B-SQP-C-00003

Revision 1

Key Words
ReadPORFLOWData.dll
Stochastic Fate and Transport Model
GoldSim©
C&WDA
Software
Quality Assurance

Retention: Permanent

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

June 4, 2013

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

Prepared for U.S. Department of Energy Under Contract No. DE-AC09-09SR22505

APPROVALS

Design Agency Qualification Lead:

Barry Lester
C&WDA Assessments
Savannah River Remediation LLC

6/5/2013
Date

Independent Reviewer:

Steven Hommel
C&WDA Assessments
Savannah River Remediation LLC

6/4/2013
Date

Cognizant Quality Function:

Vince Cordaro
Quality Assurance
Savannah River Remediation LLC

6/4/2013
Date

Management Review/Design Authority:

Kent Rosenberger
C&WDA Assessments
Savannah River Remediation LLC

6/4/2013
Date

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ACRONYNMS / ABBREVIATIONS

C&WDA	Closure & Waste Disposal Authority
DB	Database
DLL	Dynamic Link Library
GTG	GoldSim© Technology Group
HTF	H-Area Tank Farm
N/A	Not Applicable
SDF	Saltstone Disposal Facility
SP	Service Pack
SQAP	Software Quality Assurance Plan
SRR	Savannah River Remediation

1.0 INTRODUCTION

This report documents the Software Quality Assurance Plan (SQAP) for the FORTRAN-developed software: *ReadPORFLOWData.dll*, formerly called *ReadFlowFields.dll*. The change in the software's name reflects updates to the software which allow it to be used in a more general manner to read additional types and structures of PORFLOW-generated[1] data. *ReadPORFLOWData.dll* is a dynamic link library (DLL) designed to be used in conjunction with the Liquid Waste Program's area-specific GoldSim©-based Stochastic Fate and Transport Models. *ReadPORFLOWData.dll* Version 2.0 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-developed software *ReadPORFLOWData.dll* in conjunction with the Liquid Waste Program's area-specific (e.g. the H-Area Tank Farm (HTF) or Saltstone Disposal Facility (SDF)) 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 the qualification of FORTRAN-developed software *ReadPORFLOWData.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 *ReadPORFLOWData.dll*.

1.2 Background

The FORTRAN-developed software *ReadPORFLOWData.dll* is designed to allow an Area-specific Stochastic Fate and Transport Model to sample from a set of flow field data, time-dependent diffusion coefficient data, or radionuclide breakthrough curves presented in table form in one or multiple input files. This is Revision 1 of the *ReadFlowFields.dll* SQAP (*Software Quality Assurance Plan*) developed and used for performance assessment activities. To reflect the model updates that extend the software's usage to reading additional types of data, all further references to the software or associated documents will replace the name *ReadFlowFields.dll* with the name *ReadPORFLOWData.dll*.

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,

[1] Note that PORFLOW is modeling software used to simulate groundwater flow and contaminant transport. [WSRC-STI-2007-00150; SRNL-TR-2010-00213]

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 *ReadPORFLOWData.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

ReadPORFLOWData.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, time histories of diffusion coefficients, or radionuclide release breakthrough curves 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 data and when used in conjunction *ReadPORFLOWData.dll* the subsequent reading in of the chosen data set 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, *ReadPORFLOWData.dll* is not Safety Software; therefore, this software is excluded from the Safety Software Inventory List.

2.1 Developed Software

ReadPORFLOWData.dll is a dynamic link library, developed by Savannah River Remediation (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 *ReadPORFLOWData.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 the SQAP for GoldSim©: 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

ReadPORFLOWData.dll is developed to read tables containing flow fields and other flow control data, time-dependent diffusion coefficients, and radionuclide release breakthrough curves from output files generated from Area-specific Stochastic Fate and Transport Model simulations. The functional requirements of the DLL include the reading in of 1-dimensional tables of time histories for Darcy velocities, volumetric flows, saturations, cap infiltration rates, diffusion coefficients, and radionuclide release breakthrough curves generated by PORFLOW simulations. In addition, *ReadPORFLOWData.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 *ReadPORFLOWData.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

ReadPORFLOWData.dll is a FORTRAN-based DLL 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.

