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Key Words:
Performance Assessment
Software Quality Assurance

Retention:
Permanent

Software Testing and Verification of PORFLOW 6.21.0

Author: Tad Whiteside

January, 2010

Savannah River National Laboratory
Washington Savannah River Company
Savannah River Site
Aiken, SC 29808

Prepared for the U.S. Department of Energy Under
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REVIEWS AND APPROVALS

1/21/2010

Tad S. Whiteside, Author — Date
Environmental Science and Bio Technology, SRNL

1/21/2010

Gregory P. Flach, Technical Reviewer — Date
Environmental Science and Bio Technology, SRNL

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LIST OF ACRONYMS

ACRONYMS

DOE	U.S. Department of Energy
PA	Performance Assessment
QA	Quality Assurance
SRNL	Savannah River National Laboratory
SRNS	Savannah River Nuclear Solutions
SRS	Savannah River Site

1.0 SUMMARY

This report is the latest in the series of PORFLOW QA documents that identify differences between versions of PORFLOW and differences between PORFLOW and analytical results. This series is comprised of the following documents, in chronological order from oldest to newest: WSRC-STI-2007-00150, Rev. 0; G-TR-G-00002; SRNS-TR-2008-00003, Rev. 0.

This document compares 64-bit PORFLOW version 6.21.0 to 64-bit PORFLOW version 6.10.3 and 64-bit PORFLOW version 6.10.3 to 32-bit PORFLOW version 6.10.3 on the Linux operating system: Red Hat Enterprise Linux WS release 4 (Nahant Update 8).

There have been no new tests added to the test suite described in G-TR-G-00002; however a few of the input files have been modified to run on both PORFLOW version 6.10.3 and PORFLOW version 6.21.0, these modifications are described in the Method section.

Problems that differ between 64-bit PORFLOW versions 6.10.3 and 6.21.0:

- 5.8
- 5.9
- 6.5.1
- 8.2

None of the results differ between 64-bit PORFLOW version 6.10.3 and 32-bit PORFLOW version 6.10.3.

The problem numbers are from G-TR-G-00002. Only those problems that differ will be described below. The full problem descriptions can be found in WSRC-STI-2007-00150 Rev 0 and G-TR-G-00002.

The QA tests confirm PORFLOW version 6.21.0 on the Linux platform meets the needs of the tank and vault closure applications.

Solubility control should be implemented using the DIST (Mode 3) command. PROP TOTAl should be used to implement the preferred retardation definition. The DIST (Mode 1) and RETA functions do not perform correctly and are not used in this application.

2.0 OBJECTIVE

This document compares 64-bit PORFLOW version 6.21.0 to 64-bit PORFLOW version 6.10.3 and 64-bit PORFLOW version 6.10.3 to 32-bit PORFLOW version 6.10.3 on the Linux operating system: Red Hat Enterprise Linux WS release 4 (Nahant Update 8) using the problems described in WSRC-STI-2007-00150 Rev 0 and G-TR-G-00002.

3.0 METHOD

The method used to perform this QA is identical to that described in SRNS-TR-2008-00003, Rev. 0.

Due to changes in the PORFLOW source code, a few of the input files were modified to run on both the 6.10.3 and 6.21.0 versions. These modifications are:

- Changing the MATRix solver from NSPC to LUDE
- Specifying the TRANSport parameters for all species, even if those values are 0

These modifications had no impact on the results, with the exception of the solver, which resulted in minute changes of some results, well below their expected precision.

The input and output files are located on the High Performance Computing File System at the Savannah River National Lab, under the directory "/hpc/project/porflow_qa/".

4.0 SCOPE OF TEST PROBLEMS

The test problems were selected based on analytical solutions (or code-to-code comparisons) that definitively establish the code accuracy and the resulting impact of mesh and control parameter settings on the accuracy of results. Four groups of test problems are used to verify the capability of the software to represent the physical phenomena characteristic of groundwater flow and transport applications at the Savannah River Site.

They are:

Group 1: Saturated and variably saturated groundwater flow in one and two dimensions (steady-state and transient conditions).

Group 2: Contaminant transport in one, two and three dimensions (transient).

