D.L., and Appelo, C.A.J., 1999, User's guide to PHREEQC (Version 2)--a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations: U.S. Geological Survey Water-Resources Investigations Report 99-4259, 312 p.

This document is available in electronic format. A Portable Document Format (PDF) and a Postscript version are included in the doc subdirectory of the PHREEQC program distribution. These and an online HTML version can also be found at http://water.usgs.gov/software/phreeqc.html.

See http://water.usgs.gov/software/ordering_documentation.html for information on ordering printed copies of USGS publications.

D. INSTALLING

Installing PHREEQC

Note that if the software is to be installed on a server system, the person installing the software generally must have administrator rights.

To install the software, double-click phrqc242.exe to execute the installation program and follow the directions on the screen. The installation program can optionally modify the PATH environment variable so that the PHREEQC program can be executed from any directory, without needing to type the full pathname of the program's location.

By default, the software is installed in the directory C:\Program Files\USGS\phreeqc2.4.2. This is the recommended installation directory, but you may use other directories or disk drives.

Note that program components not installed initially can be installed later, and that any components damaged by, for example, being inadvertently overwritten, can be quickly reinstalled by double-clicking phrqc242.exe--a maintenance version of the installation program will be executed.

PHREEQC directory structure

The following directory structure will be created (the contents of each directory are shown to the right):

```
phreeqc2.4.2            files NOTICE.TXT, RELEASE.TXT, and this README.TXT;
                        batch file to run PHREEQC, database files
  `-----doc             documentation files
  `-----examples        examples from user's guide--used in verification tests
  `-----src             Makefile and source code
   |     `-----release  compiled executable
  `-----test            batch files to run verification tests
```

Note: It is recommended that no user files be kept in the PHREEQC directory structure. If you plan to put files in the PHREEQC directory structure, do so only by creating subdirectories.

E. COMPILING

The source code is provided so that users can generate the executable themselves. Little or no support can be provided for users generating their own versions of the software. In general, to compile a new version of the software, you will need:

a) a C compiler,
b) familiarity with the compiler and the operating system under which the compiler runs (i.e., DOS or Windows).

As provided in the phrqc242.exe distribution, the Makefile used to compile the program under Linux is provided as an example.

F. RUNNING THE SOFTWARE

If the option to modify the PATH environment variable was chosen during installation, then the following commands may be used to run

PHREEQC from an MS-DOS Command Prompt window.

command to execute PHREEQC	explanation
phreeqc	The program will query for each of the needed files.
phreeqc input	The input file is named input, the output file will be named input.out and the default database file will be used.
phreeqc input output	The input file is named input, the output file is named output, and the default database file will be used.
phreeqc input output database	All file names are specified explicitly.
phreeqc input output database screen_output	All file names are specified explicitly, and screen output is directed to the file screen_output.

If the option to modify the PATH environment variable was not chosen during installation, then two options exist. (1) the full pathname to the script that runs phreeqc can be used in place of "phreeqc" in the above commands (for example "c:\program files\usgs\phreeqc2.4.2\phreeqc". Note that because of the space present in "program files", quotation marks must be used to enter the full pathname.) Or, (2) the executable (installed in phreeqc2.4.2\src\release\phreeqc.exe) may be copied to the current directory; further, the default database file must be in the current directory and named "phreeqc.dat". The default database file is installed in phreeqc2.4.2\database\phreeqc.dat.

The environment variable PHREEQC_DATABASE can be used to specify the default database for a DOS window session. This environment variable can be set with the command:

```
set PHREEQC_DATABASE=c:\mydirectory\myproject\mydata.dat
```

This environment variable takes precedence over any default definition of the database file. If PHREEQC is invoked with at least three arguments, the third argument is the database file and it takes precedence over the environment variable or the default database.

Out of environment space error

This error can occur when assigning a value to the PHREEQC_DATABASE environment variable or running PHREEQC, including when running the verification tests. The error occurs when there is insufficient space to hold a new environment variable definition.

You can avoid this error by initiating a new command shell and specifying how much environment space you need. For example, in an MS-DOS Command Prompt window, typing

```
command /e:1024
```

will initiate a new command shell with 1024 bytes of environment space. Environment space can be between 256 and 32768 bytes.

The above command will increase the environment space for only the current Command Prompt window. To permanently increase your environment space, on Windows 9x/Me machines, click the MS-DOS icon in the upper-left corner of the Command Prompt window and select Properties. Select the Memory tab and increase the value in the Initial environment field. On

Windows NT/2000 machines, add the above command to C:\winnt\system32\config.nt and initiate and use a new MS-DOS Command Prompt window.

