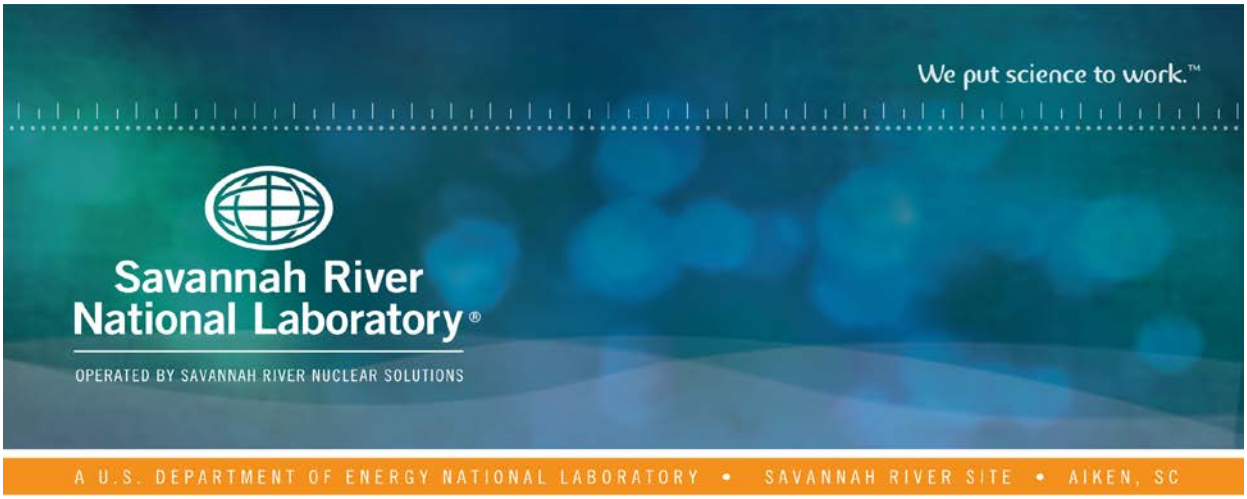
Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Disclaimer:



Software Quality Assurance Plan for The Geochemist's Workbench®

Classified as Level C

J. A. Dyer

December 2018

Q-SQP-A-00007, Revision 1

DISCLAIMER

Printed in the United States of America

Prepared for
U.S. Department of Energy

Keywords: *Performance Assessment, Geochemical Modeling, Saltstone*

Retention: *Permanent*

Software Quality Assurance Plan for The Geochemist's Workbench®

Classified as Level C

J. A. Dyer

December 2018

Prepared for the U.S. Department of Energy under contract number DE-AC09-08SR22470.

Savannah River National Laboratory®
OPERATED BY SAVANNAH RIVER NUCLEAR SOLUTIONS

APPROVALS

AUTHORS:

_____

J. A. Dyer, Environmental Modeling, SRNL Date

APPROVAL:

_____

J. A. Dyer, Design Authority/Cognizant Technical Function, Environmental Modeling, SRNL Date

_____

J. P. Lampert, Cognizant Quality Function, SRNL Quality Assurance Date

_____

D. A. Crowley, Manager Date
Design Agency, Environmental Modeling, SRNL

EXECUTIVE SUMMARY

The Geochemist's Workbench® (GWB) Release 10.0.10 is a geochemical modeling suite for simulating the reactive fate and transport of radionuclides and other metals in aqueous systems including groundwater, surface water, soil, and sediment. At the Savannah River National Laboratory, GWB plays an important role in the preparation of Performance Assessments involving cementitious materials. The software classification for GWB is Level "C." GWB was purchased from Aqueous Solutions LLC and came into existence outside of the Software Quality Assurance procedures; therefore, it is considered "existing/acquired" software. This Software Quality Assurance Plan addresses verification techniques and the required life cycle components for Level "C" existing/acquired software (i.e., "Evaluation," "Configuration Control," and "Cyber Security Analysis") with other elements optionally applied using a graded approach.

REVISION HISTORY

Date	Release	Comments
November 2012	Revision 0	GWB Release 9.0.2
December 2018	Revision 1	GWB Release 10.0.10

TABLE OF CONTENTS

LIST OF ABBREVIATIONS

CQF	Cognizant Quality Function
CTF	Cognizant Technical Function
DOE	Department of Energy
GWB	The Geochemist's Workbench®
PA	Performance Assessment
QA	Quality Assurance
SQAP	Software Quality Assurance Plan
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
SWCD	Software Classification Document

1.0 Introduction

The Geochemist's Workbench® (GWB) Release 10.0.10 is a geochemical modeling suite for simulating the reactive fate and transport of radionuclides and other metals in aqueous systems including groundwater, surface water, soil, and sediment. At the Savannah River National Laboratory (SRNL), GWB plays an important role in the preparation of Performance Assessments (PAs) involving cementitious materials. GWB was originally developed by the University of Illinois at Urbana-Champaign and is currently supported by Aqueous Solutions LLC, located in the Research Park at the University of Illinois. The principal use for GWB is to manipulate aqueous chemical reactions, calculate stability diagrams and the equilibrium states of natural waters, trace reaction processes, model reactive transport, plot the results of these calculations, and store the related data.

2.0 Scope

This Software Quality Assurance Plan (SQAP) adheres to the guidelines and minimum content requirements specified in the following documents:

- Savannah River Site (SRS) *1Q Quality Assurance (QA) Manual*, Procedure 20-1, current revision, "Software Quality Assurance" (Savannah River Site, 2018a).
- E7 Conduct of Engineering and Technical Support Procedure Manual, Procedure 5.01, current revision, "Software Engineering and Control" (Savannah River Site, 2015).

