Use of a Stochastic Model to Evaluate Uncertainty in a Performance Assessment at the Savannah River Site – 8120

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ABSTRACT

A significant effort has recently been initiated to address probabilistic issues within radiological Performance Assessments (PA's) conducted at the Savannah River Site (SRS). This effort is considered to be part of a continual process, as is the program of PA analysis and maintenance across the Department of Energy (DOE) complex. At SRS, findings in the initial probabilistic analysis of the Slit Trenches in the E-Area PA were built upon and improved in the later development of the probabilistic model for the F-Area Tank Farm.

Within the PA studies conducted at SRS, the initial effort of the uncertainty analyses was focused on the Slit Trenches as part of the E-Area PA. Specifically, a probabilistic model was developed for Slit Trench 5 within the E-Area. This model was utilized in deterministic mode to compare its results against the 2- and 3-D model results of the deterministic models. Then, utilizing the PDFs, the model was used to perform multiple realizations and produce probabilistic results. Later, a second probabilistic sensitivity and uncertainty analysis was undertaken for the F-Area Tank Farm PA. This effort is currently underway. Many improvements were made in how the flow and transport processes were incorporated within this model.

INTRODUCTION

The DOE requires that PA's be conducted to evaluate all low-level radioactive waste disposal facilities located at DOE sites. Performance objectives for disposal of Low-Level Radioactive Waste (LLW) at DOE sites are provided in DOE Order 435.1 as well as performance measures for PA exposure pathways.

One of the PA requirements of DOE Order 435.1 is to evaluate the sensitivity and uncertainty in achieving the performance goals and measures. There is, however, no clear guidance provided on how this should best be accomplished. The DOE complex-wide committee, established to review all PA's, the Low-Level Waste Disposal Facility Federal Review Group (LFRG), has indicated that a more rigorous approach to assessing sensitivity and uncertainty needs to be undertaken than has been attempted in the past. That sentiment is consistent with recommendations recently made to the DOE by the Nuclear Regulatory Commission (NRC). The DOE regards the PA process as an ongoing process in which improvements are continuously made and such improvements are evident in the PA uncertainty analyses being conducted at the Savannah River Site.

At the SRS a PA was recently completed for the low level radioactive waste disposal facilities situated within the E-Area at the Savannah River Site, South Carolina [3]. Individual facilities within E-Area include the Intermediate Level Vault (ILV), Slit and Engineered Trench, Low Activity Waste (LAW) Vaults, Components in Grout (CIG) facilities and the Naval Reactor Container Disposal Area (NRDCA). A second PA is currently in progress for the F-Area Tank Farm and two more are planned to begin within the coming year for the Saltstone Facility and H-Area Tank Farm. In addition to these studies a Composite Analysis (CA) for the SRS is currently underway. This type of investigation is slightly different than a PA in that it examines all source terms for the SRS that might add to the dose of a hypothetical future member of the public. Each of these investigations includes or will include an assessment of sensitivity and uncertainty in calculating the doses that might be received by hypothetical future members of the public.

The applicable exposure pathways have been analyzed in all PA's conducted at SRS. These include the residential, agricultural and post-drilling hypothetical intruders, atmospheric and groundwater release pathways as well as radon. The approach at SRS is to use PA's to establish facility disposal limits based on the maximum permissible exposures to hypothetical individuals over the 1000-year PA period of compliance. Limits are based on the highest exposure received by an individual through any of the analyzed pathways. Although not required by DOE Order 435.1, analyses are typically carried out for 10,000 years and longer in order to determine when a peak dose would occur.

At the SRS the groundwater pathway is the most complex, and usually the limiting pathway of all exposure pathways and usually requires the most extensive evaluation effort. Evaluations are conducted using deterministic numerical models to simulate radionuclide transport from the waste zone of the disposal facility through the vadose and saturated zones to the exposure point at the 100-m compliance well. At SRS the PORFLOW deterministic code [1] is utilized to construct these models. Traditionally, models have been constructed as 2-D cross-sectional configurations for the vadose zone and as fully 3-D configurations for the aquifer. These models are based on a conceptual model that is first established and then populated with "best estimates" values of the key flow and transport parameters. Deterministic models are convenient for calculating a result that can readily be compared to the deterministic performance measure, for example the All-Pathways 0.25 mSv/yr (25 mrem/yr) dose limit.

