WASHINGTON SAVANNAH RIVER COMPANY
INTEROFFICE MEMORANDUM

December 11, 2007 SRT-ESB-2007-00046

TO: KENT ROSENBERGER, 766-H

FROM: GREG FLACH, 773-42A GPFlach 12/11/07

DESIGN CHECKER APPROVALS:

SEBASTIAN ALEMAN: [signature] 12/12/07

LEN COLLARD: Leonard B. Collard 12/12/07

TAD WHITESIDE: Tad Whiteside 12/12/07

DESIGN CHECKS ON PORFLOW MODELING TO SUPPORT THE F-TANK FARM PA

A series of Design Checks following WSRC E7 Procedure 2.60 and related guidance documents were performed on PORFLOW modeling to support the upcoming F-Tank Farm (FTF) Performance Assessment document. Jeff Jordan and Greg Flach were the primary analysts. The checkers and associated review scope are summarized below.

Checker	Scope
Sebastian Aleman	Vadose zone flow
Len Collard	Vadose zone transport
Tad Whiteside	Aquifer transport at FTF and GSA scales

Aquifer flow fields for input to aquifer transport simulations come directly from the GSA/PORFLOW model (GSA scale), or were generated with the MESH3D program (FTF scale). Both flow fields have undergone separate QA reviews (WSRC-TR-2004-00106 and Q-SQP-G-00003, Rev. 0 respectively) and, are outside the scope of this design check. Key data inputs to the vadose zone and aquifer transport models come from information stored at \\pitstop\pitdata\PA Modeling\Baseline. These data have also been separately checked as documented in the FTF PA.

Technical findings and resolutions are presented in three separate Appendices. All technical issues have been satisfactorily resolved with respect to the present review scope, but the following actions are recommended by a Design Checker:

- The Performance Assessment document should mention that the vadose zone 2D axisymmetric radial grid sections are not limited in extent to the half-width between adjacent tanks, the closest flow obstruction. However, numerical experiments discussed herein indicate the impact is practically insignificant.
- The PA document should mention that smaller time steps, and recording thereof, would produce a modestly higher peak concentration for Nitrate, a mobile species that releases as a pulse. However, Nitrate is not a PA decision driver, so the modeling bias is acceptable.

- One logic error was noted in vadose zone transport pre-processing framework. The error did not affect any of the PORFLOW results, but should be corrected to avoid potential errors in the future should the software be reused.

Appendix A - Vadose zone flow design check

Findings (Sebastian Aleman):

1 FTF PA PORFLOW Vadose Zone Flow Design Check

A technically based design check of the FTF PA PORFLOW Vadose Zone Flow analysis effort is discussed within this section.

2 Design Check Instructions

Perform a complete design check using the design check guidelines.

- Evaluate and comment on the conceptual models used to model variably saturated groundwater flow for the FTF ancillary equipment, Type I, Type III, Type IIIA and Type IV waste tanks.
- Verify that all input parameters specified in the PORFLOW Run.dat file for each vadose zone flow run were derived from values given in the baseline spreadsheets. The exception is all input that is inserted into the Run.dat file through an INCLUDE statement. That is beyond the scope of this review because these inputs are generated directly from \\pitstop\pitdata\PA Modeling\Baseline, the contents of which have been verified separate from this design check.

3 Design Check Comment Summary and Resolution

For each item listed in the following table a brief comment summary is provided. Within the next section the details associated with each comment summary are provided.

Item	Resolution Category	Comment Summary	Resolution
1.	Will be resolved within this report revision	Why is the ancillary equipment being modeled in a cylindrical coordinate system? The ancillary equipment includes the transfer line system, pump tanks, evaporator systems, diversion boxes and valve boxes located through out the FTF. It is a spatially distributed source of contamination.	(see separate response below)

Item	Resolution Category	Comment Summary	Resolution
2.	Will be resolved within this report revision	What is the justification for extending the vadose zone beyond 70 feet radially? How sensitive is the contaminant flux leaving the vadose to the extent of the radial boundary?	(see separate response below)
3.	None	Design Input: Case F is not listed in the Liner Failure spreadsheet.	With respect to liner conditions, Case F is identical to Case B.
4.	None	All input parameters specified in the PORFLOW Run.dat file for each vadose zone flow run were derived from values given in the baseline spreadsheets	None required
5.	None	Adequate flow convergence was verified by spot checking of several vadose zone flow results.	None required

Resolution (Jeff Jordan)

Jeffrey Jordan/SRNL/Srs
11/13/2007 04:42 PM

To Gregory Flach/SRNL/Srs@srs, Sebastian Aleman/SRNL/Srs@srs
cc
bcc
Subject Re: Fw: FTF PA PORFLOW Vadose Zone Flow Design Check completed

See responses below.