ReadPORFLOWData.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.

Enhancements found in *ReadPORFLOWData.dll*, relative to Version 1.0, include:

- Allowing stochastic data to be read from single files in a nested set of folders (see included folder SaltstoneData1),
- Allowing the number of time steps in the single files to be variable, and
- Allowing for importing diffusion coefficients and radionuclide UZ release rates.

Reading stochastic data from single multi-realization files as originally done by *ReadFlowFields.dll* Version 1.0 is still allowed, but minor changes to the GoldSim© External element interface must be updated to reflect the structure described in Table 4.2-1.

Table 4.2-1: Instruction Data Passed to *ReadPORFLOWData.dll*

Number	Variable Name	Variable Meaning
1	FileExt	File extension number if desired (normally set to zero)
2	FileIndex	File number of file to be used
3	LocNumber	The location of the desired table in a file of ordered two-dimensional tables each table representing a PORFLOW flow simulation.
4	szTable	The number of dependent-variable columns in the referenced table
5	Indep	Column containing the independent Variable (time)
6	Depend	Column containing the first dependent Variable
7	Iname	0 = Data for all realizations are in a single file; 1 = Data for each realization are in a different file
8	IDU	Unit indicator for file (i.e. SDU Type (1, 2 for FDCs, 4)) **Omit if Iname = 0**
9	IRLZ	The realization number
10 thru the number of dependent variables to be returned	Variable Names	The position of dependent-variable column in the referenced table for each one-dimensional table or scalar variable to be Note that that scalar data is indicated by using the negative of the column number (-5 for column 5)
Final Line	Blank	A zero indicating that no more data is requested

Table 4.2-2: Data Extracted from the Files

Data	Form	Units
Darcy Velocities [1]	One-Dimensional Table	cm/yr
Volumetric Flows [1]	One-Dimensional Table	cm^3/yr
Saturations [1]	One-Dimensional Table	N/A
Pore Volumes [1]	Scalar	cm^3
pH Transition Times [1]	Scalar	yr
Eh Transition Times [1]	Scalar	yr
Infiltration Rate [1]	One-Dimensional Table	cm/yr
Cross Flow Rate [1]	Scalar	cm/yr
Diffusion Coefficients [2]	One-Dimensional Table	cm^2/s
Radionuclide Breakthrough Curves [3]	One-Dimensional Table	mol/yr

[1] from flow data file(s)
[2] from diffusion coefficient data file(s)
[3] from radionuclide release rate data file(s)

4.3 Life Cycle Phase: Implementation

The DLL, *ReadPORFLOWData.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 DLL is called using GoldSim©'s external function which passes the instructions through its input interface to the dynamically allocated variable *input()* in *ReadPORFLOWData.dll*. The 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 DLL, *ReadPORFLOWData.dll*, was tested using two simple GoldSim© models, TestProblemQA1.gsm and TestProblemQA2.gsm, in conjunction with the stochastic input file based on PORFLOW-generated files. The software correctly reconstructed the one-dimensional time histories and scalar variables read from the PORFLOW files, and imported into the GoldSim© environment. TestProblemQA1.gsm and its results are also used as an installation and acceptance test as described below in Section 4.5.

4.4.1 TestProblemQA1

The testing criteria for TestProblemQA1 are presented in Section 4.5 which describes the installation and acceptance phase.

4.4.1 Test Problem QA2

The testing criteria for Test Problem QA2 used to evaluate the updates implemented in *ReadPORFLOWData.dll* Version 2.0 are presented in this section.