G. TESTING

Test data sets are provided to verify that the program is correctly installed and running on the system. The tests execute the examples presented in the user's guide, which demonstrate most of the program's capabilities. The tests are run in the phreeqc2.4.2\test directory. The directory phreeqc2.4.2\examples contains the PHREEQC input data and expected results for each test.

To test the installation, in an MS-DOS Command Prompt window change to the phreeqc2.4.2\test directory:

```
c:
cd "program files"
cd usgs\phreeqc2.4.2\test
```

Execute the tests by typing the command:

```
test [start [stop]]
```

where: start = the number of the first test to perform, default = 1
stop = the number of the last test to perform, default = 18

For example:

command	what happens
test	runs all of the tests
test 1 1	runs the first test
test 2 3	runs tests 2 and 3
test 4	runs test 4 through the last test

After the tests are completed, the results are compared to the expected results (found in the PHREEQC examples directory). See the file check.log; if all goes well, there should be no differences.

Note: Sometimes different processors, or different compilers cause minor numerical differences in the results or differences in representation of exponents. In general, concentrations should differ by less than about 1e-14 (mol/kg water) between two sets of results. The pe may vary several units in some systems without redox buffering, however, all concentrations should still differ by only small amounts.

Problem 9 generates a warning message that indicates negative concentrations were generated in a kinetic run. The numerical method automatically reduces the step size until negative concentrations are eliminated and an accurate kinetic integration is obtained.

Problems 11, 12, 13, and 15 generate warning messages. The messages simply indicate a shorthand method for defining cell lengths and cell dispersivities was used in a transport calculation.

To clean up after the tests, type the command:

```
clean
```

The tests are described in the table below. Test is the test number and

the usage column indicates how a file is used, with i for input and o for output.

test	description of test and files	file name & usage	
1	Add uranium and speciate seawater		
	PHREEQC input file	ex1	i
	Printed results of calculation	ex1.out	o
2	Temperature dependence of solubility of gypsum and anhydrite		
	PHREEQC input file	ex2	i
	Printed results of calculation	ex2.out	o
	Results written to the selected-output file	ex2.sel	o
3	A. Calcite equilibrium at log Pco2 = -2.0 and 25C B. Definition of seawater C. Mix 70% ground water, 30% seawater D. Equilibrate mixture with calcite and dolomite E. Equilibrate mixture with calcite only		
	PHREEQC input file	ex3	i
	Printed results of calculation	ex3.out	o
4	A. Rain water evaporation B. Factor of 20 more solution		
	PHREEQC input file	ex4	i
	Printed results of calculation	ex4.out	o
5	Add oxygen, equilibrate with pyrite, calcite, and goethite.		
	PHREEQC input file	ex5	i
	Printed results of calculation	ex5.out	o
	Results written to the selected-output file	ex5.sel	o
6	6A. React to phase boundaries 6A1.--Find amount of k-feldspar dissolved to reach gibbsite saturation 6A2.--Find amount of k-feldspar dissolved to reach kaolinite saturation 6A3.--Find amount of k-feldspar dissolved to reach K-mica saturation 6A4.--Find amount of k-feldspar dissolved to reach k-feldspar saturation 6A5.--Find point with kaolinite present, but no gibbsite 6A6.--Find point with K-mica present, but no kaolinite 6B. Path between phase boundaries 6C. Kinetic calculation		
	PHREEQC input file	ex6	i
	Printed results of calculation	ex6.out	o
	Results written to the selected-output file	ex6A-B.sel	o
	Results written to the selected-output file	ex6C.sel	o
7	Organic decomposition with fixed-pressure and fixed-volume gas phases		
	PHREEQC input file	ex7	i
	Printed results of calculation	ex7.out	o
	Results written to the selected-output file	ex7.sel	o
8	Sorption of zinc on hydrous iron oxides		
	PHREEQC input file	ex8	i

Printed results of calculation	ex8.out	o
Results written to the selected-output file	ex8.sel	o

9 Kinetically controlled oxidation of ferrous iron.
Decoupled valence states of iron.

PHREEQC input file	ex9	i
Printed results of calculation	ex9.out	o
Results written to the selected-output file	ex9.sel	o

10 Solid solution of strontianite and aragonite.

PHREEQC input file	ex10	i
Printed results of calculation	ex10.out	o
Results written to the selected-output file	ex10.sel	o

11 Transport and ion exchange.

PHREEQC input file	ex11	i
Printed results of calculation	ex11.out	o
Results written to the selected-output file	ex11adv.sel	o
Results written to the selected-output file	ex11trn.sel	o

12 Advective and diffusive transport of heat and solutes. Constant boundary condition at one end, closed at other. The problem is designed so that temperature should equal Na-conc (in mmol/kgw) after diffusion.