This SQAP applies to SRNL organizations that use and maintain the subject software. The content of this SQAP is specified either directly in the SQAP or by reference to other documents. Deviations from this SQAP will require a new revision. All activities requiring a graded approach shall be properly documented and justified in this SQAP.

3.0 Software Classification

Based on anticipated application to U.S. Department of Energy (DOE) PAs, the Cognizant Technical Function (CTF) has classified GWB as Level "C" software per Manual 1Q, Procedure 20-1, Attachment 8.1. The classification is documented with Lotus Notes application SWCD OSR 19-337, Software Classification Document (SWCD) number K-SWCD-A-00002 (Software Classification Document, 2018), and was approved by the Cognizant Quality Function (CQF). The Level "C" class includes "software applications used to comply with regulatory laws, environmental permits or regulations and/or commitments to compliance." PA analyses establish a "reasonable expectation" per DOE M 435.1-1 (Department of Energy, 2011) that the performance objectives of DOE Order 435.1 (Department of Energy, 1999) and other regulatory requirements will be met for radionuclide waste disposal. This SQAP addresses the life-cycle requirements and verification techniques for GWB as Level "C" software.

4.0 Software QA Procedures and Plan

GWB Release 10.0.10 was purchased from Aqueous Solutions LLC. The software originally came into existence outside of the Software QA procedures; therefore, it is considered "existing/acquired" software with respect to 1Q, 20-1 and E7, 5.01. As outlined in Attachment 8.2 of Manual 1Q, Procedure 20-1 and in Section 5.1.3 of Manual E7, Procedure 5.01, the required life cycle components for Existing, Level "C" software are "Evaluation," "Configuration Control," and "Cyber Security Analysis" with other elements

optionally applied using a graded approach. Additional optional components deemed appropriate for the software are “Design,” “Implementation,” “Testing,” “Installation and Acceptance,” “Operation and Maintenance,” “Software Retirement,” “Access Control,” “Problem Reporting and Corrective Action,” and “Cyber Security Control.” The selected optional elements are discussed in more detail below.

To assure software quality, this SQAP identifies the following information, and if required, where it can be found:

- Description of the overall nature and purpose of the software (Sections 1.0 and 6.1)
- Organizations and personnel responsible for performing the work and achieving software quality, including their tasks and responsibilities (Section 5.0)
- Software engineering methods, software life cycle phases, and requirements for each phase in accordance with this procedure (Section 6.0)
- Required documentation to be maintained (within each sub-section of Section 6.0)
- Standards, conventions, techniques, or methodologies to guide the software development, as well as methods to assure compliance to the same (Section 6.2)
- Required software reviews (Sections 6.4 and 6.5)
- Software retirement (Section 6.7)
- Software configuration control and access requirements per this procedure and methodologies used (Sections 7.1 and 7.3)
- Methods for error reporting and corrective action (Section 7.4)
- Security capabilities to be implemented, using approved cyber security procedures and guidance (Section 7.5)

5.0 Roles and Responsibilities

The Design Agency is responsible for ensuring:

- The software classification process has been documented per 1Q 20-1 before developing or purchasing software or for software that meets the existing and acquired Section 5.6 of 1Q 20-1.
- When the intended use of the software changes, the current classification of the software shall be verified and then updated, if required.
- The SQAP and other required documents are developed, reviewed, approved, and sent to Site Records as required.
- Compliance with requirements and reviews as defined in the SQAP.
- The classification process is executed for software being retired.

The Design Authority/CTF is responsible for:

- Assigning and approving the software classification and making the SSIL determination

- Completing the SWCD application for unclassified software which requires getting the record document number for a new SWCD or using the record document number and next revision for an updated SWCD.
- Revising the SWCD as defined in Section 5.2 of 1Q 20-1
- Preparing, reviewing, implementing, and approving Software QA procedures, plans, and other required documents including life cycle documentation
- Reviewing, testing, and approving any changes to the software
- Identifying whether a Facility Operations Safety Committee review is required
- Reviewing the classification if the intended function or effect changes
- Completing the classification process to document the retiring of the software

The CQF is responsible for:

- Reviewing and approving the SQAP
- Reviewing and approving the SWCD

Should other SRNL business programs choose to use the software at the same Level "C" functional classification, oversight will be provided by the appropriate Manager. The Design Authority/CTF, CQF, and this SQAP would remain unchanged.

6.0 Life Cycle Plans

SRS Manual 1Q, Procedure 20-1 (Savannah River Site, 2018a) and Manual E7, Procedure 5.01 (Savannah River Site, 2015) will be used to assure quality throughout the Software Life Cycle. Software-specific implementation of QA Procedure 20-1 and E7, 5.01 for GWB is discussed in more detail below.

6.1 Function

The functional requirements define the software capabilities needed to perform the tasks of interest that will be designed into the software by in-house or vendor software designers. The functional requirements for the GWB software are described below.

6.1.1 Requirement 1: Equilibrium Calculations (High Priority)

Function: Software must have the ability to calculate the equilibrium distribution of aqueous species in a fluid for chemical systems and processes.

Performance: Vendor literature describes how to create and run a system or process equilibrium model using the **React** application within GWB.

User Interface: User must define the system or process using either the **React** interface or an input text file. In the latter case, the text file is copied into or read by the **React** interface.

External Interface: None.

Acceptance Criteria: The creation of an equilibrium model as described in the vendor literature will be tested. Comparison of test results to vendor-published results will be made.

6.1.2 Requirement 2: Activity-Activity Diagrams of Mineral Stability and Predominance of Aqueous Species in Chemical Systems (Medium Priority)

Function: Software must have the ability to calculate and plot activity-activity diagrams to show the stability of minerals and predominance of aqueous species in chemical systems.

Performance: Vendor literature describes how to create and plot an activity-activity diagram for a chemical system using the **Act2** application within GWB.