1. Why is the ancillary equipment being modeled in a cylindrical coordinate system? The ancillary equipment includes the transfer line system, pump tanks, evaporator systems, diversion boxes and valve boxes located through out the FTF. It is a spatially distributed source of contamination.

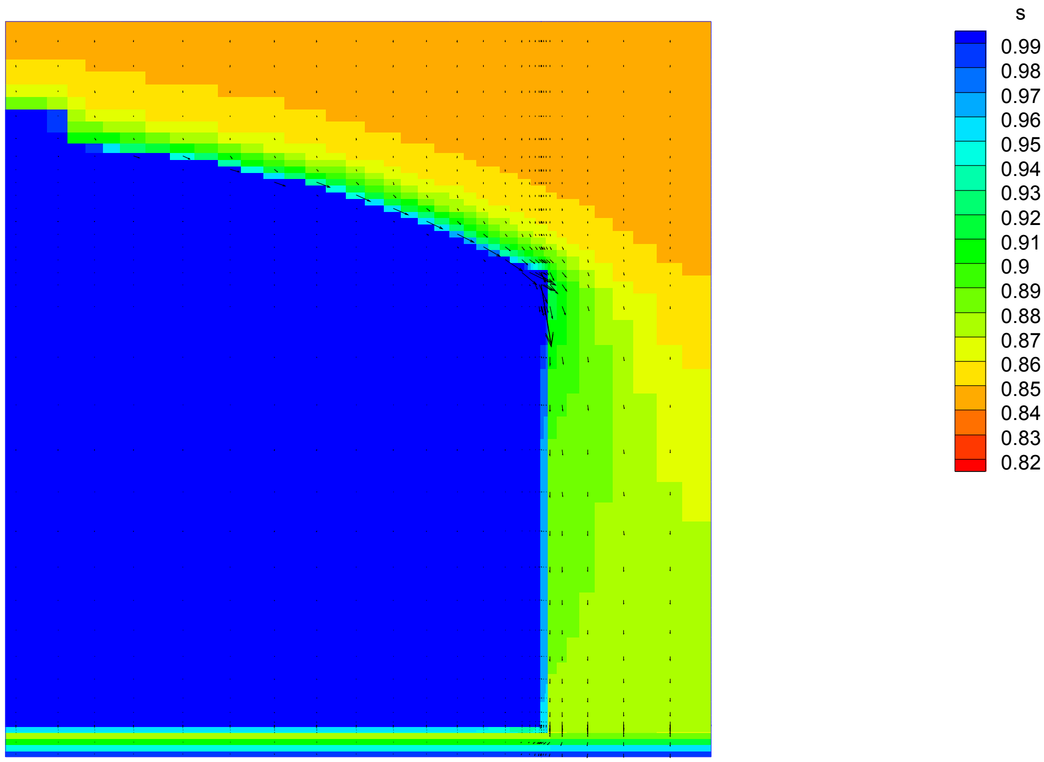
The ancillary evaluation is essentially a one-dimensional run. The materials are modeled as bands through the horizontal direction such that there is no variation in this dimension. Since there is no variation in that direction, it does not matter if it is modeled in cylindrical or cartesian coordinates. As an additional note, there are no solubility controls for the ancillary equipment.

2. What is the justification for extending the vadose zone beyond 70 feet radially? How sensitive is the contaminant flux leaving the vadose to the extent of the radial boundary?