SRS SENSITIVITY AND UNCERTAINTY APPROACH

In response to the LFRG recommendation that more rigorous sensitivity and uncertainty analyses be undertaken within PA's, SRS has initiated a probabilistic uncertainty analysis for one of the disposal facilities evaluated in the recently completed E-Area PA. The purpose of the probabilistic analyses were to gain greater understanding of the release pathways and to either question or lend added confidence to the deterministically derived facility disposal limits.

Uncertainty was addressed using a probabilistic model implemented in the commercial program GoldSim [2]. Initially, this involved establishment of a single-realization, deterministic, GoldSim model that emulated the deterministic numerical model results of the same flow system. Then, defining probability distribution functions (PDFs) that define the statistical variability for important parameters, multiple realizations were performed in which parameter values were re-sampled for each realization according to the PDFs.

Development of the probabilistic model involved construction of a modular structure within the GoldSim package [2] to simulate the waste zone, vadose zone and saturated zone such that the processes controlling the release of radionuclides could be adequately represented within this 1-D model. An example of this modular structure is shown in Figure 1, where the flow and transport processes for the waste zone, vadose zone and saturated zones, were organized within "boxes", which are referred to as containers. Within each of the containers are a series of mixing cells. These cells were populated with the appropriate materials, material properties, and water fluxes and linked to one another in an appropriate fashion such that a valid representation of the

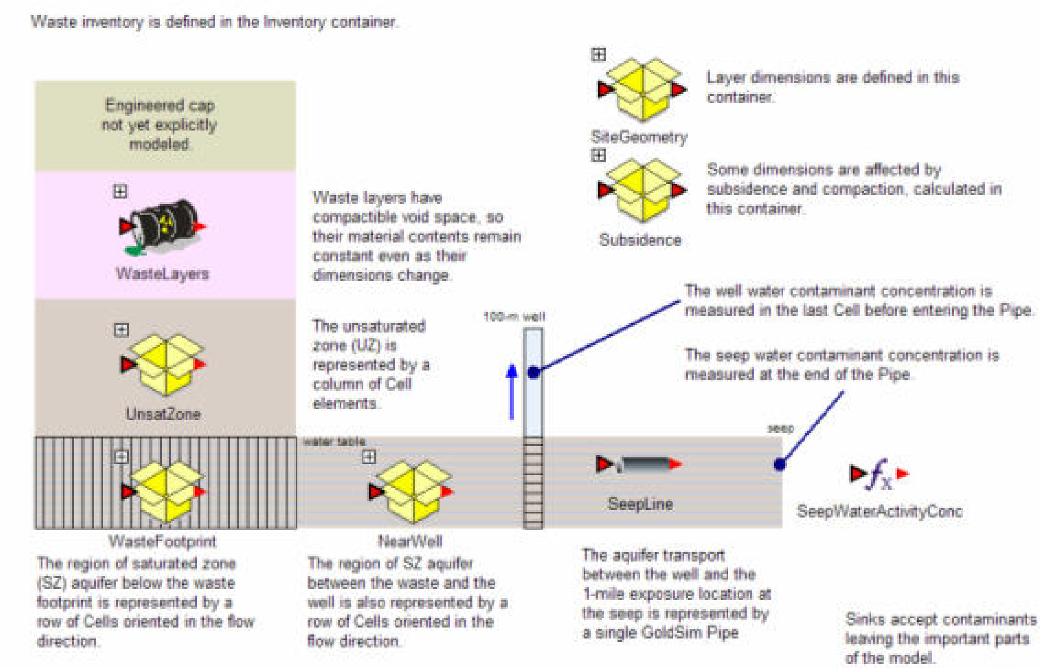

Figure 1. Probabilistic GoldSim model components

chemical and physical processes was achieved. The vadose zone was represented with a vertical "stack" of these containers to emulate the vertical downward movement of water and contaminant mass. Similarly, for the saturated zone beneath the facility and between the facility and the compliance well, a row of cells were established to emulate the lateral movement of water and contaminant mass.

SLIT TRENCH AND F-AREA TANK FARM PROBALISTIC MODELS

Within the PA studies conducted at SRS, the initial effort of the uncertainty analyses was focused on the Slit Trenches as part of the E-Area PA. Specifically, a probabilistic model was developed for Slit Trench 5 within the E-Area. This model was utilized in deterministic mode to compare its results against the 2- and 3-D model results of the deterministic models. Then, PDFs were established for selected parameters and the model was used to perform multiple realizations and to produce probabilistic results. Later, a second probabilistic sensitivity and uncertainty analysis was undertaken for the F-Area Tank Farm PA. This effort is currently underway. Many improvements were made in how the flow and transport processes were incorporated within this model.