User Interface: User must define the system using either the **Act2** interface or an input text file. In the latter case, the text file is copied into or read by the **Act2** interface.

External Interface: None.

Acceptance Criteria: The creation of activity-activity diagrams as described in the vendor literature will be tested. Comparison of test results to vendor-published results will be made.

6.1.3 Requirement 3: Reaction Path Diagrams of User-Defined Chemical Systems (Medium Priority)

Function: Software must have the ability to calculate reaction path diagrams (initial and final reaction conditions) for conditions in the user-defined chemical systems.

Performance: GWB includes an application (**Act2**) to calculate reaction path diagrams that show stability of minerals at equilibrium and an application (**React**) to calculate equilibrium conditions at the beginning and end of a specified reaction path. Both applications rely on thermodynamic data in the user-specified thermodynamic database.

User Interface: User must define the system in either the application interface or an input text file. In the latter case, the text file is copied into or read by the **Act2** interface.

External Interface: None.

Acceptance Criteria: Output from **Act2** and **React** will be compared to published calculations by Bethke (2008).

6.1.4 Requirement 4: Modifiable Thermodynamic Database (Medium Priority)

Function: Software must include a thermodynamic database that can be modified to include minerals found in the user-defined chemical systems.

Performance: The default thermodynamic database (thermo.dat) for the GWB software provides fundamental data for calculation of thermodynamic properties for an extensive list of aqueous species and minerals. However, the ability to modify and add to the default thermodynamic database is necessary.

User Interface: The default GWB database may be copied and modified using a text editor. When an application of GWB is run, the default thermo.dat database is used for thermodynamic calculations. Because the default database will be modified for modeling of user-defined chemical systems, users must specify the modified database with the GWB data command.

External Interface: None.

Acceptance Criteria: The GWB default database must be modifiable using a standard text editor.

6.1.5 Requirement 5: Reaction Transport Modeling (Medium Priority)

Function: Software must have the ability to perform transport calculations (advection, dispersion, and molecular diffusion) along with the reaction model.

Performance: GWB software includes applications (**X1t** and **X2t**) to account for transport and chemical reaction calculations. In **X1t**, an unreacted fluid of a specified composition can enter either end of a model domain and react as it passes along a linear or radial coordinate. The flow of fluid along the domain displaces reacted fluid from the opposite end. In **X2t**, transport and reactions are similar except flow can occur in two dimensions and fluid can enter and leave the domain at wells (i.e., specified locations within the domain).

User Interface: User must define the system in either the application interface or an input text file. In the latter case, the text file is copied into or read by the **X1t** or **X2t** interface.

External Interface: None.

Acceptance Criteria: An **X1t** model will be created and tested as described in the vendor literature. Comparison of test results with vendor-published results will be made.

6.2 Design

Formal design documentation and reviews are not required for the software classification within the scope of this SQAP because GWB is an acquired/existing code. Design and implementation of the GWB software is documented in the vendor-provided user's guide (Bethke and Yeakel, 2015).

6.3 Implementation

Detailed implementation processes are not required for the GWB software within the scope of this SQAP; however, in accordance with Manual 1Q, Procedure 20-1 (Savannah River Site, 2018a), a graded approach is used. Level "C" software is subject to unit and module testing conducted in accordance with Manual E7, Procedure 5.40, "Software Testing, Acceptance and Turnover" (Savannah River Site, 2015).

6.4 Testing

Testing will be performed in accordance with the five principal functional requirements outlined in Section 6.1 above. The five test cases are sample problems provided by Bethke (2008) in *Geochemical and Biogeochemical Reaction Modeling* and shall be used to verify proper functionality of the GWB software. The five tests are detailed in Appendix A. A report shall be produced to document completion of the test cases for QA purposes. The report shall explicitly identify the specific release(s) or version number(s) tested and qualified as well as the operating system and computer on which the software was installed and tested. If a new operating system is installed, revalidation shall be performed as necessary.

Any release or version of the GWB that does not have an approved installation and test report associated with it shall be considered non-qualified, non-baseline software and should not be used for quality-affecting work.

6.5 Installation and Acceptance

Upon successful completion of testing, the software is accepted for operational use. Installation and acceptance shall be documented in accordance with Manual E-7, Procedure 5.40 (Savannah River Site, 2015) for Level "C" purchased software. The 1Q Quality Assurance Manual, Procedure 20-1 (Savannah

River Site, 2018a) provides the minimum requirements for software installation, testing, and acceptance. GWB is an acquired/existing code; therefore, installation, acceptance, and testing of the software is documented by Bethke and Yeakel (2015) in the *GWB Essentials Guide*. As described in Sections 6.1 and 6.4 above, testing shall be performed in a manner consistent with vendor instructions.

Appendix A provides the installation and test report for GWB, which satisfies the qualification requirements for Release 10.0.10 of the software. Appendix A may be used as an example for qualifying future releases.

Prior to commencement of Operations and Maintenance lifecycle activities, the production baseline shall be established in accordance with the Configuration Control section of this SQAP.

6.6 Operation and Maintenance

A graded approach for Operation and Maintenance life cycle activities may be used. Because GWB is an acquired/existing code designed to be used as written, the source code itself is not anticipated to be modified by users. Input data for the GWB software will vary from project to project; however, the source code itself has been purchased for its usefulness as written.

Configuration Control shall be implemented on changes to GWB approved by the Design Agency and the Design Authority for 100% of the configuration items in the software configuration index in accordance with requirements established in the Configuration Control section of this SQAP.

Approval from the Design Agency and the Design Authority shall be required for any modifications to the approved product baseline. All modifications shall be managed in accordance with 1Q Quality Assurance Manual, Procedure 20-1, Rev. 19 (Savannah River Site, 2018a).