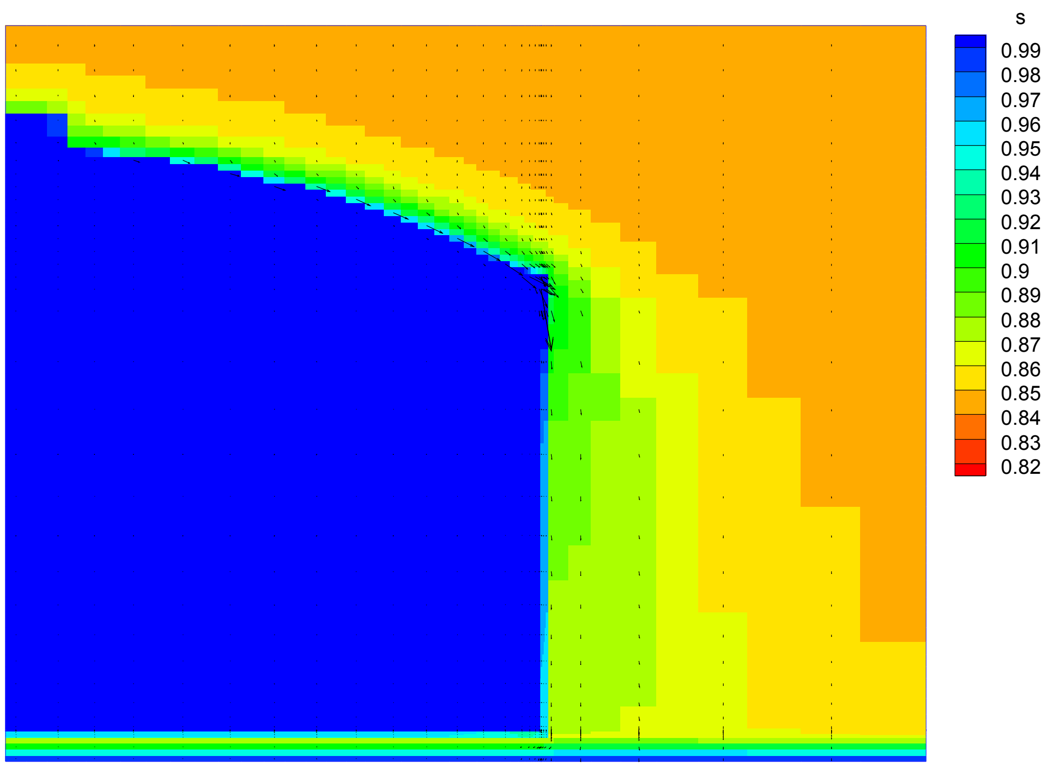
I ran an additional case to test the sensitivity. I used the minimum distance for the Type IV tanks and reran the model through the vadose zone. The results are very similar. The flow results are essentially identical - see attached. The transport concentration plots show identical trends for the parent and progeny. All of the peak values are within 2.5% and most are less than 0.5% different. I left the number of cells the same, so the grid spacing is another difference between the two runs. The time of peaks for Pu-239 are off by a larger percent, but this is due to the fact that the concentration stays relatively constant for an extended period of time, several thousand years. Overall, it can be expected that the impact would be minimal.

compare.ppt compare.xls

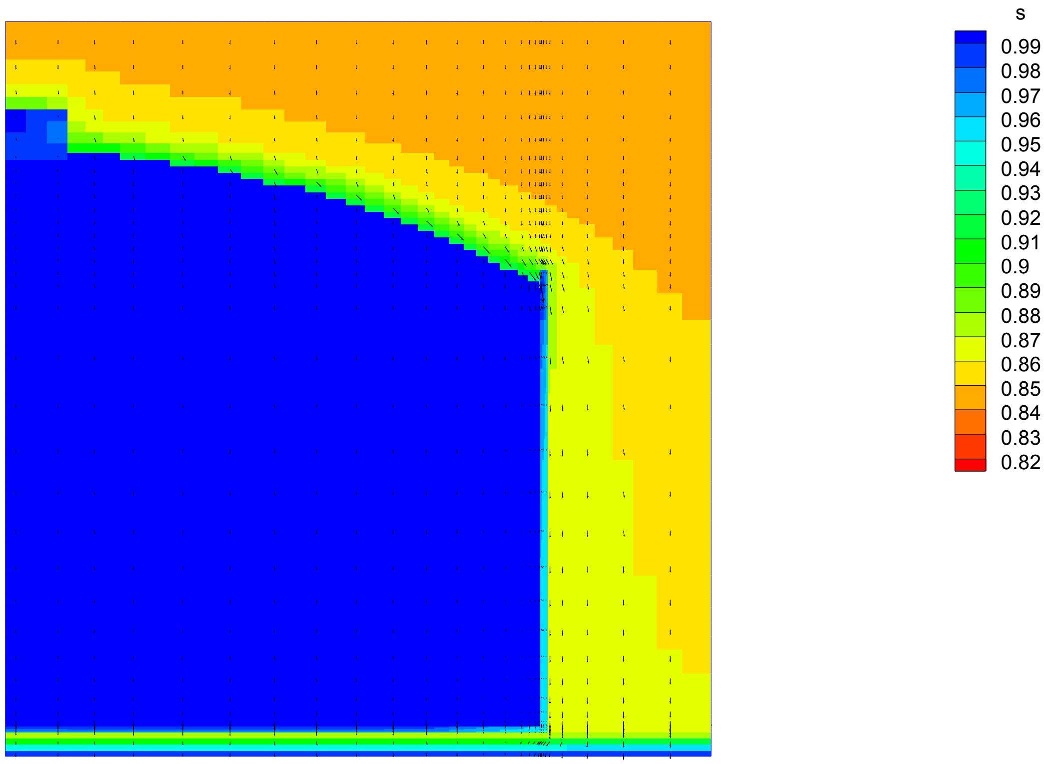
"compare.ppt" content: The first set of figures shows the saturation and velocity fields for two TypeIV grids: a) radial extent limited by the half-width between adjacent tanks and, b) radial extent assumed in FTF PA modeling. Two infiltration conditions are considered. The shorter radial distance produces higher saturation in backfilled soil at the base of the tank. The second set of figures shows flux to the water table for Pu-239 and grids a) and b) respectively. The plots are visually identical.



