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Software Quality Assurance Plan for ReadFlowFields.dll for the Savannah River Site's Liquid Waste Program

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ACRONYNMS / ABBREVIATIONS

C&WDA	Closure & Waste Disposal Authority
DB	Database
GTG	GoldSim© Technology Group
HTF	H-Area Tank Farm
N/A	Not Applicable
SP	Service Pack
SQAP	Software Quality Assurance Plan

1.0 INTRODUCTION

This report documents the Software Quality Assurance Plan (SQAP) for the FORTRAN software ReadFlowFields.dll. ReadFlowFields.dll is a dynamic link library designed to be used in conjunction with the Liquid Waste Program's area-specific GoldSim©-based Stochastic Fate and Transport Models. ReadFlowFields.dll, Version 1.0 is classified as Quality Assurance "Level C" software on the basis that it performs a reading function for models based on a commercially available software used to comply with regulatory laws, environmental permits or regulations and/or commitments to compliance. [B-SWCD-C-00040]

1.1 Scope

This SQAP has been developed in accordance with the following procedure: 1Q, *Quality Assurance Manual*, Procedure 20-1, *Software Quality Assurance*.

This SQAP provides qualification instructions for the use of the FORTRAN software ReadFlowFields.dll in conjunction with the Liquid Waste Program's area-specific (e.g. H-Area Tank Farm (HTF)) Stochastic Fate and Transport Model software and applies to any activities used to support the Savannah River Site's Liquid Waste Program.

This SQAP is applicable to FORTRAN software ReadFlowFields.dll version 1.0.

This SQAP is applicable to the qualification of FORTRAN software ReadFlowFields.dll within any operating environment (operating system, network server, laptop computer, or desktop computer), providing that operating environment supports installation and testing of FORTRAN dynamic link library ReadFlowFields.dll.

1.2 Background

The FORTRAN software ReadFlowFields.dll software is designed to allow an Area-specific Stochastic Fate and Transport Model to sample from a set of flow fields described by data assembled in one or multiple input files. This is the initial ReadFlowFields.dll SQAP (*Software Quality Assurance Plan*) developed and used for performance assessment activities.

1.3 Roles and Responsibilities

The following describes the pertinent roles and responsibilities, as needed to qualify this software.

The **Software User** is any individual who will use any of the Liquid Waste Program's Area-specific Stochastic Fate and Transport Model, with the appropriate dynamic link library function, according to provisions of this SQAP and B-SQP-C-00002. All Software Users are responsible for reading this SQAP and adhering to specified plan to ensure that any version(s) of ReadFlowFields.dll that they use for qualified work has been appropriately qualified on the environment(s) in which the software is being used.

The **Software User's Manager** is any individual with management authority over the Software User.

The **Software Developer** is the individual responsible for the development of this SQAP, the software, and associated software quality assurance documentation.

The **GoldSim© Qualification Lead** (see also B-SQP-C-00002) is the individual responsible for maintaining a record of which versions and environments have been qualified to support the Savannah River Site's Liquid Waste Program.

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

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

2.0 SOFTWARE DESCRIPTION

ReadFlowFields.dll is a FORTRAN based dynamic link library that is called by Area-specific Stochastic Fate and Transport Model software to allow the model to sample and read in the sampled flow fields generated by PORFLOW-based PA models. The Area-specific Stochastic Fate and Transport Model software are used to model the transport of radionuclide contaminants from waste disposal and closure facilities at the Savannah River Site. The Monte Carlo/Latin Hypercube functionality of the Area-specific Stochastic Fate and Transport Model software allows probabilistic sampling of the flow field and when used in conjunction with ReadFlowFields.dll the subsequent reading in of the chosen flow field from one or more input files.

Consistent with this software's use and classification, and pursuant to Section 5.10 of 1Q Procedure 20-1, ReadFlowFields.dll is not Safety Software; therefore, this software is excluded from the Safety Software Inventory List.

2.1 Developed Software

ReadFlowFields.dll is a dynamic link library, developed by SRR. As such, this software is classified as "developed".

The dynamic link library is provided with copies of the Area-specific Stochastic Fate and Transport Model, along with the necessary input files. To qualify the newly-installed software, users should follow the instructions for installation testing as defined in Section 4.5, below.