Test Problem QA2 uses the GoldSim file TestProblemQA2.gsm to test the ability of the DLL to read flow data, diffusion coefficients and radionuclide release rates from the nested folders found in the folder SaltstoneData1. The flow data imported by the DLL are presented in Tables 4.4-1 and 4.4-2. The time-dependent diffusion coefficients imported by the DLL are presented in Table 4.4-3. Due to the number of time steps involved and the size of the associated dataset, the Tc-99 release rates to the SZ imported into the GoldSim© model are graphically compared to the original data, as shown in Figure 4.4-1. The similarity between the two curves resulting from Test Problem QA2 indicates that *ReadPORFLOWData.dll* Version 2.0 shall be qualified for the intended use upon successful completion of Test Problem QA1 as described in Section 4.5.

Table 4.4-1: Flow Data Time Histories Imported in Test Problem QA2

Time (years)	SaltstoneI_DV (cm/yr)	Wall_DV (cm/yr)	Infiltration (cm/yr)	Wall_Sat
0	-4.420130E-07	-3.390220E-07	2.90E-03	9.705730E-01
50	-2.978570E-06	-3.382890E-06	6.60E-03	9.219500E-01
100	-5.903310E-05	-9.209390E-05	4.17E-02	8.937770E-01
150	-2.752710E-04	-8.078620E-04	1.06E-01	8.763770E-01
200	-6.152170E-04	-2.897200E-03	1.74E-01	8.614780E-01
250	-1.336730E-03	-1.212910E-02	3.44E-01	8.544140E-01
300	-2.435840E-03	-4.399010E-02	6.74E-01	8.510060E-01
350	-4.049690E-03	-1.373310E-01	1.25E+00	8.488480E-01
425	-5.782690E-03	-3.064630E-01	1.85E+00	8.460920E-01
500	-7.720680E-03	-5.841970E-01	2.51E+00	8.441910E-01
600	-9.964950E-03	-1.008720E+00	3.24E+00	8.433640E-01
700	-1.225130E-02	-1.562950E+00	3.96E+00	8.438560E-01
800	-1.452270E-02	-2.190760E+00	4.67E+00	8.440910E-01
900	-1.697940E-02	-8.238100E+00	5.12E+00	8.808120E-01
923	-1.816130E-02	-8.734660E+00	5.47E+00	8.827500E-01
1000	-2.135060E-02	-1.006600E+01	6.41E+00	8.884630E-01
1200	-2.621370E-02	-1.182380E+01	7.73E+00	8.953550E-01
1400	-2.124530E-01	-1.269840E+01	8.43E+00	8.971140E-01
1413	-3.226640E-01	-1.386510E+01	9.42E+00	9.014280E-01
1700	-3.319840E-01	-1.648430E+01	1.12E+01	9.082760E-01
1998	-3.416020E-01	-1.825310E+01	1.26E+01	9.127040E-01
2300	-3.436480E-01	-1.979490E+01	1.39E+01	9.165030E-01
2583	-3.493790E-01	-2.149990E+01	1.52E+01	9.199560E-01
2900	-3.507640E-01	-2.346720E+01	1.65E+01	9.232730E-01
3168	-3.539160E-01	-2.532970E+01	1.78E+01	9.263170E-01
3500	-3.547900E-01	-2.695810E+01	1.91E+01	9.289500E-01
3753	-3.526970E-01	-2.791640E+01	1.99E+01	9.305000E-01
3866	-5.526830E-01	-2.935880E+01	2.12E+01	9.328290E-01
4338	-3.665930E-01	-3.277890E+01	2.35E+01	9.368260E-01
4923	-4.195130E-01	-3.526720E+01	2.54E+01	9.395790E-01
5200	-4.634310E-01	-3.682530E+01	2.66E+01	9.412860E-01
5500	-5.345500E-01	-3.727330E+01	2.69E+01	9.417670E-01
6000	-6.306370E-01	-3.734140E+01	2.69E+01	9.418300E-01
6500	-6.682310E-01	-3.747760E+01	2.69E+01	9.420060E-01
7000	-8.499060E-01	-3.748280E+01	2.69E+01	9.419540E-01
7500	-1.000010E+00	-3.754620E+01	2.69E+01	9.419990E-01

Table 4.4-1: Flow Data Time Histories Imported in Test Problem QA2 (Continued)