6.7 Software Retirement

If the Design Agency and Design Authority decide that the GWB software is no longer needed, support for the software shall be terminated and routine use of the software shall be prevented in association with PA- or CA-related work.

When use of the software is no longer needed, the Design Authority removes the software from Service, notifies users that the software is retired, and changes the status in the Lotus Notes SWCD Application to "Retired." At that time, the software shall no longer be governed by this SQAP. If additional controls are warranted, the Design Authority shall ensure that the documented approvals of the Design Agency, Design Authority/CTF, and CQF are obtained.

7.0 Software Quality Assurance Actions

7.1 Configuration Control

Level "C" software governed by this SQAP is controlled to restrict software changes by anyone other than the designated software maintainer(s). GWB is a commercial code designed to be used as written; the user does not have access to the source code to view or make changes. Any changes to the software configuration will be approved, made, documented, and maintained by Aqueous Solutions LLC. This will take the form of periodic maintenance/new releases of the software as well as updates to the user's guides

and on-line tutorials. The maintenance updates and the user's guides and tutorials are accessible from the "Download" menu on the GWB homepage (https://www.gwb.com/update.php).

New releases will require purchase of a new user's license, which will trigger a new revision to this SQAP and acceptance testing as documented in Appendix A. Switching to a new release of GWB must be authorized by the Design Authority.

The status of each software version can be accessed in the Lotus Notes Software Classification database. The revision history is listed on page vi.

7.2 Evaluation

A software evaluation is required for Level "C" existing software. A graded approach was used to evaluate this purchased software; the evaluation results are documented in this SQAP (above) and in the Software Classification Document, K-SWCD-A-00002, Rev. 5 (Software Classification Document, 2018).

7.3 Access Control

SRNL owns two single-user licenses for the GWB software that are currently installed on two individual PCs. Installation and operation of the software requires an electronic license key. Access to the GWB software by additional users will require the purchase of additional licenses or the transfer of one of the two existing licenses to another user by the Design Authority.

7.4 Problem Reporting and Corrective Action

Problem reporting will comply with requirements of Manual 1Q, Procedure 15-1, "Control of Nonconforming Items" (Savannah River Site, 2018b) and Manual 22Q, Procedure CAP-1, "Corrective Action Program" (Savannah River Site, 2018c). The Design Authority/CTF shall report software problems/issues to the Design Agency (Manager, Environmental Modeling). The Manager will notify recipients of errant information generated by GWB, and with input from the CTF and information recipients, determine appropriate corrective action. Problem reporting and corrective action for other potential business programs will be controlled by the Design Agency.

Because GWB is purchased software, maintenance to correct software errors will be made and tested by the vendor (Aqueous Solutions LLC) according to the vendor's discretion. Revisions to the software are communicated by Aqueous Solutions LLC via new release notes that come with the software update. Comments, suggestions, and potential software errors can be communicated vi The Geochemist's Workbench Support Forum maintained by Aqueous Solutions LLC at forum.gwb.com.

7.5 Cyber Security Analysis

No additional security access controls are required to restrict the use of database and spreadsheet software or associated computer systems beyond those established in Section 7.1. At SRS, the GWB software is a stand-alone executable stored on a personal computer that is under the control of the Software Owner. The personal computer is password-protected; therefore, access to the GWB software is limited. Furthermore, an electronic license key provided by Aqueous Solutions LLC must be inserted during software installation to activate the software and related files.

8.0 Quality Assurance Records/Documentation

This record shall be controlled in accordance with the requirements of Manual 1Q, Procedure 17- 1, "Quality Assurance Records Management" (Savannah River Site, 2018d). Documents required by this plan shall be retained as QA records. Documentation may be combined, issued, and maintained as a single document, multiple parts of a single document, or multiple documents as long as all documentation, reviews, and approval requirements are met. Note that when these documents are part of a larger document, the larger document shall be controlled as a QA record.

9.0 Training

Training for the GWB shall be completed by reading this SQAP and any associated procedures or documents. No additional training is required. Management ensures that individuals receive training that is commensurate with the scope, complexity, and importance of the task.

10.0 References

Bethke, C. M. (2008) *Geochemical and Biogeochemical Reaction Modeling*, 2nd Ed., Cambridge University Press, New York.

Bethke, C. M., and Yeakel, S. (2015) *GWB Essentials Guide: The Geochemist's Workbench® Release 10.0,* Champaign, IL.

Department of Energy (2011) *Radioactive Waste Management Manual*, DOE M 435.1-1, Chg 2, June 8, 2011.

Department of Energy (1999) *Radioactive Waste Management Order*, DOE O 435.1, July 9, 1999.

Savannah River Site (2015) *Software Engineering and Control*. Conduct of Engineering and Technical Support Procedure Manual E7, Procedure 5.01, current revision.

Savannah River Site (2018a) *Software Quality Assurance*. Quality Assurance Manual 1Q, Procedure 20-1, current revision.

Savannah River Site (2018b) *Controlling of Nonconforming Items*, Quality Assurance Manual 1Q, Procedure 15-1, current revision.

Savannah River Site (2018c) *Corrective Action Program*. Contractor Assurance System Manual 22Q, Procedure CAP-1, current revision.

Savannah River Site (2018d) *Quality Assurance Records Management*, Quality Assurance Manual 1Q, Procedure 17-1, current revision.

Software Classification Document (2018) *Geochemical Modeling for Performance Assessment, The Geochemist's Workbench*, K-SWCD-A-00002, Rev. 5, October 22, 2018.

Appendix A. Installation and Test Report for The Geochemist's Workbench®, Release 10.0.10

A.1 Objective

This report provides five acceptance tests and the associated results for the qualification of The Geochemist's Workbench® (GWB), Release 10.0.10. The results are documented according to the Software Quality Assurance Plan (SQAP) for GWB and according to Quality Assurance Manual 1Q, Procedure 20-1, *Software Quality Assurance* (Savannah River Site, 2018). Acceptance of this documentation satisfies the quality assurance requirements for GWB Release 10.0.10. This appendix may also be used as a template for qualifying future releases of GWB.