2.2 Training

Due to the nature of the relationship between ReadFlowFields.dll and the Area-specific Stochastic Fate and Transport Models, the dynamic link library is automatically loaded into the GoldSim©-based model and training is not required to operate this appended software. However, as a prerequisite to using GoldSim©, users should have experience operating a computer with a Windows operating system and should read and understand this SQAP and B-SQP-C-00002. Additionally, it is recommended that new users perform vendor-provided tutorials, as described within the *GoldSim User's Guide, Volumes 1 & 2*, to become familiar with this software. [GTG-2010c]

3.0 SOFTWARE QUALIFICATION

Table 3.0-1 maps each of the software qualification requirements from 1Q Procedure 20-1 to text within the associated qualifying documentation.

Table 3.0-1: Software Requirements Matrix

Software Qualification Activities	Document	Section
Software Classification	Software Classification Document, B-SWCD-C-00040	Entire Document
Software Quality Assurance Procedures/Plans	SQAP: B-SQP-C-00003	Entire Document
Safety Software Inventory Listing	SQAP, B-SQP-C-00003	Section 2.0
Requirements, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.1
Design, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.2
Implementation, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.3
Testing, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.4
Installation and Acceptance, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.5 and Attachment 1
Operations & Maintenance, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.6
Retirement, Life Cycle Phases	SQAP, B-SQP-C-00003	Section 4.7
Configuration Management/Baseline Control	SQAP, B-SQP-C-00003	Section 5.0
Problem Reporting & Corrective Action	SQAP, B-SQP-C-00003	Section 5.1
Cyber Security Controls	SQAP, B-SQP-C-00003	Section 5.2
Risk and Safety Analysis	SQAP, B-SQP-C-00003	Section 5.2

4.0 SOFTWARE LIFE CYCLE REQUIREMENTS

Pursuant to 1Q Procedure 20-1, there are seven phases to the software life cycle that shall be considered and documented, as appropriate. These seven phases are:

- Requirements
- Design
- Implementation
- Testing
- Installation & Acceptance
- Operations & Maintenance
- Retirement

Each software life cycle phase is discussed below.

4.1 Life Cycle Phase: Requirements

ReadFlowFields.dll is developed to read in flow fields and other flow control data from output files generated from Area-specific Stochastic Fate and Transport Model simulations. The functional requirements of dynamic link library include the reading in of 1-dimensional tables of time histories of Darcy velocities, volumetric flows, saturations, and cap infiltration rates generated by PORFLOW simulations. In addition, ReadFlowFields.dll must extract scalar data, including pore volumes, transition times and saturated zone cross flow rates from tables provided in the PORFLOW generated input files. The PORFLOW generated input files contain a series of two-dimensional tables from which the data is extracted. The Area-specific Stochastic Fate and Transport Models, provide instructions to ReadFlowFields.dll indicating which file contains the appropriate data, the location of the two-dimensional tables within the file the data will be extracted from, and which columns contain the required data.

4.2 Life Cycle Phase: Design

ReadFlowFields.dll is a FORTRAN-based dynamic link library designed to take instructions from Area-specific Stochastic Fate and Transport Models and return the requested data to the GoldSim© based model. The instructions (data) to be passed from the GoldSim©-based model are listed in Table 4.2-1 below.

Table 4.2-1: Instruction Data Passed to ReadFlowFields.dll

Number	**Variable Name**	**Variable Meaning**
1	LocNumber	The location of the desired table in a file of ordered two-dimensional tables each table representing a PORFLOW flow simulation.
2	File Number	The position of the required input file name in a ReadFlowFields.dll control file
3	szTable	The number of dependent-variable columns in the referenced table
4	FileExt	File extension number if desired (normally set to zero)
5	NTimeD	The number of the columns containing Darcy velocity, volumetric flows and saturations to be returned to the GoldSim© model
6	InfilIndex	The position of the infiltration data in the output returned to the GoldSim© model
7 thru the number of variables -1	Variable Names	The position of dependent-variable column in the referenced table for each one-dimensional table or scalar variable to be returned is found (note that the column number is based on the dependent variables only so that the first three columns representing the run index and time are not considered in determining the position of the columns)
Final Line	Blank	A zero indicating that no more data is requested

ReadFlowFields.dll will then return either one-dimensional tables of time versus dependent variable or scalar variables to the GoldSim©-based model. The types of data returned to the GoldSim©-based model are listed in Table 4.2-2 below.