Time (years)	SaltstoneI_DV (cm/yr)	Wall_DV (cm/yr)	Infiltration (cm/yr)	Wall_Sat
8000	-9.880360E-01	-3.774600E+01	2.69E+01	9.422970E-01
8500	-1.172420E+00	-3.780520E+01	2.69E+01	9.423320E-01
9000	-1.242710E+00	-3.787860E+01	2.69E+01	9.423520E-01
9200	-1.207580E+00	-3.796880E+01	2.69E+01	9.424930E-01
9300	-1.441830E+00	-3.788400E+01	2.69E+01	9.423400E-01
9500	-1.454000E+00	-3.793240E+01	2.69E+01	9.423570E-01
9600	-1.522800E+00	-3.793660E+01	2.69E+01	9.423610E-01
9700	-1.339510E+00	-3.808970E+01	2.69E+01	9.426070E-01
9800	-1.575990E+00	-3.799480E+01	2.69E+01	9.424550E-01
9900	-1.620910E+00	-3.800850E+01	2.69E+01	9.424300E-01
10000	-1.497090E+00	-3.833570E+01	2.69E+01	9.428900E-01
11000	-1.908120E+00	-3.860520E+01	2.69E+01	9.430860E-01
12000	-2.826010E+00	-3.890560E+01	2.69E+01	9.432390E-01
13500	-3.750250E+00	-3.968370E+01	2.69E+01	9.441270E-01
15000	-5.086300E+00	-4.078980E+01	2.69E+01	9.453140E-01
16500	-6.250000E+00	-4.189350E+01	2.69E+01	9.462840E-01
17000	-8.157460E+00	-4.160580E+01	2.69E+01	9.458540E-01
18000	-1.193280E+01	-3.984000E+01	2.69E+01	9.440370E-01
18800	-1.661690E+01	-3.610670E+01	2.69E+01	9.398560E-01
18900	-1.838940E+01	-3.413350E+01	2.69E+01	9.377380E-01
19000	-1.981870E+01	-3.179640E+01	2.69E+01	9.352990E-01
19500	-1.987780E+01	-3.178890E+01	2.69E+01	9.352950E-01
19700	-1.991670E+01	-3.178910E+01	2.69E+01	9.352980E-01
20000	-2.183580E+01	-3.126350E+01	2.69E+01	9.348010E-01
50000	-2.420050E+01	-2.909660E+01	2.69E+01	9.321750E-01
100000	-2.420050E+01	-2.909660E+01	2.69E+01	9.321750E-01

Table 4.4-2: Scalar Flow Data Imported in Test Case QA2

Parameter	Element	Scalar Value
Wall Eh Transition Time	Wall_Eh	5919
Wall pH Transition Time	Wall_pH	8539