Group 3: Numerical dispersion.

Group 4: Keyword Commands (e.g. STATistics).

None of the results differ between 64-bit PORFLOW version 6.10.3 and 32-bit PORFLOW version 6.10.3. Only those problems that differ between PORFLOW versions 6.10.3 and 6.21.0 will be discussed below.

5.0 GROUP 1: GROUNDWATER FLOW PROBLEMS

5.8 FREE-SURFACE BOUSSINESQ FLOW WITH RECHARGE

There are minute differences between the results computed by PORFLOW versions 6.10.3 and 6.21.0. These differences are well below the precision limits.

5.9 FREE-SURFACE BOUSSINESQ FLOW WITH SEEPAGE

There are large differences between the results computed by PORFLOW versions 6.10.3 and 6.21.0. PORFLOW 6.10.3 has results that are very close to the analytical solution. PORFLOW version 6.21.0 results are identical for each of the different times and they all reach a maximum of 10 at a distance of 18m from the source. The results are included in Table 1.

Table 1. Analytical vs. PORFLOW 6.10.3 vs. PORFLOW 6.21.0

		t=9			t=36			t=81			t=144			t=225			t=324	
Distance(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)	COMSOL(m)	P-6.10.3(m)	P-6.21.0(m)
0	9	9.019	9.061	9	9.009	9.061	9	9.006	9.061	9	9.005	9.061	9	9.004	9.061	9	9.003	9.061
1	9.094	9.058	9.185	9.047	9.029	9.185	9.031	9.02	9.185	9.023	9.015	9.185	9.019	9.012	9.185	9.016	9.01	9.185
1	9.094	9.101	9.314	9.047	9.051	9.314	9.031	9.034	9.314	9.023	9.026	9.314	9.019	9.021	9.314	9.016	9.018	9.314
1	9.094	9.147	9.44	9.047	9.075	9.44	9.031	9.05	9.44	9.023	9.038	9.44	9.019	9.031	9.44	9.016	9.026	9.44
2	9.186	9.198	9.558	9.094	9.101	9.558	9.063	9.068	9.558	9.047	9.052	9.558	9.038	9.041	9.558	9.031	9.035	9.558
3	9.276	9.252	9.662	9.14	9.13	9.662	9.094	9.088	9.662	9.07	9.066	9.662	9.056	9.053	9.662	9.047	9.045	9.662
3	9.276	9.309	9.751	9.14	9.161	9.751	9.094	9.109	9.751	9.07	9.082	9.751	9.056	9.066	9.751	9.047	9.056	9.751
4	9.362	9.37	9.822	9.186	9.195	9.822	9.125	9.132	9.822	9.094	9.1	9.822	9.075	9.08	9.822	9.063	9.067	9.822
5	9.443	9.433	9.878	9.231	9.231	9.878	9.156	9.157	9.878	9.117	9.119	9.878	9.094	9.096	9.878	9.078	9.081	9.878
5	9.443	9.498	9.919	9.231	9.271	9.919	9.156	9.184	9.919	9.117	9.14	9.919	9.094	9.113	9.919	9.078	9.095	9.919
6	9.52	9.564	9.949	9.276	9.313	9.949	9.186	9.214	9.949	9.14	9.163	9.949	9.112	9.132	9.949	9.094	9.111	9.949
7	9.59	9.629	9.969	9.319	9.358	9.969	9.217	9.246	9.969	9.163	9.188	9.969	9.131	9.152	9.969	9.109	9.128	9.969
9	9.711	9.692	9.982	9.403	9.406	9.982	9.276	9.281	9.982	9.209	9.215	9.982	9.168	9.174	9.982	9.14	9.146	9.982
10	9.761	9.751	9.99	9.444	9.456	9.99	9.305	9.319	9.99	9.231	9.244	9.99	9.186	9.198	9.99	9.156	9.167	9.99
11	9.805	9.806	9.995	9.482	9.509	9.995	9.334	9.359	9.995	9.253	9.276	9.995	9.204	9.224	9.995	9.171	9.189	9.995