Table 4.2-2: Data Extracted from the Flow Field Files

Data	**Form**	**Units**
Darcy Velocities	One-Dimensional Table	cm/yr
Volumetric Flows	One-Dimensional Table	cm^3/yr
Saturations	One-Dimensional Table	N/A
Pore Volumes	Scalar	cm^3
pH Transition Times	Scalar	yr
Eh Transition Times	Scalar	yr
Infiltration Rate	One-Dimensional Table	cm/yr
Cross Flow Rate	Scalar	cm/yr

4.3 Life Cycle Phase: Implementation

The dynamic link library ReadFlowFields.dll was written and compiled in FORTRAN using Intel® Fortran Compiler XE 12.1, used in conjunction with using Microsoft© Visual Studio 2010 Version 10.0.30319.1. The dynamic link library is called using GoldSim©'s external function which passes the instructions through its input interface to the dynamically allocated variable *input()* in ReadFlowFields.dll. The dynamic link library ReadFlowFields.dll then assigns the requested data to the 1-dimensional variable array *output()* with the structure of the vector variable controlled by the output interface of the external function element. The required structure of the external function interface and the general structure of the FORTRAN model are described in Appendix C of GTG-2010c.

4.4 Life Cycle Phase: Testing

The dynamic link library ReadFlowFields.dll was tested using a simple GoldSim© model TestProblem1.gsm in conjunction with the stochastic input file based on PORFLOW flow model output files. The software correctly reconstructed the one-dimensional time histories and scalar variables read from the PORFLOW model generated files, and imported into the GoldSim© environment. TestProblem1.gsm and its results are also used as an installation and acceptance test as described below in Section 4.5. In addition to the DLL test problem, the correctness of the linkage between the Area-specific models (e.g. the H-Area Tank Farm (HTF) Stochastic Fate and Transport Model, Version 1.0) is checked as part of the model's QA plan.

4.5 Life Cycle Phase: Installation & Acceptance

The test case noted in Section 4.4 is also used to demonstrate acceptable installation and performance of ReadFlowFields.dll. As a prerequisite to performing this test, the Software User must have a registered version of GoldSim© that is Version 10.50 (SP2) or newer. The test case uses the aforementioned GoldSim© model file (*TestProblem1.gsm*) in conjunction with ReadFlowFields.dll for verification purposes. The test case is set up to read the flow parametric study flow-field data for the seventh sample a TypeII tank, for the Case E configuration, to evaluate the capability of the software to link to and interface correctly with a GoldSim© external element. Instructions for performing the test case, and evaluating the results, are described below (see Tables 4.5-1, 4.5-2, and 4.5-3).

The test case was developed by creating a simple GoldSim© model that is set up to use ReadFlowFields.dll to read the flow data for a Type II Tank. To evaluate the correctness of the dynamic link library, ReadFlowFields.dll was used to import the specific the parameters listed in Table 4.2-2, into the GoldSim© model.

Software users should run the simplified GoldSim© model and then compare the results to those posted in Table 4.5-2. Results should match to three significant figures. Software Users should then document the results of the test case using the ReadFlowFields.dll Software Quality Assurance Test Form (see Attachment 1) and submit the completed form to the ReadFlowFields.dll Qualification Lead, consistent with the instructions provided in Section 5.0. If the Software User intends to qualify the DLL with multiple versions of GoldSim© or on different operating systems, they must complete and document a separate ReadFlowFields.dll Software Quality Assurance Test Form for each version of the GoldSim© and for each test environment to be qualified. For the purposes of this SQAP a test environment is the combination of the hardware (i.e., desktop computer, laptop computer, or server) and the operating system (e.g., Windows 7).