A.2 Software Description

GWB is a geochemical modeling suite for simulating the reactive fate and transport of radionuclides and other metals in aqueous systems including groundwater, surface water, soil, and sediment. At the Savannah River National Laboratory, GWB plays an important role in the preparation of Performance Assessments involving cementitious materials. GWB was originally developed by the University of Illinois at Urbana-Champaign and is currently supported by Aqueous Solutions LLC, located in the Research Park at the University of Illinois. The principal use for GWB is to manipulate aqueous chemical reactions, calculate stability diagrams and the equilibrium states of natural waters, trace reaction processes, model reactive transport, plot the results of these calculations, and store the related data.

A.3 Method

Testing will be performed in accordance with the five principal functional requirements outlined in Section 6.1 of the SQAP following the installation of the software, but prior to general use. The five test cases are sample problems provided by Bethke (2008) in *Geochemical and Biogeochemical Reaction Modeling* and shall be used to verify proper functionality of the GWB software. By completing each test and documenting that the results satisfy the specified acceptance criteria, the software shall be qualified.

A.4 Qualification Tests

The five acceptance tests are presented in Table A.4-1. Testing was performed on a LENOVO 43536F0 computer with a 64-bit Microsoft Windows 10 Enterprise operating system (Version 1703, OS Build 15063.1387). If a new operating system is installed, revalidation will be performed as necessary.

A.4.1 Requirement 1: Equilibrium Calculations (High Priority)

Function: Software must have the ability to calculate the equilibrium distribution of aqueous species in a fluid for chemical systems and processes.

Performance: Vendor literature describes how to create and run a system or process equilibrium model using the **React** application within GWB.

User Interface: User must define the system or process using either the **React** interface or an input text file. In the latter case, the text file is copied into or read by the **React** interface.

External Interface: None.

Acceptance Criteria: The creation of an equilibrium model as described in the vendor literature will be tested. Comparison of test results to vendor-published results will be made.

Table A.4-1. Test Cases for The Geochemist's Workbench® Qualification Testing.

Test Case	Capability Tested	Section
TC-01	Requirement 1: Equilibrium Calculations (High Priority)	A.4.1
TC-02	Requirement 2: Activity-Activity Diagrams of Mineral Stability and Predominance of Aqueous Species in Chemical Systems (Medium Priority)	A.4.2
TC-03	Requirement 3: Reaction Path Diagrams of User-Defined Chemical Systems (Medium Priority)	A.4.3
TC-04	Requirement 4: Modifiable Thermodynamic Database (Medium Priority)	A.4.4
TC-05	Requirement 5: Reaction Transport Modeling (Medium Priority)	A.4.5

A.4.2 Requirement 2: Activity-Activity Diagrams of Mineral Stability and Predominance of Aqueous Species in Chemical Systems (Medium Priority)

Function: Software must have the ability to calculate and plot activity-activity diagrams to show the stability of minerals and predominance of aqueous species in chemical systems.

Performance: Vendor literature describes how to create and plot an activity-activity diagram for a chemical system using the **Act2** application within GWB.

User Interface: User must define the system using either the **Act2** interface or an input text file. In the latter case, the text file is copied into or read by the **Act2** interface.

External Interface: None.

Acceptance Criteria: The creation of activity-activity diagrams as described in the vendor literature will be tested. Comparison of test results to vendor-published results will be made.

A.4.3 Requirement 3: Reaction Path Diagrams of User-Defined Chemical Systems (Medium Priority)

Function: Software must have the ability to calculate reaction path diagrams (initial and final reaction conditions) for conditions in the user-defined chemical systems.

Performance: GWB includes an application (**Act2**) to calculate reaction path diagrams that show stability of minerals at equilibrium and an application (**React**) to calculate equilibrium conditions at the beginning and end of a specified reaction path. Both applications rely on thermodynamic data in the user-specified thermodynamic database.

User Interface: User must define the system in either the application interface or an input text file. In the latter case, the text file is copied into or read by the **Act2** interface.

External Interface: None.

Acceptance Criteria: Output from **Act2** and **React** will be compared to published calculations by Bethke (2008).

A.4.4 Requirement 4: Modifiable Thermodynamic Database (Medium Priority)

Function: Software must include a thermodynamic database that can be modified to include minerals found in the user-defined chemical systems.

Performance: The default thermodynamic database (thermo.dat) for the GWB software provides fundamental data for calculation of thermodynamic properties for an extensive list of aqueous species and minerals. However, the ability to modify and add to the default thermodynamic database is necessary.

User Interface: The default GWB database may be copied and modified using a text editor. When an application of GWB is run, the default thermo.dat database is used for thermodynamic calculations. Because the default database will be modified for modeling of user-defined chemical systems, users must specify the modified database with the GWB data command.

External Interface: None.

Acceptance Criteria: The GWB default database must be modifiable using a standard text editor.

A.4.5 Requirement 5: Reaction Transport Modeling (Medium Priority)

Function: Software must have the ability to perform transport calculations (advection, dispersion, and molecular diffusion) along with the reaction model.

Performance: GWB software includes applications (**X1t** and **X2t**) to account for transport and chemical reaction calculations. In **X1t**, an unreacted fluid of a specified composition can enter either end of a model domain and react as it passes along a linear or radial coordinate. The flow of fluid along the domain displaces reacted fluid from the opposite end. In **X2t**, transport and reactions are similar except flow can occur in two dimensions and fluid can enter and leave the domain at wells (i.e., specified locations within the domain).