13	9.875	9.854	9.998	9.556	9.563	9.998	9.39	9.401	9.998	9.298	9.31	9.998	9.24	9.253	9.998	9.201	9.213	9.998
14	9.901	9.895	9.999	9.59	9.618	9.999	9.417	9.447	9.999	9.319	9.347	9.999	9.258	9.283	9.999	9.217	9.24	9.999
16	9.941	9.928	9.999	9.654	9.672	9.999	9.47	9.494	9.999	9.362	9.386	9.999	9.293	9.316	9.999	9.247	9.268	9.999
18	9.966	9.953	10	9.711	9.726	10	9.52	9.543	10	9.403	9.428	10	9.328	9.352	10	9.276	9.299	10
20	9.982	9.972	10	9.761	9.777	10	9.568	9.594	10	9.443	9.472	10	9.362	9.39	10	9.305	9.332	10
23	9.993	9.984	10	9.825	9.825	10	9.634	9.645	10	9.501	9.518	10	9.411	9.43	10	9.348	9.367	10
25	9.997	9.992	10	9.859	9.868	10	9.674	9.696	10	9.538	9.565	10	9.444	9.472	10	9.376	9.405	10
28	9.999	9.996	10	9.901	9.905	10	9.729	9.746	10	9.59	9.614	10	9.49	9.517	10	9.417	9.445	10
31	10	9.998	10	9.933	9.935	10	9.777	9.794	10	9.638	9.664	10	9.534	9.563	10	9.457	9.487	10
35	10	9.999	10	9.961	9.958	10	9.831	9.839	10	9.697	9.713	10	9.59	9.611	10	9.508	9.531	10
39	10	10	10	9.979	9.975	10	9.874	9.878	10	9.749	9.761	10	9.641	9.659	10	9.556	9.577	10
43	10	10	10	9.989	9.986	10	9.909	9.913	10	9.795	9.807	10	9.689	9.707	10	9.601	9.624	10
47	10	10	10	9.994	9.993	10	9.935	9.941	10	9.834	9.849	10	9.732	9.755	10	9.644	9.671	10
53	10	10	10	9.998	9.997	10	9.963	9.962	10	9.882	9.887	10	9.788	9.8	10	9.702	9.719	10
58	10	10	10	9.999	9.999	10	9.977	9.978	10	9.913	9.92	10	9.828	9.842	10	9.745	9.765	10
64	10	10	10	10	10	10	9.988	9.988	10	9.941	9.946	10	9.869	9.881	10	9.791	9.809	10
71	10	10	10	10	10	10	9.995	9.994	10	9.964	9.966	10	9.906	9.914	10	9.837	9.851	10
79	10	10	10	10	10	10	9.998	9.998	10	9.98	9.98	10	9.938	9.941	10	9.879	9.887	10
87	10	10	10	10	10	10	9.999	9.999	10	9.99	9.99	10	9.96	9.962	10	9.913	9.919	10
96	10	10	10	10	10	10	10	10	10	9.995	9.995	10	9.977	9.978	10	9.941	9.945	10
106	10	10	10	10	10	10	10	10	10	9.998	9.998	10	9.988	9.988	10	9.963	9.965	10
117	10	10	10	10	10	10	10	10	10	9.999	9.999	10	9.994	9.994	10	9.979	9.98	10
129	10	10	10	10	10	10	10	10	10	10	10	10	9.998	9.998	10	9.989	9.989	10
142	10	10	10	10	10	10	10	10	10	10	10	10	9.999	9.999	10	9.995	9.995	10
157	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	9.998	9.998	10
173	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	9.999	9.999	10
191	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
200	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10

6.0 GROUP 2: CONTAMINANT TRANSPORT PROBLEMS

6.5 IMPACT OF PORFLOW RETARDATION MODEL ON VARIABLY SATURATED SOLUTE TRANSPORT

Problem 1A:
PORFLOW version 6.10.3 does not implement *water content* correctly for any of the scenarios (parent and daughter at 25 and 50 years). PORFLOW version 6.21.0 has corrected this bug.

