SRNL-L3200-2013-00022

Date: June 4, 2013

To: Dave Crowley

From: Frank Smith
Tom Butcher
Greg Flach

Copy: Jeff Jordan
Kent Rosenberger
Richard Sheppard

Subject: **Design Checking of PORFLOW Modeling Supporting the Saltstone FY13 Special Analysis**

PORFLOW modeling in support of the Saltstone FY13 Special Analysis (SA) has been design checked per Procedure Manual E7, 2.60 *Technical Reviews* following guidance provided by WSRC-IM-2002-00011, Rev. 2, *Technical Report Design Check Guidelines*. The purpose of this memorandum is to summarize technical findings and resolutions originating from multiple SRNL design checkers. Additional quality assurance checks were performed by Savannah River Remediation LLC, but are not documented here.

PORFLOW models for the Saltstone FY13 SA (SRR 2013) are based on the 2009 Performance Assessment (PA) (SRR 2009, Flach et al. 2009) and subsequent modeling to support a response to NRC Request for Additional Information (RAI) PA-8 (SRR 2011, Flach 2011). FY13 SA differences from the RAI PA-8 analysis are defined by SRR (2013) and Sheppard (2013). Notable changes to the nominal RAI PA-8 model include revised degradation of cementitious materials (Flach and Smith 2013) and associated hydraulic properties, and a revised Tc-99 shrinking-core model to implement combined redox and solubility controls. These new Saltstone model developments are discussed by Jordan and Flach (2013).

Frank Smith, Tom Butcher, and Greg Flach performed independent checks on various components of the overall PORFLOW modeling effort, as described below.

Frank Smith

Frank Smith checked the PORFLOW modeling technical report (Jordan and Flach, 2013) and performed selected spot checking of PORFLOW model input and output files for vadose zone flow and transport calculations and for aquifer transport calculations. Comments on the technical report were furnished to the analysts in a copy of the draft document with changes tracked. All comments were satisfactorily addressed in the final version of the report.

Because a very large number of PORFLOW calculations were performed, it was only possible to manually check a small subset of the input and output files in detail. However, the creation of the PORFLOW input decks is automated through pre-processing scripts so manual checking of only a small fraction of the files was deemed sufficient to provide confidence that the intended functions for implementing the conceptual models were performed correctly. More comprehensive checking of input parameter values was performed by Greg Flach. In addition to spot checking PORFLOW input and output, the Excel spreadsheets used by pre-processing scripts to assign material properties and chemistry were spot checked. This checking verified the correct implementation of concrete degradation in the calculations as described in the technical report. Again, a large number of these spreadsheets were used and only a small fraction could be checked manually. The checking focused on the Tc-99 runs verifying that solubility constraints and slag oxidation, which control the release of Tc-99, were implemented as described in the technical report. Flow solutions were also qualitatively checked by examining Tecplot plots of the flow.

Appendix A summarizes technical findings and resolutions. No errors were found in the PORFLOW calculations. A suggested improvement is included in Appendix A addressing the difficulty in checking such a large number of calculations each of which has large PORFLOW input and output files and several associated spreadsheet inputs. Most of the checking involved, for example, examining the PORFLOW input for one particular case in detail and then using TextPad to identify the differences between this case and others. If the differences between the two input files showed the expected changes, such as Tc solubility for example, the second case was confirmed to be correct.

Tom Butcher

Tom Butcher reviewed the conceptual approach to PORFLOW modeling described in the technical report authored by Jordan and Flach (2013): *PORFLOW Modeling Supporting the FY13 Saltstone Special Analysis*, SRNL-STI-2013-00280. The review specifically considered the reasonableness of the overall conceptual approach, and findings are summarized below.

The first aspect of model development discussed was the degradation of cementitious materials comprising Saltstone Disposal Units (SDU) 1, 2 and 4. The authors selected a method of representing physical degradation by assuming a smooth transition of each cementitious material (roof, floor, walls, columns and grout) from an initial matrix state to a fully-degraded soil-like material as represented by adjoining soils. To achieve this smooth transition the hydraulic properties were blended over the degradation-time in linear fashion. Other blending approaches were modeled (i.e., concrete-gravel blend and accounting for fractured medium attributes) to demonstrate that blending to adjacent soils is a reasonable choice for SDU steady-state flow modeling.