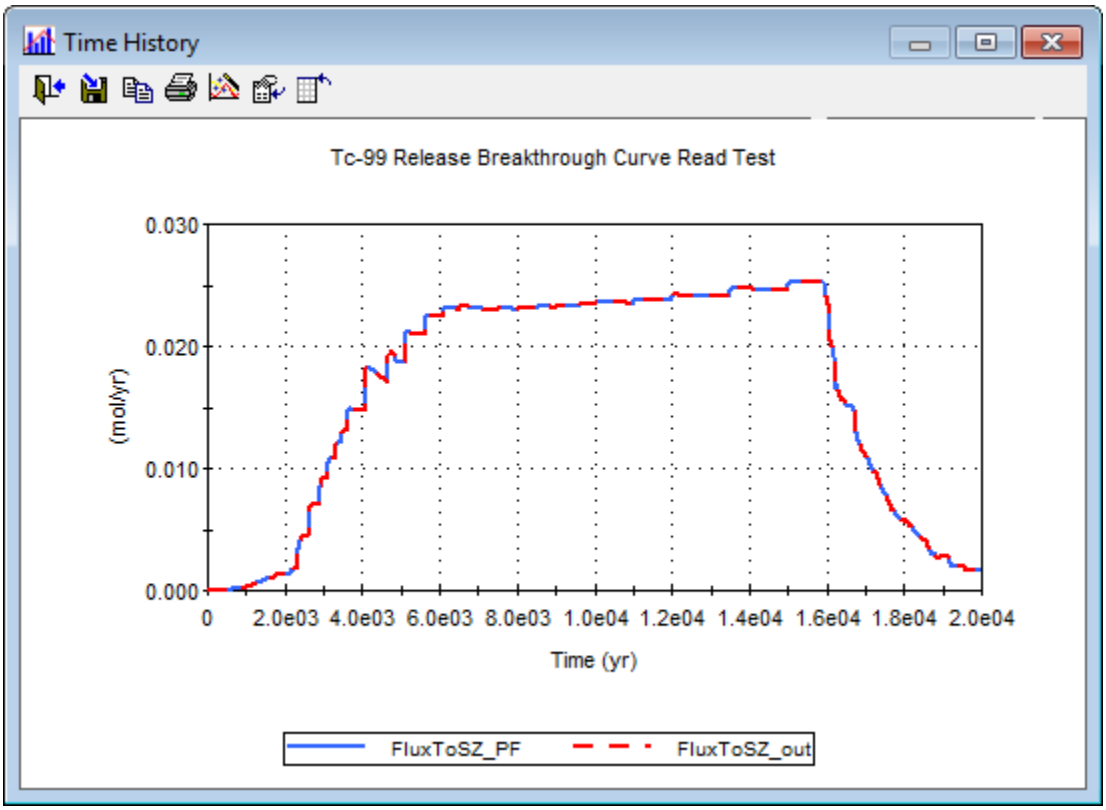
Table 4.4-3: Diffusion Coefficient Time Histories Imported in Test Problem QA2

Time (years)	UZ (cm^2/s)	Floor (cm^2/s)	Saltstone (cm^2/s)	Wall (cm^2/s)
0	5.296E-06	1.433E-07	9.989E-09	5.296E-06
50	5.296E-06	3.298E-07	9.989E-09	5.296E-06
100	5.296E-06	5.169E-07	9.989E-09	5.296E-06
150	5.296E-06	7.040E-07	9.989E-09	5.296E-06
200	5.296E-06	8.403E-07	9.989E-09	5.296E-06
224	5.296E-06	1.008E-06	9.989E-09	5.296E-06
290	5.296E-06	1.243E-06	9.989E-09	5.296E-06
350	5.296E-06	1.449E-06	9.989E-09	5.296E-06
400	5.296E-06	1.636E-06	9.989E-09	5.296E-06
450	5.296E-06	1.836E-06	9.989E-09	5.296E-06
507	5.296E-06	2.115E-06	1.097E-08	5.296E-06
600	5.296E-06	2.477E-06	1.303E-08	5.296E-06
700	5.296E-06	2.848E-06	1.516E-08	5.296E-06
800	5.296E-06	3.234E-06	1.728E-08	5.296E-06
900	5.296E-06	3.583E-06	1.941E-08	5.296E-06
1000	5.296E-06	4.154E-06	2.258E-08	5.296E-06
1200	5.296E-06	4.915E-06	2.689E-08	5.296E-06
1407	5.296E-06	5.296E-06	3.114E-08	5.296E-06
1600	5.296E-06	5.296E-06	3.520E-08	5.296E-06
1800	5.296E-06	5.296E-06	3.964E-08	5.296E-06
2000	5.296E-06	5.296E-06	4.471E-08	5.296E-06
2300	5.296E-06	5.296E-06	5.105E-08	5.296E-06
2600	5.296E-06	5.296E-06	5.739E-08	5.296E-06
2900	5.296E-06	5.296E-06	6.405E-08	5.296E-06
3200	5.296E-06	5.296E-06	6.913E-08	5.296E-06
3400	5.296E-06	5.296E-06	7.357E-08	5.296E-06
3600	5.296E-06	5.296E-06	7.991E-08	5.296E-06
4000	5.296E-06	5.296E-06	8.942E-08	5.296E-06
4500	5.296E-06	5.296E-06	9.989E-08	5.296E-06
5000	5.296E-06	5.296E-06	1.107E-07	5.296E-06
5500	5.296E-06	5.296E-06	1.211E-07	5.296E-06
6000	5.296E-06	5.296E-06	1.316E-07	5.296E-06
6500	5.296E-06	5.296E-06	1.424E-07	5.296E-06
7000	5.296E-06	5.296E-06	1.481E-07	5.296E-06
7035	5.296E-06	5.296E-06	1.484E-07	5.296E-06
7036	5.296E-06	5.296E-06	1.535E-07	5.296E-06
7500	5.296E-06	5.296E-06	1.636E-07	5.296E-06