User Interface: User must define the system in either the application interface or an input text file. In the latter case, the text file is copied into or read by the **X1t** or **X2t** interface.

External Interface: None.

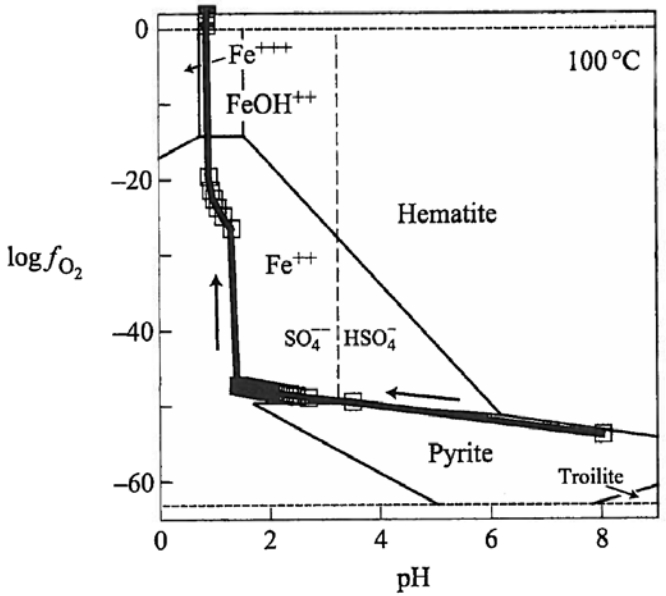
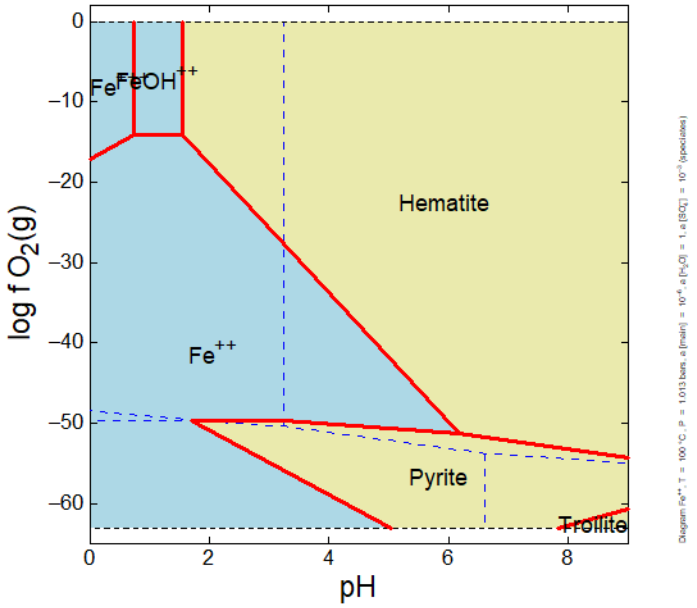
Acceptance Criteria: An **X1t** model will be created and tested as described in the vendor literature. Comparison of test results with vendor-published results will be made.

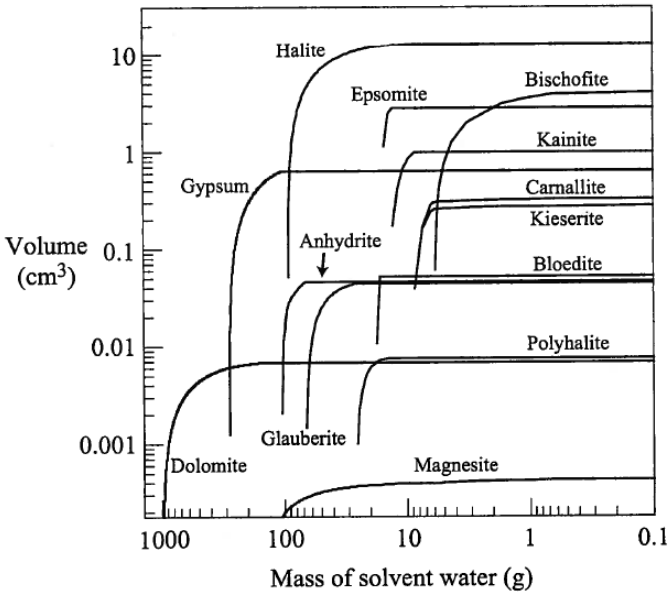
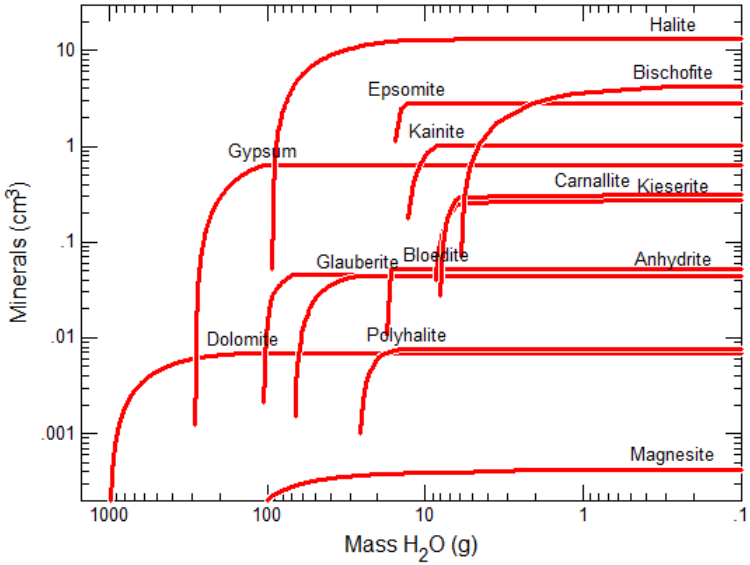
A.5 GWB Testing Results

Table A.5-1 provides the results of the five functional test cases for Release 10.0.10 of the GWB software.