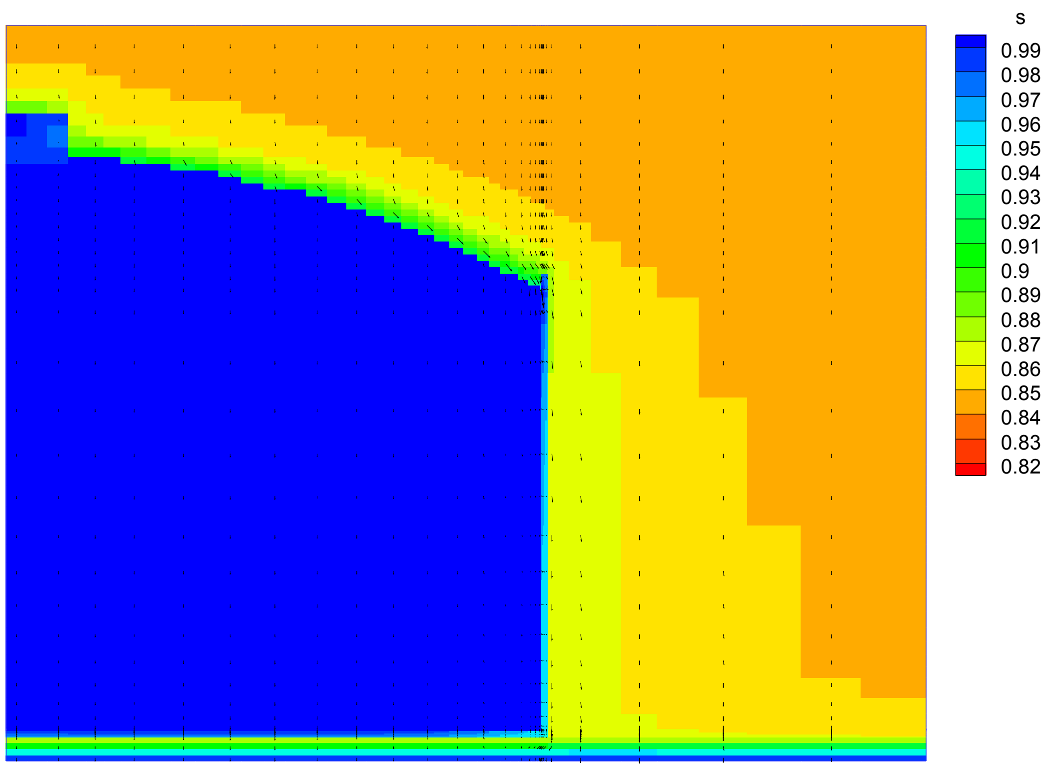
a) Shorter radial extent grid (higher infiltration)



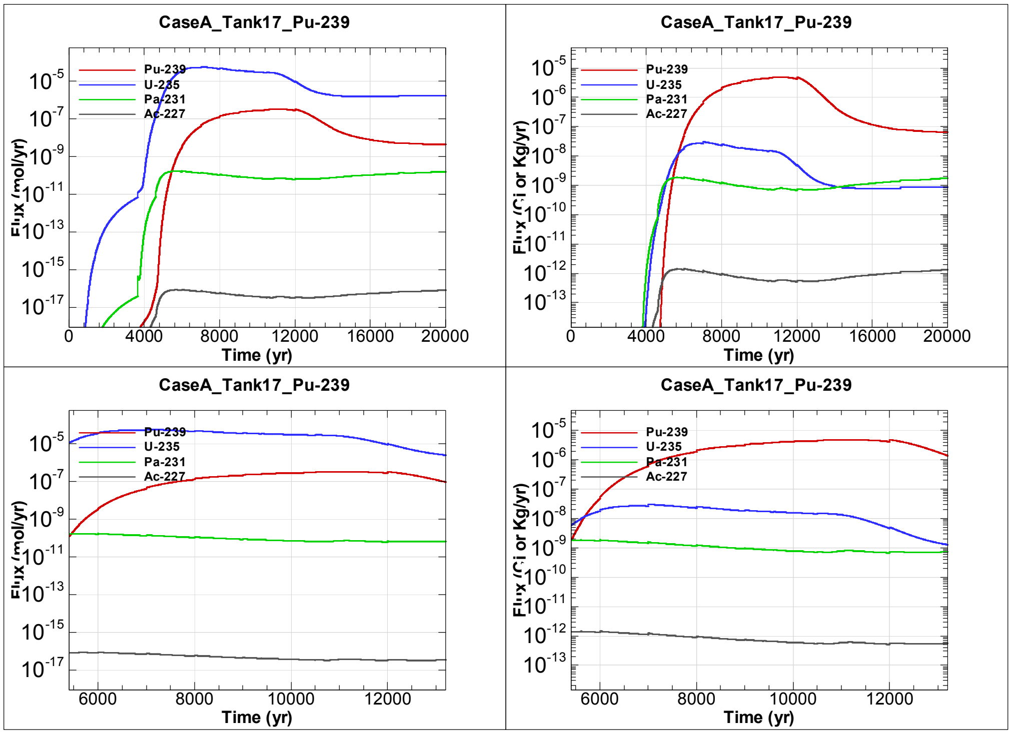
a) Longer radial extent (PA) grid (higher infiltration)