Table 4.4-3: Diffusion Coefficient Time Histories Imported in Test Problem QA2 (Continued)

Time (years)	UZ (cm^2/s)	Floor (cm^2/s)	Saltstone (cm^2/s)	Wall (cm^2/s)
8000	5.296E-06	5.296E-06	1.741E-07	5.296E-06
8500	5.296E-06	5.296E-06	1.849E-07	5.296E-06
9000	5.296E-06	5.296E-06	1.899E-07	5.296E-06
9001	5.296E-06	5.296E-06	1.922E-07	5.296E-06
9200	5.296E-06	5.296E-06	1.963E-07	5.296E-06
9400	5.296E-06	5.296E-06	1.995E-07	5.296E-06
9500	5.296E-06	5.296E-06	2.017E-07	5.296E-06
9600	5.296E-06	5.296E-06	2.029E-07	5.296E-06
9624	5.296E-06	5.296E-06	2.042E-07	5.296E-06
9700	5.296E-06	5.296E-06	2.058E-07	5.296E-06
9800	5.296E-06	5.296E-06	2.080E-07	5.296E-06
9900	5.296E-06	5.296E-06	2.102E-07	5.296E-06
10000	5.296E-06	5.296E-06	2.220E-07	5.296E-06
11000	5.296E-06	5.296E-06	2.429E-07	5.296E-06
12000	5.296E-06	5.296E-06	2.695E-07	5.296E-06
13500	5.296E-06	5.296E-06	3.012E-07	5.296E-06
15000	5.296E-06	5.296E-06	3.330E-07	5.296E-06
16500	5.296E-06	5.296E-06	3.583E-07	5.296E-06
17383	5.296E-06	5.296E-06	3.742E-07	5.296E-06
18000	5.296E-06	5.296E-06	3.900E-07	5.296E-06
18800	5.296E-06	5.296E-06	3.995E-07	5.296E-06
18900	5.296E-06	5.296E-06	3.995E-07	5.296E-06
19000	5.296E-06	5.296E-06	4.059E-07	5.296E-06
19500	5.296E-06	5.296E-06	4.154E-07	5.296E-06
19700	5.296E-06	5.296E-06	4.186E-07	5.296E-06
100000	5.296E-06	5.296E-06	4.186E-07	5.296E-06

Figure 4.4-1: *ReadPORFLOWData.dll* Test Case Results for Test Problem QA2



4.5 Life Cycle Phase: Installation & Acceptance

The first case (TestProblemQA1.gsm) noted in Section 4.4 is also used to demonstrate acceptable installation and performance of *ReadPORFLOWData.dll*. As a prerequisite to performing this test, the Software User must have a registered version of GoldSim© that is Version 10.50 (SP3) or newer. The test case uses the aforementioned GoldSim© model file (*TestProblem1.gsm*) in conjunction with *ReadPORFLOWData.dll* for verification purposes. The test problem is set up to read flow-field data for a sample Type II waste tank to evaluate the capability of the software to link to and interface correctly with a GoldSim© external element. Instructions for performing the test, and evaluating the results, are described below (see Tables 4.5-1, 4.5-2, and 4.5-3).