Table 4.5-1: Installation Test (Test Case 1)

Step	Task/Action	Expected Result from Task/Action
1	Contact the ReadFlowFields.dll Qualification Lead to request the test case files.	User has the following test case files: TestProblem1.gsm and ReadFlowFields.dll
Open the GoldSim© test case model file.		
2	On the computer desktop, go to Start → Programs → GoldSim©.	The GoldSim© Launch Window will appear (see Figure 4.5-1). Note: The appearance of this window may vary between software versions.
3	Click "Open Model"	An Open file dialogue pops up.
4	Navigate to and select the model file: *TestProblem1.gsm.*	The model file opens (see Figure 4.5-2).
Run the model deterministically.		
5	In the GoldSim© Tool Bar, go to Run → Run Model.	The "GoldSim© Run Controller" appears (see Figure 4.5-3).
6	On the "GoldSim© Run Controller" click the "Run" button.	The model will begin to run deterministically and read in the desired data. This should take approximately two to three seconds.
7	If a warning message appears, asking to display the "run log file", select "No".	The warning message closes.
Verify and document the model results.		
8	To check your results for the time series listed in Table 4.5-2, double-click on each look-up table and click on the "View Data" button.	The results found in each look-up table element should be comparable (to three significant figure) to the results presented in Table 4.5-2
9	To check your results for the scalar parameters listed in Table 4.5-3, move your cursor over the green arrow on each expression element.	The results found in each expression element should be comparable (to three significant figures) to the results presented in Table 4.5-3
10	Document the results of Test Case 1 using the GoldSim© Software Quality Assurance Test Form (see Attachment 1).	Test Case 1 and verification testing is complete.

