Software Quality Assurance Plan (SQAP) for The Geochemist's Workbench™

November 2010

Prepared by: Savannah River Remediation LLC
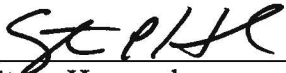Closure and Waste Disposal Authority
Aiken, SC 29808

SRR
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Remediation

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APPROVALS

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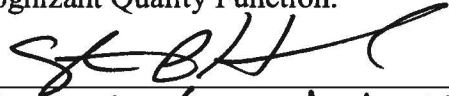
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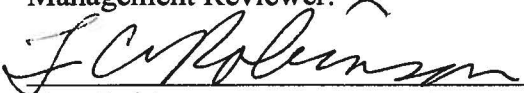
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ACRONYMS/ABREVIATIONS

C&WDA	Closure and Waste Disposal Authority
CQF	Cognizant Quality Function
CTF	Cognizant Technical Function
GWB	Geochemist's Workbench
LWO	Liquid Waste Organization
OS	Operating System
QA	Quality Assurance
RID	Requirement Identifier
SQAP	Software Quality Assurance Plan
SRR	Savannah River Remediation
SRS	Savannah River Site
TC	Test Case
UIUC	University of Illinois at Urbana-Champaign

1.0   SCOPE

This Software Quality Assurance Plan (SQAP) was developed in accordance with the 1Q Quality Assurance Manual, Procedure 20-1, Rev. 11.   This document defines the software quality assurance requirements for the software: The Geochemist's Workbench™ (GWB). The GWB is Level C software (see software classification document). [B-SWCD-C-00032]

This is existing software, acquired from and developed by the University of Illinois at Urbana-Champaign (UIUC). This document evaluates the GWB to determine the acceptability of the software for its intended use. The principal use of this software is to manipulate 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.   The software contains tools for balancing reactions, calculating activity diagrams, computing speciation in aqueous solutions, plotting the results of these calculations, and storing the related data. [SRR-CWDA-2010-00105] The GWB shall be used within Closure & Waste Disposal Authority (C&WDA) to support conceptual modeling of waste releases for use in performance assessment calculations and modeling and other similar activities [WSRC-STI-2007-00544].

2.0   ROLES AND RESPONSIBILITIES

The Software Owner is the individual or organization assigned to perform the detailed design, development, implementation, and testing activities for the GWB. The Software Owner reviews and approves change requests and ensures that all required reviews and approvals are completed for the project deliverables.

The Cognizant Technical Function (CTF) is a technical individual or individuals within C&WDA assigned to review and approve the software lifecycle document(s), to ensure that all required reviews and approvals are completed, and to accept the software for operational use.

The Cognizant Quality Function (CQF) is the Quality Assurance (QA) designated individual responsible for quality assurance support to the electronic aids. The CQF reviews and approves the SQAP.

The Management Reviewer is the manager within C&WDA Assessments who shall review and approve the SQAP.

3.0   SOFTWARE QUALITY ASSURANCE REQUIREMENTS

The GWB is an acquired/existing code, subject to the evaluation requirements described in 1Q Quality Assurance Manual, Procedure 20-1, Rev. 11. To ensure completeness, Table 3.0-1 provides a roadmap between the documentation requirements for quality assurance and the requirements described within this SQAP. The requirements described within the following sections must be satisfied for the qualification of the GWB.

Table 3.0-1: Roadmap to QA Software Documentation Requirements

Software QA Documentation Requirement	SQAP Approach for Satisfying Requirement
Software Classification	Software Classification Document for the Geochemist's Workbench [B-SWCD-C-00032]
Software Quality Assurance Plan	This entire document: SRR-CWDA-2010-00154
Lifecycle Activities – Requirements Phase	SRR-CWDA-2010-00154, Section 3.1.1
Lifecycle Activities – Design Phase	SRR-CWDA-2010-00154, Section 3.1.2
Lifecycle Activities – Implementation Phase	SRR-CWDA-2010-00154, Section 3.1.2
Lifecycle Activities – Testing Phase	SRR-CWDA-2010-00154, Section 3.1.3
Lifecycle Activities – Installation and Acceptance Phase	SRR-CWDA-2010-00154, Section 3.1.3
Lifecycle Activities – Operations and Maintenance	SRR-CWDA-2010-00154, Section 3.1.4
Lifecycle Activities – Retirement	SRR-CWDA-2010-00154, Section 3.1.5
Configuration Control	SRR-CWDA-2010-00154, Section 3.2
Evaluation	This entire document: SRR-CWDA-2010-00154
Problem Reporting & Corrective Action	SRR-CWDA-2010-00154, Section 3.3
Failure Analysis	SRR-CWDA-2010-00154, Section 3.4
Software Security Controls	SRR-CWDA-2010-00154, Section 3.5

3.1   Lifecycle Activities

This section describes the requirements related to the lifecycle activities for GWB.

3.1.1   Lifecycle Activities – Technical/Functional Requirements

The 1Q Quality Assurance Manual, Procedure 20-1, Rev. 11, Section D.2 provides the minimum requirements for developing software requirements. The requirements described below meet these requirements.

3.1.1.1   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.exe application of GWB.

User Interface: User must define the system or process either in the React.exe interface or in a text file. In the latter case, the text file is copied or read into the React.exe interface.

External Interface: None

Acceptance Criteria: The creation of an equilibrium model as described in the vendor literature will be tested.

3.1.1.2 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.exe application of GWB.