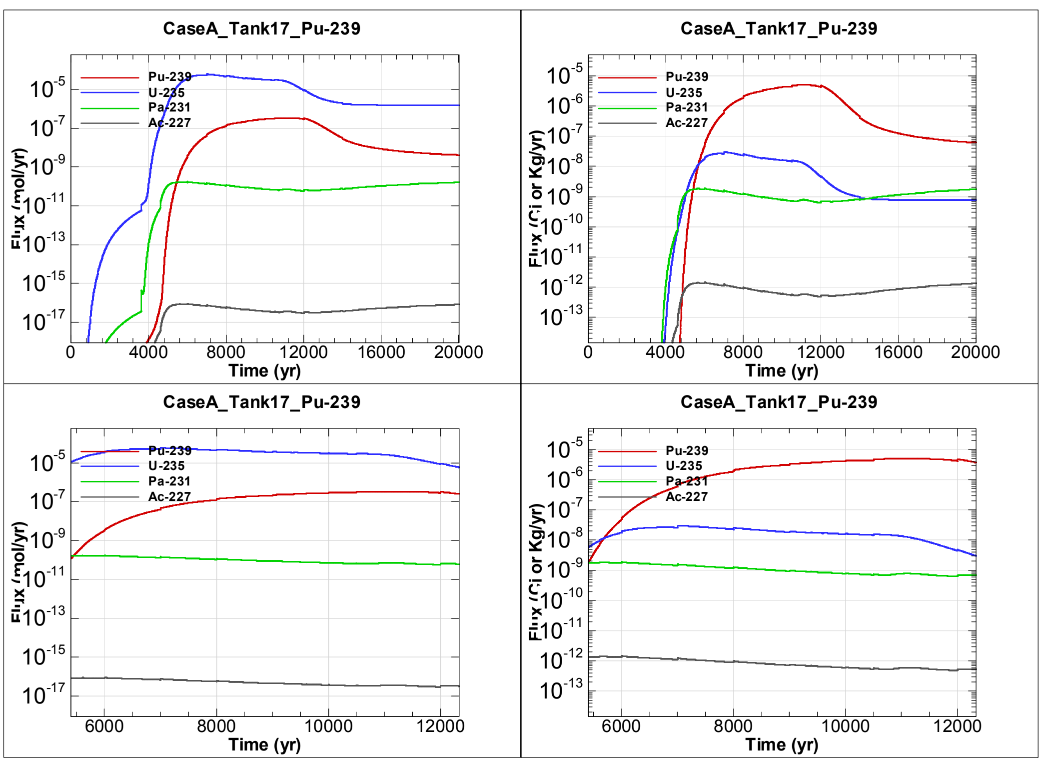
a) Shorter radial extent grid (lower infiltration)



b) Longer radial extent (PA) grid (lower infiltration)



a) Shorter radial extent



b) Longer radial extent (PA)

"compare.xls" content: The "New" and "Old" peak flux data in the table correspond to grids a) and b) respectively. The differences are practically insignificant. The notation "_mol" refers to units of "zmol".

New

!nuclide	inventory	moles	time (yr)	flux (_mol/yr per rad)	flux*FluxScale (	flux*FluxSc	flux*FluxScale/VZt	flux*FluxScale/VZto	flux*FluxScale/VZtoSZ/Moles/ActRat(I)*Inventory (Ci|kg/yr)
Pu-239	1.48E+01 Ci	9.97E-01 mol	1.20E+04	5.21E+13	5.21E-08	3.28E-07	3.28E-07	3.28E-07	4.86E-06
U-235			7.00E+03	9.50E+15	9.50E-06	5.97E-05	5.98E-05	2.05E-09	3.03E-08
Pa-231			6.00E+03	2.79E+10	2.79E-11	1.76E-10	1.76E-10	1.30E-10	1.92E-09
Ac-227			6.00E+03	1.43E+04	1.43E-17	8.99E-17	9.01E-17	9.97E-14	1.48E-12