Figure 4.5-1: GoldSim© Launch Window

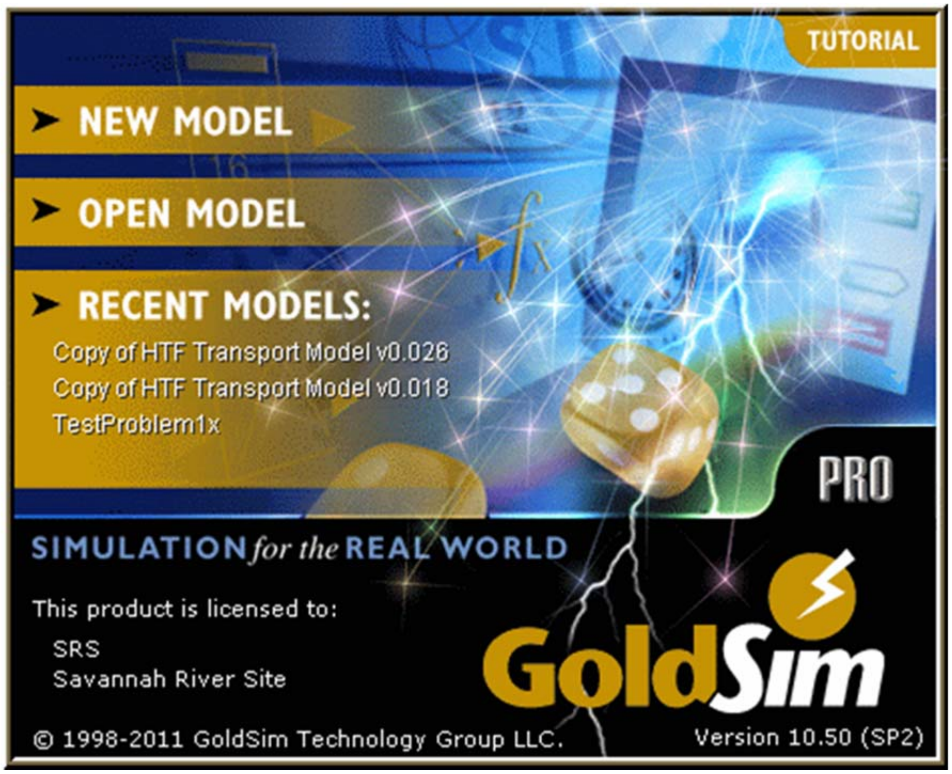

Figure 4.5-2: GoldSim© Test Case Model File

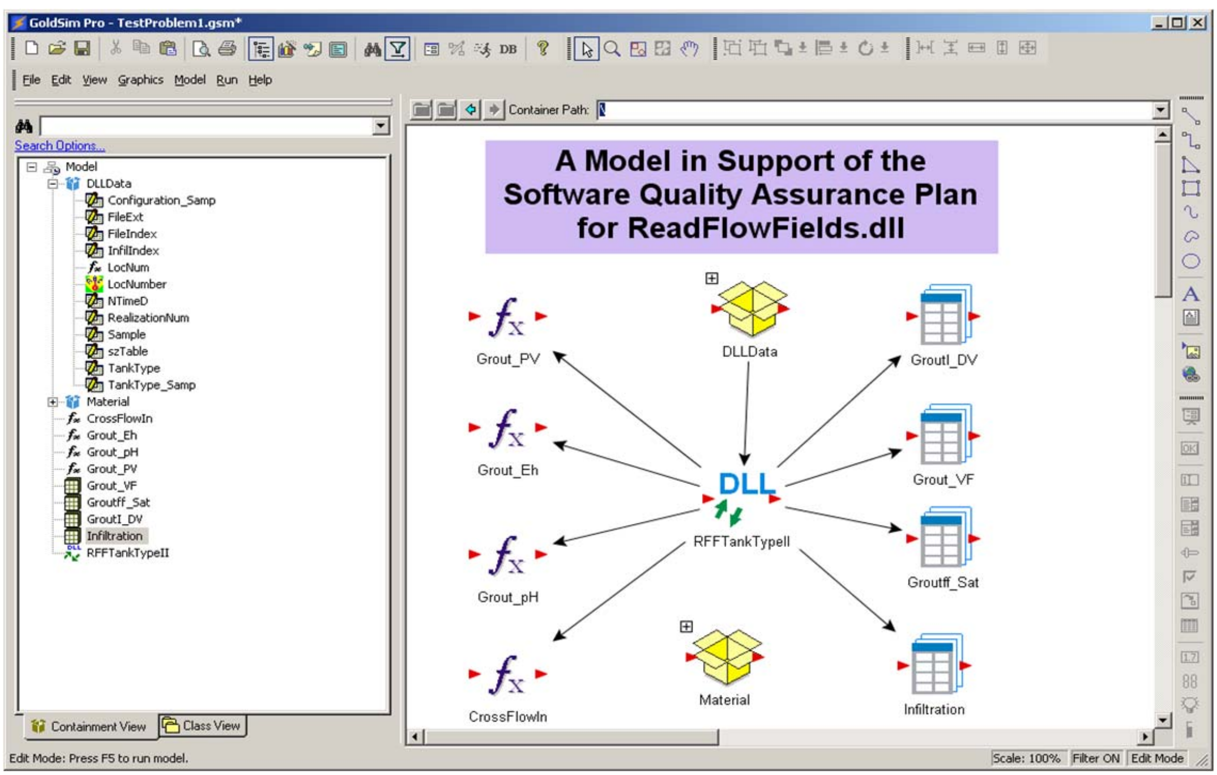

Figure 4.5-3: GoldSim© Run Controller

Table 4.5-2: Installation Test Results for Time Series Data (Test Case 1)

Time (years)	GroutI_DV (cm/yr)	Grout_VF(cm3/yr)	Groutff_Sat	Infiltration (cm/yr)
0	-2.54E-06	245.231	0.306777	0.0079
50	-5.36E-06	517.027	0.359191	0.0193
100	-2.80E-06	58.0989	0.896134	0.2773
200	-9.94E-07	7.30542	1	0.7702
300	-3.87E-07	2.9006	1	2.8099
400	-3.13E-07	2.17609	1	5.4561
500	-4.14E-07	2.918	1	7.9257
600	-4.96E-07	3.5422	1	11.2577
800	-5.75E-07	4.09484	1	15.6259
1000	-6.23E-07	4.42473	1	18.965
1200	-6.59E-07	4.67965	1	21.275
1400	-7.10E-07	5.04597	1	24.1625
1700	-1.44E-06	10.4502	1	27.3389
2200	-3.91E-07	3.33928	1	28.4476
2506	-0.0614787	414793	0.447414	28.8899
2550	-0.704092	3678140	0.447259	29.0906
2700	-1.71824	8892310	0.446532	29.2068
3100	-5.88881	30084800	0.442594	29.2982
3500	-19.5533	95176600	0.42399	29.3473
4000	-28.7086	128519000	0.405284	29.3994
4500	-29.1802	129194000	0.404479	29.4567
5100	-29.2884	129817000	0.404952	29.5087
5500	-29.337	130828000	0.405556	29.5426
6000	-29.3517	132540000	0.406386	29.5548
6500	-29.3457	135572000	0.407495	29.5661
7000	-28.9841	144044000	0.408765	29.5832
8000	-28.9011	154183000	0.409887	29.6002
8500	-28.8919	155532000	0.410052	29.6116
9000	-28.9032	155590000	0.410075	29.623
9500	-28.9145	155648000	0.410097	29.6343
10000	-28.9202	155677000	0.410109	29.64
11000	-28.9202	155677000	0.410109	29.64
12000	-28.9202	155677000	0.410109	29.64
12687	-28.9202	155677000	0.410109	29.64