8.0 GROUP 4: KEYWORD COMMANDS

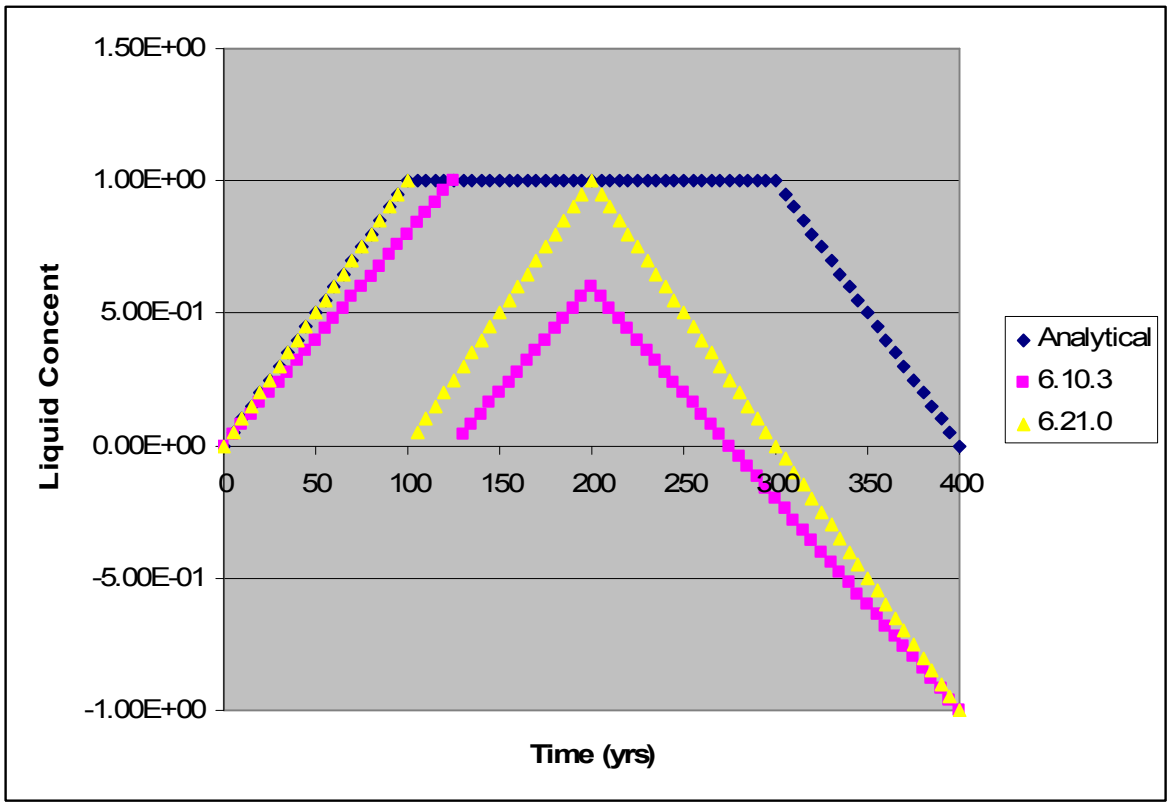
8.2 DISTRIBUTION AND RETARDATION

This group of problem was implemented in G-TR-G-00002 to properly test the DIST and RETA commands. There are still problems with these commands, which is why they are more fully described below.

Problem 2:
This problem implements the command DIST (Mode 1). This command is **not** implemented correctly in either PORFLOW version 6.10.3 or PORFLOW version 6.21.0. However, they both produce the same output.

Problem 3:
This problem implements the command RETA. This command is **not** implemented correctly in either PORFLOW version 6.10.3 or PORFLOW version 6.21.0, and both produce different output. The output of PORFLOW version 6.21.0 is identical to that produced by PORFLOW version 5.97.0, so a change was made to the code; however this current implementation of RETA is still flawed. See Figure 1 for the comparison of the output from these versions with the analytical solution.

Figure 1 Analytical vs. PORFLOW 6.10.3 vs PORFLOW 6.21.0



9.0 REFERENCES

Whiteside, T., 2007, Software Testing and Verification for PORFLOW Version 6.10.3, G-TR-G-00002, Rev. 0.

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