Old

!nuclide	inventory	moles	time (yr)	flux (_mol/yr per rad)	flux*FluxScale (	flux*FluxSc	flux*FluxScale/VZt	flux*FluxScale/VZto	flux*FluxScale/VZtoSZ/Moles/ActRat(I)*Inventory (Ci|kg/yr)
Pu-239	1.48E+01 Ci	9.97E-01 mol	1.12E+04	5.33E+13	5.33E-08	3.35E-07	3.36E-07	3.36E-07	4.97E-06
U-235			7.00E+03	9.47E+15	9.47E-06	5.95E-05	5.97E-05	2.04E-09	3.02E-08
Pa-231			6.00E+03	2.78E+10	2.78E-11	1.75E-10	1.75E-10	1.29E-10	1.91E-09
Ac-227			6.00E+03	1.42E+04	1.42E-17	8.95E-17	8.97E-17	9.93E-14	1.47E-12

Comparison

Pu-239			7.05%	-2.25%	-2.25%	-2.27%	-2.26%	-2.26%	-2.25%
U-235			0.00%	0.29%	0.29%	0.29%	0.28%	0.29%	0.30%
Pa-231			0.00%	0.40%	0.40%	0.34%	0.40%	0.39%	0.42%
Ac-227			0.00%	0.42%	0.42%	0.40%	0.40%	0.39%	0.41%

Appendix B - Vadose zone transport design check

Instructions (Greg Flach):

Design check instructions for
F Tank Farm PA vadose zone transport modeling using PORFLOW

Selected PORFLOW vadose zone transport runs were performed around October 25 for the purpose of comparing to similar GoldSim simulations, specifically, Cases A and D, and species N, Pu-239 and Tc-99. The associated PORFLOW files are available from \\g-flach\TankPA_25Oct2007. The Case A runs are also part of the production/final runs for a larger suite of radionuclides found at \\g-flach\TankPA. Key input information to PORFLOW modeling, which has or will be design-checked separately, is available at \\pitstop\pitdata\PA Modeling\Baseline.

The following aspects of the PORFLOW vadose runs in \\g-flach\TankPA_25Oct2007 should be checked using \\pitstop\pitdata\PA Modeling\Baseline:

- Confirm that inventory information in .\Inventory is appropriately reflected in PORFLOW input. The relevant files are
  - Tanks, rads: Appendix A_10-22-07_MBB.txt
  - Tanks, nonrads: NonRads Appendix B_10-11-07_MBB.txt
  - Ancillary equipment, rads: Archive\Ancillary Inventory_10-22-07_MBB.txt
  - Ancillary equipment, nonrads: NonRad Ancillary Inventory_10-15-07_MBB_RES.txt
- Confirm that abbreviated chain, decay and regeneration information in .\Decay are appropriately reflected in PORFLOW input. The relevant files are
  - Chains_0.5yr*.dat
- Confirm that solubility and Kd information in .\Chemistry are appropriately reflected in PORFLOW input. The relevant files are
  - solubility: Waste Layer Solubility Oct 172.txt
  - distribution coefficient: Kd Oct 11_MHL.txt
  - see also: .\Design Inputs\Solubility Transition Time Oct 10 MHL.xls
- Confirm that material properties and degradation functions in .\Properties are appropriately reflected in PORFLOW input. The relevant files are
  - Hydraulic Properties_11-1_MHL-RES.xls
- Confirm that the Case A and D scenarios, described in .\Design Inputs\Flow Cases_10-9-07_MHL.xls, are adequately implemented in PORFLOW
- Confirm that peak flux and time of peak flux (Flux.tab files), and water table flux (*.flx) information is correctly generated w.r.t. magnitude and units
- Review the overall setup of PORFLOW transport simulations for technical adequacy.

To the extent practical, an exhaustive check of RUN.dat files is desired. However, spot checks may be used. Design check findings may be transmitted as a Word file or Email.

<u>Subsequent information</u>

This spreadsheet relates each cementitious Material zone to each Pore Volume zone.

For Case A (intact scenario), the concept is that contamination zone pore water chemistry is controlled by the overlying tank fill grout. The roof, tank grout, basemat are based on pore volumes through the entire feature, i.e., the non-FF and FF zones combined.

For Case D (fast flow path scenario), water entering the contamination has bypassed the grout, and the contamination zone chemistry is based on pore volumes through that same region. The FF subregions do not have geochemical controls, and the intact portion of the roof, grout, and basemat regions is based on pore volumes through the same region.

For Cases A and D, the wall and annulus chemistry is related to pore volumes through those regions. The center riser and dome ring are linked to the roof condition.

Also, at the top directory level (\\g-flach\TankPA_25Oct2007) the "Cement_change_pore.xls" spreadsheet can be used to see when the Eh (Re --> Ox) and pH (II --> III) changes occur.

Findings and Resolution (Len Collard and Greg Flach):

1 FTF PA PORFLOW Vadose Zone Transport Design Check

A technically based design check of the FTF PA PORFLOW Vadose Zone Transport analysis effort is discussed within this section.