PHREEQC input file	ex12	i
Printed results of calculation	ex12.out	o
Results written to the selected-output file	ex12.sel	o

13 A. 1 mmol/l NaCl/NO3 enters column with stagnant zones. Implicit definition of first-order exchange model.
B. 1 mmol/l NaCl/NO3 enters column with stagnant zones. Explicit definition of first-order exchange factors.
C. 1 mmol/l NaCl/NO3 enters column with stagnant zones. 5 layer stagnant zone with finite differences.

PHREEQC input file	ex13a	i
Printed results of calculation	ex13a.out	o
Results written to the selected-output file	ex13a.sel	o
PHREEQC input file	ex13b	i
Printed results of calculation	ex13b.out	o
Results written to the selected-output file	ex13b.sel	o
PHREEQC input file	ex13c	i
Printed results of calculation	ex13c.out	o
Results written to the selected-output file	ex13c.sel	o

14 Transport with equilibrium_phases, exchange, and surface reactions

PHREEQC input file	ex14	i
Printed results of calculation	ex14.out	o
Results written to the selected-output file	ex14.sel	o

15 1D Transport: Kinetic Biodegradation, Cell Growth, and Sorption

PHREEQC input file	ex15	i
database file	ex15.dat	i
Printed results of calculation	ex15.out	o
Results written to the selected-output file	ex15.sel	o

16 Inverse modeling of Sierra springs

PHREEQC input file	ex16	i
Printed results of calculation	ex16.out	o

17 Inverse modeling of Black Sea water evaporation

	PHREEQC input file	ex17	i
	Printed results of calculation	ex17.out	o
18	Inverse modeling of Madison aquifer		
	PHREEQC input file	ex18	i
	Printed results of calculation	ex18.out	o

H. CONTACTS

Inquiries about this software distribution should be directed to:

U.S. Geological Survey
Hydrologic Analysis Software Support Program
437 National Center
Reston, VA 20192

e-mail: h2osoft@usgs.gov

APPENDIX B

RELEASE.TXT

Features not documented in WRIR 99-4259.

Version 2.4:

Added identifier -warnings to PRINT keyword.

An integer following -warnings gives the maximum number of warnings to print into the output file. A negative number allows all warnings to be printed.

Example: -warnings 20

Changed the results of the function CELL_NO in Basic programs.

Function cell_no in Basic now prints a number equivalent to -solution in SELECTED_OUTPUT data block. It gives the solution number for initial solution calculations and the solution being used in batch reaction calculations. Result is the same as previous versions for ADVECTION or TRANSPORT calculations.

Version 2.3:

DATABASE--New keyword data block

It must be the first keyword in the input file. The character string following the keyword is the pathname for the database file to be used in the calculation. The file that is specified takes precedence over any default database name, including environmental variable PHREEQC_DATABASE and command line arguments.

LLNL_AQUEOUS_MODEL_PARAMETERS--New keyword data block

Added new keyword to make aqueous model similar to EQ3/6 and Geochemists Workbench when using llnl.dat as the database file. Values of Debye-Huckel a and b and bdot (ionic strength coefficient) are read at fixed temperatures. Linear interpolation occurs between temperatures.

New options for SOLUTION_SPECIES are
-llnl_gamma a , where a is the ion-size parameter.
-co2_llnl_gamma , indicates the temperature dependent function for the bdot term given in -co2_coefs of LLNL_AQUEOUS_MODEL_PARAMETERS will be used. Applies to uncharged species only.

```
LLNL_AQUEOUS_MODEL_PARAMETERS
-temperatures
        0.0100   25.0000   60.0000  100.0000
      150.0000  200.0000  250.0000  300.0000
#debye huckel a (adh)
-dh_a
        0.4939    0.5114    0.5465    0.5995
        0.6855    0.7994    0.9593    1.2180
#debye huckel b (bdh)
-dh_b
        0.3253    0.3288    0.3346    0.3421
        0.3525    0.3639    0.3766    0.3925
-bdot
```

```
         0.0394    0.0410    0.0438    0.0460
         0.0470    0.0470    0.0340    0.0000
#cco2   (coefficients for the Drummond (1981) polynomial)
-co2_coefs
        -1.0312              0.0012806
          255.9                 0.4445
      -0.001606
```

Added function SURF to Basic.

SURF("element", "surface") gives the amount of element in the diffuse layer for "surface". "surface" should be the surface name, not the surface-site name (that is, no underscore).

Allow decimals in definition of secondary master species.

