

**Software Release Notice
Acquired Software**

1. Software Name: **MINTEQA2/PRODEFA2** Software Version: **4.03**

2. Software Function: MINTEQA2 is a equilibrium speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model is useful for calculating the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressures. PRODEFA2 is the associated input file editor.

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

MINTEQA2/PRODEFA2 version 4.02 was not compatible with the Windows XP and later operating systems. MINTEQA2/PRODEFA2 version 4.03 addressed the incompatibility problems with the previous version. There are no major computational changes between MINTEQA2/PRODEFA2 version 4.02 and version 4.03 however there may be some minor differences due to accumulated rounding errors. All changes are in an attached document named 4.03 changes.

4. Software Installation

4a. Computer Platform(s): PC/Pentium level processor
 4b. Operating System(s): Windows XP (can run on older versions)
 4c. Programming Language(s): Fortran v.9.0

4d. Installation Testing: A set of 12 standard installation problems were performed
 Passed Performed by: Lynn Sabido
 Testing Performed On: PC computer with XP operating system
 Description of Testing Performed:
 A set of 12 examples for an installation test, no discrepancies, see the attached CD.

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

Installation Performed by: Computer information systems administrator	Date:
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Remarks:

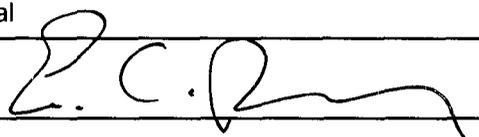
5. Software Assessment

Validation Status:
 Full Validation Limited Validation Date of Validation: 11/13/06
 Not Validated, Explain: Validation is up for approval

Software User: Paul Bertetti, James Myers, Dave Turner, and Lynn Sabido	Date: 11/13/06
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Remarks: Regression testing was completed by running Validation tests from the last Validation (MINTEQA2/PRODEFA2, 4.02) using MINTEQA2/PRODEFA2, 4.03. The Result files were compared for discrepancies. Files with no unexplainable discrepancies are considered successful tests. The comparison files for old and new results are contained in the attached cd. There were no discrepancies in the validation test files.

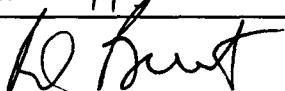
6. Approval

Manager: 	Date: 3/27/2007
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Remarks:

7. QA Verification

SRN Number: **415**

Verified by: 	Date: 3/27/2007
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Remarks:

The following notes are from the EPA website:
<http://www.epa.gov/ceampubl/mmedia/minteq/mintreln.htm>

MINTEQA2 Release Notes

Version: 4.03

Corrections & Improvements to Prior Versions

New versions of MINTEQA2, PRODEFA2, FRMT and UNFRMT were generated for modern operating systems (Win2K/XP) due to the failure of the Lahey compiled versions to correctly operate on these systems. Intel FORTRAN v9.0 was used to recompile the codes with attendant minor changes in operation in MINTEQA2 and PRODEFA2. The new versions will run on all MS Windows versions. The programs are now run directly; the DOS batch files that launched the programs have been removed. To initiate a MINTEQA2 simulation enter the runtime image's name; "MINTEQA2". PRODEFA2, FRMT and UNFRMT all operate in a similar fashion.

ANSI extended codes that perform screen manipulations were removed from MINTEQA2 and PRODEFA2 due to the complexity of loading the various versions of the ANSYS device driver for the differing command interpreters (COMMAND.COM, CMD.EXE) in the various operating systems. Screen IO for these programs is now sequentially generated and scrolls in the normal manner for command interpreters.

The new version of MINTEQA2 requires versions of TYPE6.UNF and THERMO.UNF generated by the new Intel compiled version of UNFRMT. If users have their own customized versions of these databases, they should first run the new FRMT program and then the new UNFRMT version to generate Intel FORTRAN direct access versions of these files.

A new component database (MMHG&TBT.DBS) containing Monomethylmercury (MMHg) and Tributyltin (TBT) is

distributed with this version of MINTEQA2. A testing input file (MMHG&TBT.INP) and comparison output file (test_output\MMHG&TBT.OUT) are included. To run the tests, see RELEASE.TXT. Refer to the "MMHG&TBT.pdf" paper in the \docs directory for further information.

No direct changes to the science simulated by the model have been made but users should note that, to date, small changes (on the order of $10e-19$) occur in some numerical mass balance results generated by MINTEQA2 executing the testing input files. No programmatic reason for this discrepancy has yet been found and no scientific assessment of the significance of these differences has been obtained. The differences may be due to accumulated rounding errors for numerical operations or compilation switch incompatibility but this has not been ascertained at this time. Testing consists of running the newly compiled MINTEQA2 code with the input files provided and comparing the results generated with the standard test results contained in the test_output subdirectory. Current testing results are found in RELEASE.TXT.