2 Design Check Comment Summary and Resolution

For each item listed in the following table a brief comment summary is provided.

Item	Resolution Category	Comment Summary	Resolution
1.		In initial inspections I discovered that some liners were not being assigned the appropriate class of material as specific times. Greg Flach discovered that his most recent correction also corrected those misassignments and I was assigned a newer set of files to inspect. All information below is based on the newer set of files.	No action

Item	Resolution Category	Comment Summary	Resolution
2.		I regenerated all the input files for the vadose zone runs, then performed comparisons. For many of the numbers I could not get an exact match, with differences appearing in the 3rd or 4th digit after the decimal point. I started from text files, such as matlProp.tab. Subsequently I was planning to ensure that all the raw data as stated below were properly captured in the text files, but I did not have sufficient time to complete that aspect. The differences in the numbers are likely the result of how the numbers are being generated by the modelers (not the checker). In many circumstances the modelers' script to generate the input files is echoing numbers to an external program to perform rudimentary algebraic calculations. The echo only carries three digits to the right of the decimal point. In some cases the external programs operate in double precision, while in other cases in single precision. I attempted to reproduce these actions in Fortran, but still could not produce an exact match. I did check all the inventory information for correctness. This included the proper combining of NO2 and NO3 to produce N.	The originators agree that some values in the Porflow flow input files were generated with less than single (real*4) precision, for the reasons given by the checker. This makes exhaustive checking through an automated process difficult. While inconvenient for design checking, the values are sufficiently accurate for their intended purpose. The numerical values in matlProp.tab come from \\pitstop\pitdata\PA Modeling\Baseline, which has been separately checked.
3.		I checked the decay chains using the original files produced by Larry Koffman. Everything matched exactly. However, the set of parents did not enter the changed world of assuming secular equilibrium at 0.5 years, rather than at 5 years. I did a spot check on a parent in the production folder that should reflect a change and it correctly did so.	No action.

Item	Resolution Category	Comment Summary	Resolution
4.		I checked that the Kd information was correct using text files that already incorporated when the number of pore volumes flushes exceeded key thresholds. I did not check that the pore volume flushes were calculated correctly, although I was in the process and did not note any problems.	No action.
5.		Solubilities were not traced back to the raw data, because of time limitations.	No action.
6.		The CaseA and CaseD scenarios were spot-checked and appeared to be properly implemented.	No action.
7.		Water table flux information (i.e. contaminant flux at the water table) were spot checked. A Flux.out.z file was inspected for comparison to its *.flx files. Conversions from zMoles/rad to Moles were appropriately performed, although various roundoffs appeared, such that I could not exactly match the modelers' values.	No action.
8.		The overall setup of the transport simulations was examined. A true axisymmetric setting does not exist, because no tank is completely surrounded by other tanks. The lateral extent of the model is somewhat questionable, because on any side where a neighbor tank appears, the distance in that direction may be less than the distance assumed in the model.	This issue also arose in the vadose flow design check performed by Sebastian Aleman (Finding #2), and was satisfactorily resolved in that context.
9.		The MakeFile value of 2*Pi used to produce the source term as moles/radian should be 6.2831853 rather than 6.283183 as was used. The subsequent conversion back to moles uses a correct value of 0.1591549.	Agreed. The small error introduced is acceptable, and will be corrected before any future usage.

Item	Resolution Category	Comment Summary	Resolution
10.		The LOCATE commands refer to material 19 as S_VERT_LINER and material 20 as P_VERT_LINER. However the FOR commands reverse the names in the comments after the exclamation point.	The comment associated with the LOCAte command is correct. The comments associated with the FOR commands indicate an error in the pre-processing logic used, in which the properties for the S_VERT_LINER and P_VERT_LINER zones are reversed. Fortuitously, the same properties have been specified for the two liners to date, so the actual PORFLOW input is unaffected (apart from the misleading comments). The logic error will be fixed to avoid any future problems.
11.		The read statements for the steady-state flow fields do restart the count for the diagnostics, except for the first read. This will cause the number for the diagnostic step to be influenced by the time step from the flow field runs.	Agreed. No impact on results.