Some redox states do not average to integers, for convenience in identifying them, decimal numbers may be used within the parentheses that define the redox state, example S(0.3) could be used in the MASTER_SPECIES data block for the valence state of aqueous species S6-2.

Eliminate echo of input file in PRINT data block.

-echo_input T/F turns echoing on and off. Default is true, initial value is true.

Added option for an equilibrium-phase to dissolve only.

"dis" is added at the end of a line defining an equilibrium-phase. No data fields may be omitted. Should not be used when adding an alternative reaction.

Example:

```
EQUILIBRIUM_PHASES
Dolomite 0.0  0.001 dis
```

Version 2.2:

Added function EDL to Basic.

EDL("element", "surface") gives the amount of element in the diffuse layer for "surface". "surface" should be the surface name, not the surface-site name (that is, no underscore).

Special values for "element" include:

```
"charge" - gives surface charge, equivalents.
"sigma"  - surface charge density, C/m**2.
"psi"    - potential at the surface, Volts.
"water"  - mass of water in the diffuse layer, kg.
```

End of Features not documented in WRIR 99-4259.

Revisions and bug fixes

Version 2.4.2: Date: Fri June 15, 2001

Fixed spreadsheet bug. Program was not ignoring columns that could not be identified as either element names or allowed data (ph, pe, number, description, etc). Also, the program failed if a spreadsheet solution

number was negative.

Version 2.4.1: Date: Mon June 4, 2001
Fixed spreadsheet bugs with isotopes.

Version 2.4: Date: Fri June 1, 2001

Added structure for spreadsheet for use by PhreeqcI.

Isotope value initialized incorrectly if only an -uncertainty was defined in SOLUTION_SPREAD.

Fixed segmentation violation when primary and secondary master species were defined improperly.

Corrected enthalpies of reaction in llnl.dat. Previous release had erroneously had enthalpies of formation in -delta_H parameter; the values should be enthalpies of reaction. Enthalpies of reaction were calculated from the enthalpies of formation and these values are now included in the -delta_H parameter. This change will have very little impact on calculations because the analytical expression has precedence over -delta_H in calculating temperature dependence of log K, and nearly all species and minerals have an analytical expression or lack both an analytical expression and an enthalpy of reaction.

Corrected bugs in punch of solid solution components that caused both selected output and output file errors: moles were incorrect in selected output, and total moles and mole fraction were incorrect in output file.

Added surface complexation constants for Fe+2; two complexes for weak sites and one complex for strong sites. phreeqc.dat and wateq4f.dat modified.

Comment for units of parameters for calcite rate equation was wrong. Rate equation now uses cm^2/L for area parameter. Previously the correct units would have been 1/decimeter. phreeqc.dat and wateq4f.dat modified.

Fixed a bug when rates were equal within tolerance, but negative concentrations occurred because of small initial concentrations.

Added -warnings to PRINT keyword for specification of maximum number of warnings to print. Negative number allows all warnings to be printed.

Function CELL_NO in Basic now prints a number equivalent to -solution in SELECTED_OUTPUT data block. This does not change printing for ADVECTION or TRANSPORT calculations.

Kinetics time is halved for advective part of reaction in transport; time incorrectly accounted for before.

-punch_ identifiers printed -1 instead of the correct solution number for batch-reaction calculations.

-high_precision is no longer reset to false with every SELECTED_OUTPUT data block.

SELECTED_OUTPUT file name stored for use by PhreeqcI.

Alkalinity for NH3 corrected to 1.0 in llnl.dat.

Fixed bug with USER_PRINT of kinetics. Did not find correct kinetics information in some cases.

Fixed bug in default values for SOLUTION_SPREAD. Cannot use phase name and SI for pH or pe, and bug did not allow PHREEQC to run. Now PHREEQC runs, but warns that this is not allowed.

Version 2.3: Date: Tue January 2, 2001

Added new keyword DATABASE. It must be the first keyword in the input file. The character string following the keyword is the pathname for the database file to be used in the calculation. The file that is specified takes precedence over any default database name, including environmental variable PHREEQC_DATABASE and command line arguments.

Fixed bug in SOLUTION_SPREAD. If first heading in the spread-sheet input was an identifier--pH, pe, units, etc--then the headings were interpreted as an identifier and bad things happened.

Added new keyword to make aqueous model similar to LLNL and Geochemists Workbench when using llnl.dat as the database file. Values of Debye-Huckel a and b and bdot (ionic strength coefficient) are read at fixed temperatures. Linear interpolation occurs between temperatures.