Table 4.5-2: Installation Test Results for Time Series Data (Test Case 1) (Continued)

Time (years)	GroutI_DV (cm/yr)	Grout_VF(cm3/yr)	Groutff_Sat	Infiltration (cm/yr)
13000	-28.9202	155677000	0.410109	29.64
13500	-28.9202	155677000	0.410109	29.64
14500	-28.9202	155677000	0.410109	29.64
16700	-28.9202	155677000	0.410109	29.64
17500	-28.9202	155677000	0.410109	29.64
20000	-28.9202	155677000	0.410109	29.64
100000	-28.9202	155677000	0.410109	29.64

Table 4.5-3: Installation Test Results for Scalar Data (Test Case 1)

Parameter	Element	Scalar Value
Pore Volume of Grout (cm3)	Grout_PV	8.67389 E+08
Grout Eh Transition Time (yr)	Grout_Eh	6976
Grout pH Transition time (yr)	Grout_pH	15952
Grout Crossflow Rate (cm/yr)	CrossFlowIn	480

4.6 Life Cycle Phase: Operations & Maintenance

The graded approach for qualification of developed, Class C software requires justification for exceptions to documenting Operations & Maintenance Phase requirements (per 1Q Procedure 20-1). Operation of this software is performed by running GoldSim© based software, as described within the vendor-provided *GoldSim User's Guide, Volume 2, Appendix C*. [GTG-2010c].

This software is developed to support Performance Assessments. As such, any problems associated with the use of this software should be reported to the C&WDA Assessment Manager in accordance with Section 5.1. Maintenance will be performed by updating this software as necessary.

4.7 Life Cycle Phase: Retirement

The graded approach for qualification of developed, Class C software requires justification for exceptions to documenting Retirement Phase requirements (per 1Q Procedure 20-1). Routine use of this software shall be terminated at such a time that (1) suitable replacement software has been identified and qualified, (2) it has been determined that the need for this software no longer exists, or (3) conditions have changed that prevent this software from remaining qualified.

5.0 CONFIGURATION MANAGEMENT/BASELINE CONTROL

Configuration control is a method established to control, uniquely identify, describe, and document the configuration of each version of a computer program. ReadFlowFields.dll is a dynamic link library comprised of a FORTRAN module that performs a generalized reading function for use in conjunction with GoldSim©'s external function allowing time series and scalar variables to be read from external files and imported into the Liquid Waste Program's Area-specific Stochastic Fate and Transport Models. The software is automatically provided along with any versions of the Liquid Waste Program's Area-specific Stochastic Fate and Transport Models that have been implemented with the logic to read in flow data from external files. For this reason, the dynamic link library falls under the control of the Liquid Waste Program's GoldSim© Qualification Lead as opposed to the Software Developer.

Table 5.0-1 outlines the necessary steps to ensure proper configuration management of ReadFlowFields.dll software under this SQAP.