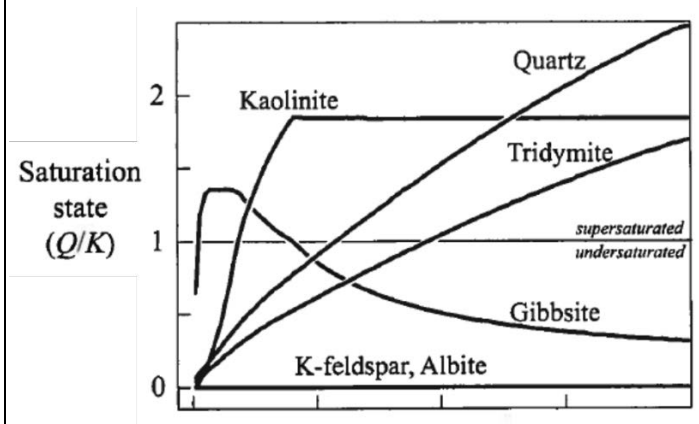
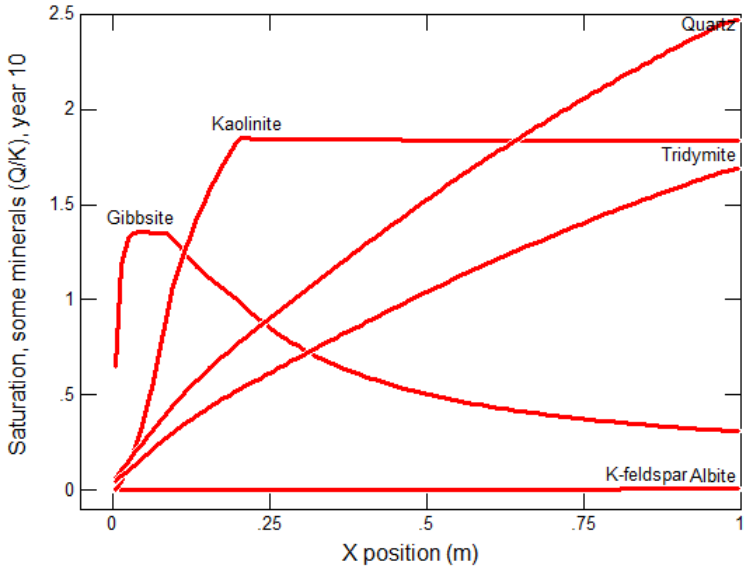
Table A.5-1. Results of The Geochemist's Workbench® (Release 10.0.10) Qualification Testing

Computer Name or Identifier: V0056315		**Operating System:** Microsoft Windows 10 Enterprise; Version 1703, OS Build 15063.1387	
Test Case	**Published Results**	**Test Case Results**	**Test Pass/ Fail**
TC-01	Table 6.4. *Calculated molalities (m), activity coefficients (γ), and log activities (a) of the most abundant species in seawater* Species / *m* / *γ* / log *a* Cl^- 0.5500 0.6276 −0.4619 Na^+ 0.4754 0.6717 −0.4958 Mg^{++} 0.3975×10^{-1} 0.3160 −1.9009 SO_4^{--} 0.1607×10^{-1} 0.1692 −2.5657 K^+ 0.1033×10^{-1} 0.6276 −2.1881 $MgCl^+$ 0.9126×10^{-2} 0.6717 −2.2125 $NaSO_4^-$ 0.6386×10^{-2} 0.6717 −2.3676 Ca^{++} 0.5953×10^{-2} 0.2465 −2.8334 $MgSO_4$ 0.5767×10^{-2} 1.0 −2.2391 $CaCl^+$ 0.3780×10^{-2} 0.6717 −2.5953 NaCl 0.2773×10^{-2} 1.0 −2.5571 HCO_3^- 0.1498×10^{-2} 0.6906 −2.9851 $CaSO_4$ 0.8334×10^{-3} 1.0 −3.0792 $NaHCO_3$ 0.4447×10^{-3} 1.0 −3.3519 $O_2(aq)$ 0.2151×10^{-3} 1.1735 −3.5980 $MgHCO_3^+$ 0.1981×10^{-3} 0.6717 −3.8760 KSO_4^- 0.1869×10^{-3} 0.6717 −3.9013 $MgCO_3$ 0.1068×10^{-3} 1.0 −3.9715 $SiO_2(aq)$ 0.8188×10^{-4} 1.1735 −4.0174 KCl 0.5785×10^{-4} 1.0 −4.2377 CO_3^{--} 0.5437×10^{-4} 0.1891 −4.9879	Aqueous species / molality / mg/kg sol'n / act. coef. / log act. Cl- 0.5499 1.881e+04 0.6276 -0.4620 Na+ 0.4754 1.055e+04 0.6717 -0.4958 Mg++ 0.03975 932.3 0.3160 -1.9009 SO4-- 0.01606 1489. 0.1692 -2.5657 K+ 0.01033 389.8 0.6276 -2.1881 MgCl+ 0.009125 526.1 0.6717 -2.2126 NaSO4- 0.006386 733.5 0.6717 -2.3676 Ca++ 0.005954 230.3 0.2465 -2.8334 MgSO4 0.005767 669.8 1.0000 -2.2391 CaCl+ 0.003780 275.5 0.6717 -2.5954 NaCl 0.002772 156.3 1.0000 -2.5572 HCO3- 0.001498 88.22 0.6906 -2.9851 CaSO4 0.0008334 109.5 1.0000 -3.0791 NaHCO3 0.0004447 36.05 1.0000 -3.3519 O2(aq) 0.0002151 6.640 1.1734 -3.5980 MgHCO3+ 0.0001981 16.31 0.6717 -3.8759 KSO4- 0.0001869 24.37 0.6717 -3.9013 MgCO3 0.0001068 8.687 1.0000 -3.9715 SiO2(aq) 8.188e-05 4.747 1.1734 -4.0174 KCl 5.784e-05 4.161 1.0000 -4.2378 CO3-- 5.437e-05 3.148 0.1891 -4.9879	*Pass*