User Interface: User must define the system either in the Act2.exe interface or in a text file. In the latter case, the text file is copied or read into the Act2.exe interface.

External Interface: None

Acceptance Criteria: The creation of activity-activity diagrams as described in the vendor literature will be tested.

3.1.1.3 Requirement 3: Activity-Activity Diagrams of Reaction Paths of User-Defined Chemical Systems (Medium Priority)

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

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

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

External Interface: None

Acceptance Criteria: The output of Act2.exe and React.exe will be compared to published calculations.

3.1.1.4 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 GWB software default thermodynamic database (thermo.dat) 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 text editor.

3.1.2 Lifecycle Activities – Design and Implementation

The 1Q Quality Assurance Manual, Procedure 20-1, Rev. 11, Sections D.3 and D.4 provide the minimum requirements for software design and implementation. The following documentation meets these requirements.

As the GWB is an acquired/existing code, the design and implementation of the software is documented within the following vendor-generated document: *GWB Essentials Guide* (Bethke, C. M., 2005 1980). [SRR-CWDA-2010-00105]

3.1.3 Lifecycle Activities – Installation, Testing, and Acceptance

The 1Q Quality Assurance Manual, Procedure 20-1, Rev. 11, Sections D.5 and D.6 provide the minimum requirements for software installation, testing, and acceptance.

As the GWB is an acquired/existing code, the installation, acceptance, and testing of the software is documented within the following vendor-generated document: *GWB Essentials Guide* (Bethke, C. M., 2005 1980). [SRR-CWDA-2010-00105] Testing shall be performed in a manner that is consistent with vendor instructions.

The code, and any associated input and configuration files, shall be placed under configuration management controls as described in Section 3.2, below.

3.1.4 Lifecycle Activities – Operation and Maintenance

Approval from the Reviewing Manager and the Software Owner 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. 11, Section D.7, and Section 3.2 of this SQAP.

3.1.5 Lifecycle Activities – Retirement

When the retirement is foreseeable, this SQAP shall be revised to address the specifics of the retirement process that will terminate support and prevent routine use of the electronic aid. Retirement of old versions of software shall be managed as part of the standard revision process.

3.2 Configuration Management/Baseline Control

During the development of this SQAP, documentation and files shall be managed according to C&WDA document management practices, per SRR-CWDA-2009-00053. After development, any changes to this document (or any related documents) shall be subject to approval from the Reviewing Manager, CTF, CQF and the Software Owner. In the event of any updates or changes, a Revision History section shall be added to this SQAP to describe the changes.

Vendor-created documents related to GWB have been submitted to the Liquid Waste Organization (LWO) document library, per SRR-CWDA-2009-00053. The LWO Document Library is a Savannah River Site (SRS)-internal Lotus Notes application that serves as a file and document repository.

Additionally, any files provided by the vendor (including GWB executable files, data files, and database files) shall be subject to configuration management and baseline controls.

After successful installation and testing according to vendor instructions, these files shall be controlled by limiting user-access (through password protection) to the computer containing the vendor-provided files.

3.3 Problem Reporting and Corrective Action

Software users who identify errors within the GWB shall notify the Software Owner. The Software Owner or Reviewing Manager, or delegate, shall assess the error(s) to determine impact and path forward, and (if required) shall contact the ORNL for correction. Since the GWB is a purchased code, maintenance to correct software errors will be made and tested by the vendor according to the vendor's discretion.

3.4 Failure Analysis

As the GWB is existing, "Class C" software, and the code was developed by UIUC and is widely distributed and used throughout the Department of Energy complex, a failure analysis of this code is deemed unnecessary.

3.5 Software Security Controls

Computer Security shall be applied per Cyber Security Manual 10Q. If users identify any security-related issues, they should be reported according to Section 3.3.

3.6 Acquisition or Procurement

The GWB is existing software that has been acquired from UIUC. A controlled copy of the software is maintained by the primary user(s) at the Savannah River National Laboratory (SRNL), therefore procurement instructions are not necessary.

3.7 Tools, Techniques, Methods, Standards, Practices, and Conventions

There are no tools, techniques, methods, standards, practices and conventions to describe, other than those reflected in the other sections. This section shall remain within the SQAP in case future revisions require text to be added.

3.8 Quality Assurance Records/Documentation

This document shall be submitted to Document Control. In addition, any documents containing results from CTF or CQF reviews shall be submitted to Records Management as QA records.

4.0 TRAINING

Training for the GWB shall be completed by reading this SQAP and any associated procedures or documents. No additional training is required.

5.0   REFERENCES

1Q Quality Assurance Manual, Procedure 20-1.

10Q Computer Security Manual.

B-SWCD-C-00032, Software Classification Document for The Geochemist's Workbench^{TM}, Aiken, SC. November 2010.

SRR-CWDA-2009-00053, Dyer, C., et al., Closure & Waste Disposal Authority (C&WDA) Desktop Guidelines for General Office Practices, Savannah River Site, Aiken, SC, May 2010.

SRR-CWDA-2010-00105 (Copyright), *GWB Essentials Guide,* The Geochemist's Workbench Release 8.0, Department of Geology, University of Illinois, Urbana, IL, August 3, 2010. http://www.geology.uiuc.edu/Hydrogeology/hydro_gwb.htm.

WSRC-STI-2007-00544, Denham, M. E., *Conceptual Model of Waste Release from the Contaminated Zone of Closed Radioactive Waste Tanks,* Savannah River Site, Aiken, SC, Rev. 2, April 2010.