Since SDU cementitious materials are expected to physically degrade in the form of cracking for some degradation phenomena (causing changes in material properties), the authors considered discrete fracture models (DFM) as an alternative the blending approach (equivalent continuum model, ECM) described in the previous paragraph. Fractured cementitious media analog representations were set up to test flow and solute transport through a degraded SDU with fully-penetrating fractures. Fracture spacing, hydraulic conductivity of the grout, and infiltration rates were varied in the various test cases. As can be expected, different transport behavior was observed between the two types of models under

some conditions. Lateral diffusion into the fracture zone is evident in the DFM simulation for 1.0 meter fracture spacing and 10 cm/yr infiltration rate, whereas the ECM simulation shows a uniform flushing front. However, at slower flow rates and smaller fracture spacings the DFM and ECM results were observed to be similar, because the transport timescales were sufficiently long for approximate equilibrium between fracture and matrix to occur. Results from the various comparisons indicate that the ECM approach is a good approximation to, or conservative relative to, the alternative DFM approach depending on fracture spacing and flow rate. A set of simulations was specifically run for Tc-99 to account for the additional influences of redox and solubility with a similar result with respect to peak flux.

A key risk driver for SDUs is Tc-99. Slag is used in all SDU grouts and concretes (except SDU 1 and 4 roof) because Tc-99 mobility is limited by solubility under reducing conditions. These reducing capacities are consumed by dissolved oxygen entering the system through infiltrating liquid. A series of model verification tests were performed by simulating the disposal system in a simple analytical model and separately in one and two-dimensional modeling of slag oxidation. Models accounted for dissolved oxygen transport by both advection and diffusion. The test cases demonstrated adequate agreement between the numerical simulation and analytical solutions.

Tc-99 release has a dual dependence on redox state and solid-phase concentration of Tc-99. Since solubility and redox controls cannot be simultaneously implemented by the Kd construct in PORFLOW the authors created a user-defined variable to implement a more sophisticated Kd function that can account for both effects. Test cases were run demonstrating implementation of solubility control and combined redox and solubility control.

Based on the above considerations, the conceptual models selected for implementing degradation of the various concrete and grout materials in the disposal system and contaminant transport appear reasonable. Lacking knowledge of the exact morphology of a concrete or grout at its end-state, a sufficiently wide range of cases were evaluated to help demonstrate that the selected modeling approach is a good approximation to, or conservative relative to, alternative models.

Greg Flach

Greg Flach checked that Jeff Jordan correctly implemented certain modeling scenarios, cases, and inputs defined by Savannah River Remediation LLC in PORFLOW vadose zone flow and transport simulations. These cases are defined by Sheppard (2013) and described in the PORFLOW modeling report (Jordan and Flach 2013). The specific cases checked were

- Base case flow (“Case_sa”)
- Flow parametric study cases (“Case_param.#)
- Base case transport (“Case_sa”)
- Tc-99 sensitivity Cases 1) through 5) described in Section 5.0 of SRNL-STI-2013-00280

Appendix B enumerates a few technical findings, all of which has been satisfactorily resolved.

References

Flach, G. P., *Oxidation of Fractured Cementitious Materials in Performance Assessments*, SRNL-L4321-2011-00004, March 24, 2011.

Flach, G. P., J. M. Jordan, and T. Whiteside, *Numerical Flow and Transport Simulations Supporting the Saltstone Disposal Facility Performance Assessment*, SRNL-STI-2009-00115, Rev. 1, June 2009.

Flach, G. P., and F. G. Smith III, *Degradation of Cementitious Materials Associated With Saltstone Disposal Units*, SRNL-STI-2013-00118, March 2013.

Jordan, J. M., and G. P. Flach, 2013, *PORFLOW Modeling Supporting the FY13 Saltstone Special Analysis*, SRNL-STI-2013-00280, Rev. 0.

Procedure Manual E7, 2.60, *Technical Reviews*.

Savannah River National Laboratory, 2004, *Technical Report Design Check Guidelines*, WSRC-IM-2002-00011, Rev. 2.

Sheppard, R. E., *PORFLOW Input to Support the Development of the SDF FY13 Special Analysis*, SRR-CWDA_2013-00064, Rev. 1, April 30, 2013.

SRR Closure & Waste Disposal Authority, *Performance Assessment for the Saltstone Disposal Facility at the Savannah River Site*, SRR-CWDA-2009-00017, Rev. 0, October 2009.

SRR Closure & Waste Disposal Authority, *Comment Response Matrix for Nuclear Regulatory Commission RAI-2009-02 Second Request for Additional Information (RAI) on the Saltstone Disposal Facility Performance Assessment (SRR-CWDA-2009-00017, Revision 0, dated October 29, 2009)*, SRR-CWDA-2011-00044, Rev. 1, August 2011.

SRR Closure & Waste Disposal Authority, *FY2013 Special Analysis for the Saltstone Disposal Facility at the Savannah River Site*, SRR-CWDA-2013-00062, Rev. 0, June 2013.