File: RELEASE.TXT

MINTEQA2 Model System Release Notes version 4.03 May 2006 Center for Exposure Assessment Modeling (CEAM) National Exposure Research Laboratory - Ecosystems Research Division Office of Research and Development (ORD) U.S. Environmental Protection Agency (U.S. EPA) 960 College Station Road Athens, Georgia 30605-2700 706/355-8400

CORRECTIONS AND IMPROVEMENTS TO MINTEQA2 VERSION 4.02

New versions of MINTEQA2, PRODEFA2, FRMT and UNFRMT were generated for modern operating systems (Win2K/XP) due to the failure of the Lahey compiled versions to correctly operate on these systems. Intel FORTRAN v9.0 was used to recompile the codes with attendant minor changes in operation in MINTEQA2 and PRODEFA2. The new versions will run on all MS Windows versions. The programs are now run directly; the DOS batch files that launched the programs have been removed. To initiate a MINTEQA2 simulation enter the runtime image's name; "MINTEQA2". PRODEFA2, FRMT and UNFRMT all operate in a similar fashion. -----
----- ANSI extended codes that perform screen manipulations were removed from MINTEQA2 and PRODEFA2 due to the complexity of loading the various versions of the ANSI.SYS device driver for the differing command

interpreters (COMMAND.COM, CMD.EXE) in the various operating systems. Screen IO for these programs is now sequentially generated and scrolls in the normal manner for command interpreters. ----- The new version of MINTEQA2 requires versions of TYPE6.UNF and THERMO.UNF generated by the new Intel compiled version of UNFRMT. If users have their own customized versions of these databases, they should first run the new FRMT program and then the new UNFRMT version to generate Intel FORTRAN direct access versions of these files. -----

----- A new component database (MMHG&TBT.DBS) containing Monomethylmercury (MMHg) and Tributyltin (TBT) is distributed with this version of MINTEQA2. A testing input file (MMHG&TBT.INP) and comparison output file (test_output\MMHG&TBT.OUT) are included. To run the test users can: 1) Rename the COMP.DBS to save it and rename the MMHG&TBT.DBS to COMP.DBS; then run the model. Or, 2) Edit the DBASE.INI file directly and change the line "COMPONENT DATABASE: comp.dbs" to "COMPONENT DATABASE: mmhg&tbt.dbs"; then run the model. Or, 3) Run PRODEFA2 to generate the correct DBASE.INI file prior to running the model. Refer to the "MMHG&TBT.pdf" paper in the \docs directory for further information.

No direct changes to the science simulated by the model have been made but users should note that, to date, small changes (on the order of $10e-19$) occur in some numerical mass balance results generated by MINTEQA2 executing the testing input files. No programmatic reason for this discrepancy has yet been found and no scientific assessment of the significance of these differences has been obtained. The differences may be due to accumulated rounding errors for numerical operations or compilation switch incompatibility but this has not been ascertained at this time. Testing consists of running the newly compiled MINTEQA2 code with the input files provided and comparing the results generated with the standard test results contained in the test_output subdirectory. Current testing results are:

test1a - passes

test 1b - passes

test 2a - fails

test 2b - fails

test 2c - fails

test 3 - passes

test 4 - passes

test 5a - passes

test 5b - fails

test 5c - passes

test 6 - passes

test30 - fails

The tests fail in the following way; all differences occur in Part 3 of the output files in

"Parameters of the component most out of balance" section.

test	pgm variable	component_id/name	results	standard results
test2a	array t	330/H+1	-7.200e-20	-7.115e-20
test2b	array t	330/H+1	-1.050e-19	-1.042e-19
test2c	array t	330/H+1	-7.200e-20	-7.115e-20
test5b	array y	330/H+1	0	-4.337e-19
test30	array t	330/H+1	0	-1.158e-21
test30	array t	2/H2O	0	-1.158e-21
test30	array y	580/PO4-3	0	1.548e-21

"array t" holds the total concentration values, "array y" holds the residual values, "results" are what is generated with the newly compiled code, "standard results" are numbers from the comparison files in the test_output directory.

The numbers in question on the reports are generated in the SOLIDX routine inside nested loops; the total concentration and residual storage arrays are declared and sized in the MINTEQA2 include file.