Computer Name or Identifier: V0056315		**Operating System:** Microsoft Windows 10 Enterprise; Version 1703, OS Build 15063.1387	
Test Case	**Published Results**	**Test Case Results**	**Test Pass/ Fail**
TC-02	Chapter 15, Figure 15.9 (Bethke 2008) 		*Pass*

Computer Name or Identifier: V0056315		**Operating System:** Microsoft Windows 10 Enterprise; Version 1703, OS Build 15063.1387	
Test Case	**Published Results**	**Test Case Results**	**Test Pass/ Fail**
TC-03	Chapter 24, Figure 24.9 (Bethke 2008) 		*Pass*

Computer Name or Identifier: V0056315		**Operating System:** Microsoft Windows 10 Enterprise; Version 1703, OS Build 15063.1387	
Test Case	**Published Results**	**Test Case Results**	**Test Pass/ Fail**
TC-04	Original Database "thermo.tdat" -end- 624 minerals (BaO)2^(SiO2)3(c) type= formula= mole vol.= 122.8000 cc mole wt.= 486.9117 g 4 species in reaction -4.000 H+ 2.000 Ba++ 3.000 SiO2(aq) 2.000 H2O 24.8965 23.3104 21.2301 19.2286 17.2446 15.6907 14.3849 13.0572 (BaO)2^SiO2(c) type= formula= mole vol.= 66.6800 cc mole wt.= 366.7431 g 4 species in reaction -4.000 H+ 2.000 Ba++ 1.000 SiO2(aq) 2.000 H2O 48.3839 44.5743 40.1033 36.0058 31.9993 28.8545 26.2582 23.8785 (UO2)3(PO4)2(c) type= formula= mole vol.= 0.0000 cc mole wt.= 1000.0261 g 3 species in reaction -2.000 H+ 2.000 HPO4-- 3.000 UO2++ -25.2122 -26.3391 -27.9315 -29.7108 -31.9013 -34.0653 500.0000 500.0000 (VO)3(PO4)2(c) type= formula= mole vol.= 0.0000 cc mole wt.= 390.7651 g 3 species in reaction -2.000 H+ 3.000 VO++ 2.000 HPO4-- 48.8314 48.8314 500.0000 500.0000 500.0000 500.0000 500.0000 500.0000	Modified database to include Ettringite, Monosulfate, and Hydrotalcite -end- 634 minerals * Molar volume of CSH set to give a mineral density of 2.72 g/cc for sa Ettringite type= formula= Ca6Al2O6(SO4)3^32H2O mole vol.= 716.92 cc mole wt.= 1255.0990 g 5 species in reaction -12.000 H+ 6.000 Ca++ 2.000 Al+++ 3.000 SO4-- 38.000 H2O 500.0000 57.1500 500.0000 500.0000 500.0000 500.0000 500.0000 500.0000 Monosulfate type= formula= Ca4Al2O6(SO4)^12H2O mole vol.= 319.15 cc mole wt.= 622.5190 g 5 species in reaction -12.000 H+ 4.000 Ca++ 2.000 Al+++ 1.000 SO4-- 18.000 H2O 500.0000 72.6600 500.0000 500.0000 500.0000 500.0000 500.0000 500.0000 * Molar volume of Hydrotalcite set to give a mineral density of 2.72 g/ Hydrotalcite type= formula= Mg4Al2O7^10H2O mole vol.= 162.989 cc mole wt.= 443.331 g 4 species in reaction -14.000 H+ 4.000 Mg++ 2.000 Al+++ 17.000 H2O 500.0000 73.7800 500.0000 500.0000 500.0000 500.0000 500.0000 500.0000 (BaO)2^(SiO2)3(c) type= formula= mole vol.= 122.800 cc mole wt.= 486.9117 g 4 species in reaction -4.000 H+ 2.000 Ba++ 3.000 SiO2(aq) 2.000 H2O 24.8965 23.3104 21.2301 19.2286 17.2446 15.6907 14.3849 13.0572 (BaO)2^SiO2(c) type= formula=	*Pass*

Computer Name or Identifier: V0056315		**Operating System:** Microsoft Windows 10 Enterprise; Version 1703, OS Build 15063.1387	
Test Case	**Published Results**	**Test Case Results**	**Test Pass/ Fail**
TC-05	Chapter 27, Figure 27.3 (Bethke 2008) 		*Pass*

A.6 Conclusions

The results from these five test cases demonstrate that the GWB software is functioning correctly as intended and is appropriate for use in qualified work. As a result, GWB, Release 10.0.10 passes acceptance testing and is considered qualified for use within the environment tested.

A.7 References

Bethke, C. M. (2008) *Geochemical and Biogeochemical Reaction Modeling*, 2nd Ed., Cambridge University Press, New York.

Savannah River Site (2018) *Software Quality Assurance*. Quality Assurance Manual 1Q, Procedure 20-1, current revision.

Distribution:

dave.crowley@srnl.doe.gov
john.dickson@srnl.doe.gov
james.dyer@srnl.doe.gov
gregory.flach@srs.gov
nancy.halverson@srnl.doe.gov
steven.hommel@srs.gov
jocelyn.lampert@srnl.doe.gov
barry.lester@srs.gov
jeremiah.mangold@srs.gov
luke.reid@srnl.doe.gov
kent.rosenberger@srs.gov
Records Management (EDWS)
EM File, 773-42A – Rm. 243
(1 file copy and 1 electronic copy)