Table 5.0-1: ReadFlowFields.dll Software Configuration Managements Activities

Responsible Individual(s)	Step	Task/Activities
Software User and Software User's Manager	1	Identify the need to run a qualified version of the dynamic link library ReadFlowFields.dll.
Software User	2	Ensure that your computer contains a qualified version of GoldSim©, per B-SQP-C-00002.
	3	Perform Installation and Acceptance Tests, as described in Section 4.5 of this SQAP.
	4	Document the results of the Installation and Acceptance Tests by completing the ReadFlowFields.dll Software Qualification Test Form (see Attachment 1).
	5	Submit the completed ReadFlowFields.dll Software Quality Assurance Test Form to the GoldSim©l Qualification Lead.
GoldSim© Qualification Lead	6	Review and approve the completed ReadFlowFields.dll Software Quality Assurance Test Form.

In addition to these steps, the GoldSim© Qualification Lead shall maintain control of the Installation and Acceptance Test files (described in Section 4.5) and keep a record of all instances of GoldSim© software and associated dynamic link libraries that have been qualified according to this SQAP.

After qualification, the Software User shall notify the GoldSim© Qualification Lead of any changes to the computing environment that would adversely affect the qualification of GoldSim© (e.g., the operating system is updated or the software is removed).

5.1 Problem Reporting and Corrective Action

Software Users shall report all software problems to the C&WDA Assessments Manager. The C&WDA Assessments Manager shall document the issue in accordance with Manual 1B, Procedure 4.23, Corrective Action Program, including determining impacts and a path forward. The Software Developer will revise the software and requalify as needed. Users will be notified of revisions.

5.2 Software Security Controls (Risks and Safety)

Computer Security shall be applied per the 10Q, *Cyber Security Manual*. Any Software User who identifies a security-related issue shall immediately report the issue according to Cyber Security Manual 10Q.

5.3 Quality Assurance Records/Documentation

This document shall be submitted to Document Control as a Quality Assurance record. In addition, electronic copies of completed Attachment 1 forms (ReadFlowFields.dll Software Quality Assurance Test Form) shall be submitted to Records Management in accordance with Manual 1B, Procedure 3.31, Records management.

6.0 REFERENCES

1Q Manual, Procedure 20-1, *Quality Assurance Manual*, *Software Quality Assurance*, Savannah River Site, Aiken, SC, Rev. 13, October 14, 2011.

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7.0 GLOSSARY

Deterministic Simulation	A simulation in which the input parameters are represented using single values (i.e., they are "determined" or assumed to be known with certainty). [GTG-2010c]
GoldSim©	A highly graphical, object-oriented computer program for carrying out dynamic, probabilistic simulations. [GTG-2010c]
Model	An abstract representation of system.
Monte Carlo Simulation	A method for propagating (translating) uncertainties in model inputs into uncertainties in model results. [GTG-2010c]
Performance Assessment	An analysis that estimates the impact (e.g., dose) of a system (e.g., liquid waste closure system), usually over time and within the bounds of a regulatory framework.
Probabilistic Simulation	A simulation in which the uncertainty in input parameters is explicitly represented by defining them as probability distributions. [GTG-2010c]
Realization	A single model run within a Monte Carlo simulation. It represents one possible path the system could follow through time. [GTG-2010c]
Simulation	The implementation of a mathematical model of a system within a specific computational tool (or set of tools). [GTG-2010c]
Stochastic	A process that often has some underlying trend or pattern, but inherently has a random component, and as a result, can only be described statistically.

ATTACHMENT 1: READFLOWFIELDS.DLL SOFTWARE QUALITY ASSURANCE TEST FORM

ReadFlowFields.dll Version Example: Version 1.0	
GoldSim Version Example: Version 10.50	
Computer ID Example: V0042##	
Operating System Example: Windows 7	

Software User Training

Per Section 2.2 of the SQAP, Software User:	**Software User Initials:**
Has experience operating a computer with a Windows operating system. (Required)	
Has read and understood the SQAP. (Required)	
Has performed vendor-provided GoldSim© software tutorials. (Recommended, but not required)	

Quality Assurance Test Results

Test Case	**Pass**	**Fail**
	(Check One)	
Test Case 1: Installation and Verification Test Upon completion of Test Case 1, results within the executed GoldSim model file match (to three significant figures) the results as indicated in Tables 4.5-1, 4.5-2 and 4.5-3.		

Approvals

Software User	Print	
	Sign	
	Date	

ReadFlowFields.dll Qualification Lead	Print	
	Sign	
	Date	