New options for SOLUTION_SPECIES are
-llnl_gamma a , where a is the ion-size parameter.
-co2_llnl_gamma , indicates the temperature dependent function for the bdot term given in -co2_coefs of LLNL_AQUEOUS_MODEL_PARAMETERS will be used. Applies to uncharged species only.

```
LLNL_AQUEOUS_MODEL_PARAMETERS
-temperatures
         0.0100   25.0000   60.0000  100.0000
       150.0000  200.0000  250.0000  300.0000
#debye huckel a (adh)
-dh_a
         0.4939    0.5114    0.5465    0.5995
         0.6855    0.7994    0.9593    1.2180
#debye huckel b (bdh)
-dh_b
         0.3253    0.3288    0.3346    0.3421
         0.3525    0.3639    0.3766    0.3925
-bdot
         0.0394    0.0410    0.0438    0.0460
         0.0470    0.0470    0.0340    0.0000
#cco2   (coefficients for the Drummond (1981) polynomial)
-co2_coefs
        -1.0312              0.0012806
          255.9                 0.4445
      -0.001606
```

Fixed bug in basic interpreter. A number like "..524" would cause an infinite loop.

Added function SURF to Basic.
SURF("element", "surface") gives the amount of element in the diffuse layer for "surface". "surface" should be the surface name, not the surface-site name (that is, no underscore).

Fixed option to "runge_kutta" from "runge-kutta" to match documentation for KINETICS.

Fixed UO2+2 and Mn+2 reaction stoichiometry for Hfo surface complexation in wateq4f.dat.

Added option for an equilibrium-phase to dissolve only.
"dis" is added at the end of a line defining an equilibrium-phase. No data fields may be omitted. Should not be used when adding an alternative reaction.
Example:
EQUILIBRIUM_PHASES
Dolomite 0.0 0.001 dis

R-K integration failed when only the final rate generated negative concentrations.

Allow decimals in definition of secondary master species, for example S(0.3).

Fixed bug if description was more than about 85 characters; now allows about 400 characters.

Fixed bug for surface/exchange sites related to phases. Was checking internal copies of surfaces/exchange with negative numbers.

Fixed bug in quick prep that did not set the correct pointer for gas phases.

Fixed segmentation fault that occurred if all elements for phase-boundary mineral were not in the solution. Only applied to a phase used to define concentration in an initial solution calculation.

Added option to eliminate echo of input file in PRINT data block. -echo_input T/F turns echoing on and off. Default is on.

Release 2.2: Date: Wed March 1, 2000

Fixed bug in MIX if no solutions are defined.

Changed printout for surface.
Only gives net surface charge for diffuse layer calculation.
Prints correct value for the surface charge and surface charge density for diffuse-layer calculation.

Added function EDL to Basic.
EDL("element", "surface") gives the amount of element in the diffuse layer for "surface". "surface" should be the surface name, not the surface-site name (that is, no underscore).

Special values for "element" include:
"charge" - gives surface charge, equivalents.
"sigma" - surface charge density, C/m**2.
"psi" - potential at the surface, Volts.
"water" - mass of water in the diffuse layer, kg.

Changed distribution to be more consistent with other USGS water-resources applications.

Release 2.1: Date: Wed January 19, 2000

Added additional #ifdef's for PhreeqcI.

Fixed problem with formats for USER_PUNCH and others with Microsoft C++ 3 digit exponents.

Initial Release 2.0: Date: Wed December 15, 1999

Version: C_54 = Version 2.0

APPENDIX C

```
CHECK.LOG

Comparing files ..\EXAMPLES\ex1.out and EX1.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex2.out and EX2.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex2.sel and EX2.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex3.out and EX3.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex4.out and EX4.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex5.out and EX5.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex5.sel and EX5.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex6.out and EX6.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex6A-B.sel and EX6A-B.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex6C.sel and EX6C.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex7.out and EX7.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex7.sel and EX7.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex8.out and EX8.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex8.sel and EX8.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex9.out and EX9.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex9.sel and EX9.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex10.out and EX10.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex10.sel and EX10.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex11.out and EX11.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex11adv.sel and EX11ADV.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex11trn.sel and EX11TRN.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex12.out and EX12.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex12.sel and EX12.SEL
```

```
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13a.out and EX13A.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13b.out and EX13B.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13c.out and EX13C.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13a.sel and EX13A.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13b.sel and EX13B.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex13c.sel and EX13C.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex14.out and EX14.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex14.sel and EX14.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex15.out and EX15.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex15.sel and EX15.SEL
FC: no differences encountered

Comparing files ..\EXAMPLES\ex16.out and EX16.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex17.out and EX17.OUT
FC: no differences encountered

Comparing files ..\EXAMPLES\ex18.out and EX18.OUT
FC: no differences encountered
```