The test problem was developed by creating a simple GoldSim© model that uses *ReadPORFLOWData.dll* to read the flow data for the Type II waste tank. To evaluate the correctness of the DLL, *ReadPORFLOWData.dll* was used to import the specific the parameters listed in Table 4.2-2, into the GoldSim© model.

Software users should follow the instructions in Table 4.5-1 to 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 problem using the *ReadPORFLOWData.dll* Software Quality Assurance Test Form (see Attachment 1) and submit the completed form to the *GoldSim* 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 *ReadPORFLOWData.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 Problem QA1)

Step	Task/Action	Expected Result from Task/Action
1	Contact the *GoldSim* Qualification Lead to request the test problem files.	User has the following test problem files: TestProblemQA1.gsm, ReadPFdata.in, GoldSim_CaseAFlowFields.txt, GoldSim_CaseBFlowFields.txt, GoldSim_CaseCFlowFields.txt, GoldSim_CaseDFlowFields.txt, GoldSim_CaseEFlowFields.txt, GoldSim_StochasticFlowFields.txt and ReadPORFLOWData.dll
Open the GoldSim© test problem 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: *TestProblemQA1.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. Note: If GoldSim© provides a warning message "Starting a new simulation will destroy your existing results. Are you sure you want to run again?" then click Yes and go to Step 7.	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 element (i.e., the four GoldSim© elements on the right of Figure 4.5-2) 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 (i.e., the four GoldSim© elements on the left of Figure 4.5-	The results found in each expression element should be comparable (to three significant figures) to the results presented in Table 4.5-3

	2).	
10	Document the results of Test Problem QA1 using the *ReadPORFLOWData.dll* Software Quality Assurance Test Form (see Attachment 1).	Test Problem QA1 and verification testing is complete.