Item	Resolution Category	Comment Summary	Resolution
12.		Shorter recording time steps for highly mobile contaminants should be considered. For example, in one previous analysis peak fluxes at common recorded time steps for H-3 were 28% lower than those recorded for shorter time steps.	The originators agree that shorter time steps would result in a modestly higher peak concentration for a mobile species that releases as a pulse. To investigate further, a Tracer species (Kd=0, no solubility limit, no decay) was simulated at 0.1 year steps in both the vadose and aquifer models. A 35% higher peak concentration was observed at a 100 meter distance. However, for Kd=2 mL/g in the aquifer, the peak concentration for 0.1 year steps is only 6% higher. An examination of water table flux and Kd assumptions for the full suite of parents indicates that only the nitrate results are sensitive to time steps below 1 year. The current Nitrate results are not close to the MCL, so a refined simulation, while desirable, is not required. However, the PA should make note of that the nitrate results could be biased low by approximately 1/3.
13.		I have not seen any drafts of the PA report, so I am not aware of exactly how the PORFLOW results are being represented. Responses to at least Comment 8 and Comment 12 above need to be included in the final PA report – not merely in the resolution column of the design check, unless the design checks will be included in their entirety in the report.	Technical review of the Performance Assessment document is beyond the scope of this design check. Suggested discussion related to Comments 8 and 12 has been provided to the PA document preparation team for inclusion. The draft final PA report will be provided to the Design Checker for concurrence that the higher-level discussion adequately incorporates the two issues identified in Comments 8 and 12.

Appendix C - Aquifer transport design check

Instructions (Greg Flach):

Design check instructions for
F Tank Farm PA aquifer transport modeling using PORFLOW

PORFLOW aquifer transport runs have been performed for Case A and 79 rad and non-rad species. The associated PORFLOW files are available from

\\hpcfs\hpc_project\tankpa\Tmp_storage\All, Near-field (1 and 100 m) results for Case A and All sources
\\g-flach\TankPA\AquiferGSA, Far-field (seepage face) results for Case A, All sources, and key rads
\\g-flach\TankPA_overflow, Near-field results for Case A, key individual sources, and key rads
\\g-flach\TankPA\GSA_PORFLOW\GSA_PORFLOW_FTF\Transport\LOCAte, 1 meter and 100 meter monitoring locations
\\g-flach\TankPA\GSA_PORFLOW\GSA_TRANSPORT_uncert\Transport\LOCAte, seepage face monitoring locations

Key input information to PORFLOW modeling, which has been or will be design-checked separately, is available at \\pitstop\pitdata\PA Modeling\Baseline.

The following aspects of the PORFLOW aquifer transport runs should be checked:

- Spot check that the 1 meter, 100 meter and seepage face monitoring locations are correctly defined in PORFLOW.
- Confirm that water table flux tables are correctly drawn from the associated vadose run directories. Vadose zone results are found at \\g-flach\TankPA\Vadose*.
- Confirm that abbreviated chain, decay and regeneration information in \\pitstop\pitdata\PA Modeling\Baseline\Decay are appropriately reflected in PORFLOW input. The relevant files are
    - Chains_0.5yr*.dat
- Confirm that Kd information in \\pitstop\pitdata\PA Modeling\Baseline\Chemistry is appropriately reflected in PORFLOW input. The relevant file is
    - distribution coefficient: Kd Oct 11_MHL.txt
- Confirm that material properties \\pitstop\pitdata\PA Modeling\Baseline\Properties are appropriately reflected in PORFLOW input. The relevant files are
    - Hydraulic Properties_11-1_MHL-RES.xls
- Confirm that peak concentration and time of peak concentration (Stat*.tab files), information is correctly generated w.r.t. magnitude and units
- Review the overall setup of PORFLOW transport simulations for technical adequacy.

To the extent practical, an exhaustive check of RUN.dat files is desired. However, spot checks may be used. Design check findings may be transmitted as a Word file or Email.

Findings (Tad Whiteside):

Tad Whiteside/SRNL/Srs	To	Gregory Flach/SRNL/Srs@srs
12/04/2007 02:35 PM	cc	Heather Burns/SRNL/Srs@Srs
	bcc	
	Subject	Re: Design check on Porflow FTF Model Aquifer Transport

Design check for F Tank Farm PA aquifer transport modeling using PORFLOW

The following aspects of the PORFLOW aquifer transport runs should be checked:

- Spot check that the 1 meter, 100 meter and seepage face monitoring locations are correctly defined in PORFLOW.

Checked - they are

- Confirm that water table flux tables are correctly drawn from the associated vadose run directories. Vadose zone results are found at \\g-flach\TankPA\Vadose*.

Checked - they are

- Confirm that abbreviated chain, decay and regeneration information in \\pitstop\pitdata\PA Modeling\Baseline\Decay are appropriately reflected in PORFLOW input.

Checked - it is

- Confirm that Kd information in \\pitstop\pitdata\PA Modeling\Baseline\Chemistry is appropriately reflected in PORFLOW input.

Checked - it is

- Confirm that material properties \\pitstop\pitdata\PA Modeling\Baseline\Properties are appropriately reflected in PORFLOW input.

Checked - it is

- Confirm that peak concentration and time of peak concentration (Stat*.tab files), information is correctly generated w.r.t. magnitude and units

Checked - it is

- Review the overall setup of PORFLOW transport simulations for technical adequacy.

Checked - they are

Tad Whiteside

Resolution (Greg Flach):

None required.