Appendix A - Design checking performed by Frank Smith

Design Check: Technical report, PORFLOW implementation	**Date:** 5/30/2013
Design check scope, instructions, and/or general comments: <insert PORFLOW cases/files>	

No.	Comment	Proposed Resolution	Analyst Response	Checker Concur? Y,N
1	Very difficult to independently check such a large number of cases and corresponding PORFLOW input and output files.	Reduce the size of PORFLOW input files for vadose transport by not repeating material properties that do not change between time steps. Is it possible to have a single MaterialPalette.xls file for all cases?	Will investigate in future modeling efforts. No action taken, due to schedule constraints.	Y
2	Spot checking performed on vadose flow and transport calculations for approximately five cases and five flows/case for Vault 1, Vault 2 and Vault 4 "_mpad" files. Primarily checked Tc input. No problems found.	No action needed	OK	Y
3	Spot checking performed on five cases chosen at random in the folder AquiferZ_mpad/Transport. Checked Tc input for all five cases examined and Cs-135 and I-129 in two cases. No problems found.	No action needed	OK	Y

If checker has no comments, check here. ☒ Add additional rows above, as needed.

Analyst Name (print): Jeff Jordan and Greg Flach	**E-Signature (or sign/date/scan hardcopy):** (Not required if no comments)
Checker Name (print): Frank Smith	**E-Signature (or sign/date/scan hardcopy):**

Appendix B - Design checking performed by Greg Flach

Design Check: PORFLOW implementation	**Date:** 5/30/2013
Design check scope, instructions, and/or general comments: PORFLOW setup of a) base case vadose zone flow and transport, and aquifer transport, and b) flow parametric study	

No.	Comment	Proposed Resolution	Analyst Response	Checker Concur? Y,N
1	Base case (Case_sa) vadose zone flow: For SDU 2, the FF_ROOF_HDPE and FF_FLOOR_HDPE zones do not fail along with the FLOOR_HDPE_GCL and ROOF_HDPE_GCL zones. For SDU 1 and 4, no problems were detected.	Fix discrepancy. However, no action is required because the issue only affects ~7 inch wide portions of the HDPE/GCL liners and flow can easily pass around these small zones; thus the discrepancy should have insignificant impact.	No action taken, due to schedule constraints.	Y
2	Flow parametric study: a) For SDU 2 and 4 cases involving joint MCC change to "RelPermEqOne", this specification is not occurring in PORFLOW input files. b) For SDU 2 Best-Estimate (BE) cases, the FF_GROUT7 degradation is paired with FF_GROUT6 instead of FF_GROUT5. c) For parametric case V2_21, one of the time series has values out of order.	a) Re-run affected cases with relative permeability = 1 b) Assess impact and re-run if needed c) Fix and re-run	a) PORFLOW input corrected and simulations re-run b) No action proposed. The FF_GROUT7 discrepancy occurs around 40k years, which is well past the 0-20k year time period of primary interest. The issue will thus not affect the results of interest. Furthermore, the out-year results will probably not be significantly affected. c) Input corrected and simulation re-run	Y

Design Check: PORFLOW implementation	**Date:** 5/30/2013
Design check scope, instructions, and/or general comments: PORFLOW setup of a) base case vadose zone flow and transport, and aquifer transport, and b) flow parametric study	

No.	Comment	Proposed Resolution	Analyst Response	Checker Concur? Y,N
3	Base case (Case_sa) vadose zone transport: a) The sorption coefficients for soils are all zero. b) The SDU 2 upper mudmat should be ReModerate initially instead of OxModerate c) Similarly the SDU 1, 4 walls should be ReModerate initially. d) SDU 1 joint Kd should be Zero instead of Sandy. e) Saltstone Kd values for Ba and Sr are not as specified by Sheppard (2013).	a) Re-run using specified Kd values b) Re-run with specified setting c) Re-run with specified setting d) Re-run with specified Kd e) Re-run with specified Kd	a) Kd values corrected and simulations re-run b) Schedule constraints do not accommodate a re-run of the full suite of species. However, re-runs of I-129 and Ra-226 indicate insignificant impact to the water table flux; many other species have no redox sensitivity. Also, Tc-99 uses a separate slag shrinking core model and is not impacted. Th-230, U-234, Pu-238, and Cm-242 were also re-run, but no action is proposed for the remainder of the full suite considering the dose insignificance of these species. c) Schedule constraints do not accommodate a re-run of the full suite of species. No action is proposed following b). d) No action is proposed because impact should be insignificant. e) Re-runs made with corrected Kd values.	Y
6	Tc sensitivity cases: Cases 1) through 5) described in SRNL-STI-2013-00280 (draft final) were checked. No problems detected.	No action needed	OK	Y

If checker has no comments, check here. ☐ Add additional rows above, as needed.

Analyst Name (print): Jeffrey Jordan	**E-Signature (or sign/date/scan hardcopy):** (Not required if no comments)
Checker Name (print): Greg Flach	**E-Signature (or sign/date/scan hardcopy):**