Figure 4.5-1: GoldSim© Launch Window

Figure 4.5-2: GoldSim© Test Problem Model File

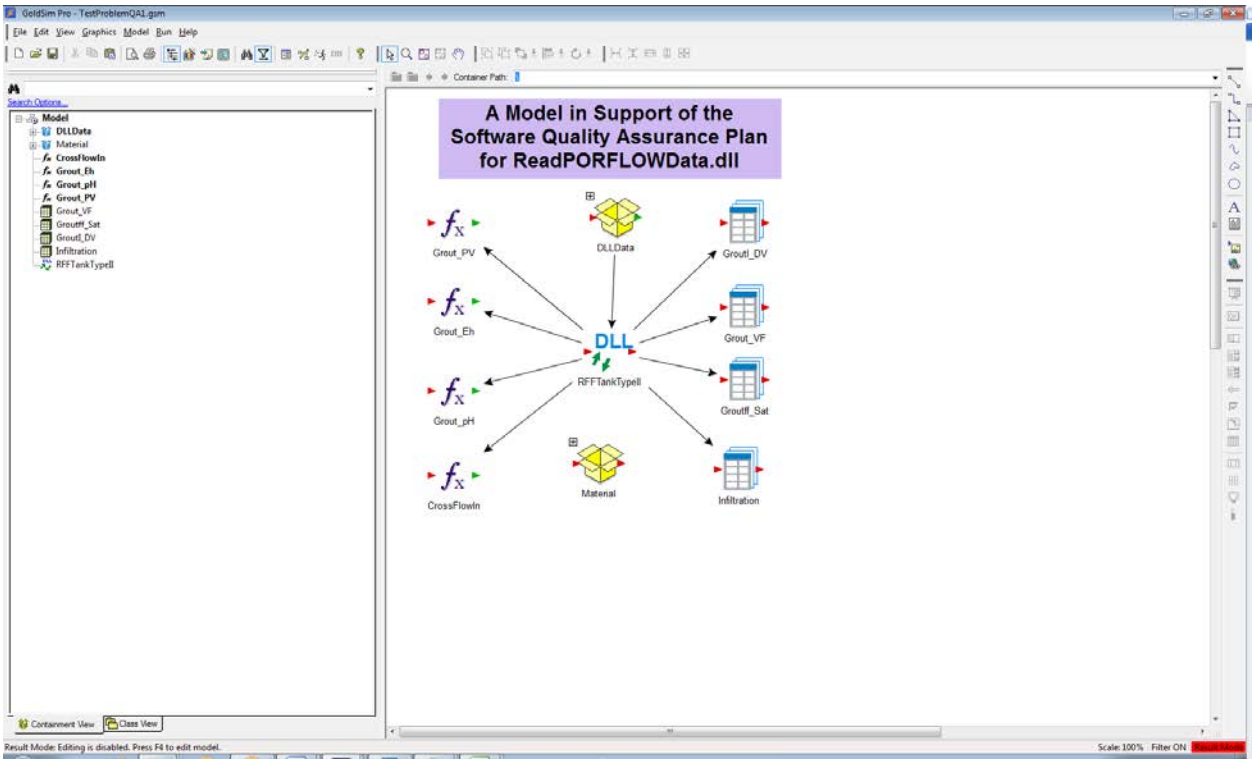


Figure 4.5-3: GoldSim© Run Controller

Table 4.5-2: Installation Test Results for Time Series Data (Test Problem QA1)

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 Problem QA1) (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 Problem QA1)

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© 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. *ReadPORFLOWData.dll* is a DLL 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 PORFLOW data from external files. For this reason, the DLL 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 *ReadPORFLOWData.dll* software under this SQAP.

Table 5.0-1: *ReadPORFLOWData.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 *ReadPORFLOWData.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 *ReadPORFLOWData.dll* Software Qualification Test Form (see Attachment 1).
	5	Submit the completed *ReadPORFLOWData.dll* Software Quality Assurance Test Form to the GoldSim© Qualification Lead.
GoldSim© Qualification Lead	6	Review and approve the completed *ReadPORFLOWData.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 (*ReadPORFLOWData.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.

10Q Manual, *Cyber Security Manual,* Savannah River Site, Aiken, SC, Rev. 3, October 2, 2009.

B-SQP-C-00002, Hommel, S., *Software Quality Assurance Plan for GoldSim© for Savannah River Site's Liquid Waste Program,* Savannah River Site, Aiken, SC, Rev. 0, April 23, 2012.

B-SWCD-C-00040, Lester, B., *Software Classification Document for ReadFlowFields.dll,* Savannah River Site, Aiken, SC, Rev. 0, June 4, 2012.

GTG-2010c (Copyright), *GoldSim User's Guide, Volumes 1 & 2,* GoldSim Technology Group LLC, Issaquah, WA, January 2010.

SRNL-TR-2010-00213, Whiteside, T., *Software Testing and Verification of PORFLOW Versions 6.30.1 and 6.30.2,* Savannah River Site, Aiken, SC, Rev. 0, July 2010.

WSRC-STI-2007-00150, Aleman, S., *PORFLOW Testing and Verification Document,* Savannah River Site, Aiken, SC, Rev. 0, June 2007.

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]
Fortran	A general-purpose programming language that is especially suited to numeric computation and scientific computing.
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.
PORFLOW	Modeling software used to simulate groundwater flow and contaminant transport. [WSRC-STI-2007-00150; SRNL-TR-2010-00213]
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: *READPORFLOWDATA.DLL* SOFTWARE QUALITY ASSURANCE TEST FORM

***ReadPORFLOWData.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 SQAPs for GoldSim© (B-SQP-C-0002) and *ReadPORFLOWData.dll* (B-SQP-C-0003). (Required)	
Has performed vendor-provided GoldSim© software tutorials. (Recommended, but not required)	

Quality Assurance Test Results

Test Case	**Pass** (Check One)	**Fail** (Check One)
Test Case 1: Installation and Verification Test Upon completion of Test Case QA1, results within the executed GoldSim© model file match (to three significant figures) the results as indicated in Tables 4.5-2 and 4.5-3.		

Approvals

Software User	Print	
	Sign	
	Date	

***ReadPORFLOWData.dll* Qualification Lead**	Print	
	Sign	
	Date	