With respect to both uncertainty analyses, the GoldSim and PORFLOW models are based on the same conceptual models, therefore the materials, properties and basic model features are the same. The difference between the two models is that one, PORFLOW, is constructed as multi-dimensional and the other, GoldSim, is 1-D. The challenge was to adequately abstract the data from the multi-dimensional model into the 1-D model such that similar or virtually identical output can be obtained.

Since GoldSim is a transport code and does not calculate water flow, an abstraction of water fluxes from the PORFLOW model was made to incorporate into the GoldSim model. The fact that the Slit Trenches and F-Tank Farm have predominantly vertical downward flow in the vadose zone and horizontal flow in the saturated zone made the extraction of the relevant fluxes fairly simple. Since both zones are essentially 1-D flow fields, fluxes were extracted at various elevations, or horizontal positions, within the PORFLOW model domains. Using these fluxes, equivalent flows were established for use in the GoldSim model.

For the Slit Trench 5 analysis, the first step was to establish simplified test models for both the PORFLOW and GoldSim model codes [1,2] using identical fluxes and geochemical properties. The identical model node representation enabled a determination of whether the codes were capable of producing identical results. This exercise led to the identification of a difference in the way each code calculates contaminant retardation within the flow field. When this difference was accounted for the models produced identical results. Such a realization highlights the benefit of using separate model codes to check one another.

Following this, a more detailed GoldSim model was constructed that could be used to compare against the results of the PA deterministic PORFLOW models. This model was constructed as described earlier and schematically shown in Figure 1. An iterative simulation study was used to establish the minimum number of nodes (or mixing cells) needed such that GoldSim could adequately calculate mechanical dispersivity and produce desired temporal resolution. Within the aquifer portion of the GoldSim model it was discovered that a GoldSim “Pipe” element could not be used because of its inability to represent a time-varying boundary condition at the pipe inlet.

For the Slit Trench 5 probabilistic model, comparisons were made for 4 radionuclides, two non-sorbing radionuclides (C-14 and I-129) and two sorbing radionuclides (Tc-99 and Np-237). With non-sorbing radionuclides it was simple to achieve calibration but more difficult to do so with sorbing radionuclides. This difficulty was not fully resolved within the Slit Trench 5 probabilistic model; however the issue was more fully addressed later when the F-Area Tank Farm probabilistic model was developed.

Once a satisfactory conformance between the GoldSim and PORFLOW deterministic models results was obtained for the Slit Trench 5 model, it was utilized in stochastic mode to perform the uncertainty analysis. PDFs were established for infiltration, the degree of Waste Zone compaction, bulk density, particle density, water content and Kd. The same 1,000-year period of performance was evaluated with 1000 independent realizations, with re-sampling of PDF parameters for each realization.

F-Area Tank Farm model was established to simulate releases from multiple waste tanks. A highly similar approach as that of the Slit Trench 5 probabilistic model was used to develop this model. This includes the use of a modular structure, the use of the same conceptual models for both PORFLOW and GoldSim models, and the method of extracting water fluxes from PORFLOW that was described earlier. The PORFLOW model and GoldSim models were developed simultaneously in this PA which resulted in a greater degree of interaction in which discrepancies between the PORFLOW and GoldSim model representations were resolved in real time. This proved to be very beneficial for the development of both models. Transport simulations were conducted for an abbreviated Pu-239 decay chain, including Pu-239, U-235, Pa-231, Ac-227 and Tc-99.

The earlier difficulty in matching GoldSim and PORFLOW results for sorbing radionuclides was examined in more detail during this investigation and a problem was traced to the saturated zone portion of the GoldSim model. In this zone, a PORFLOW stream trace was fully 3-D and penetrated several aquitards. This phenomenon had not been adequately captured in the GoldSim representations and was addressed by assigning each GoldSim aquifer zone mixing cell a mixture of sandy and clayey material with a multiplier to adjust the ratio. Sand and clay each have different retardation coefficients associated with individual radionuclides, hence the mix of media gave an equivalent retardation coefficient that resulted in closer adherence of arrival times for contaminants at the compliance point for the GoldSim and PORFLOW models.

RESULTS

The results of the initial Slit Trench 5 probabilistic analysis are shown in Figure 2 where PORFLOW results are plotted against the deterministic GoldSim results. To facilitate the comparison, PORFLOW output was utilized to compute doses to hypothetical individuals in separate post-processing calculations. Dose calculations were then performed directly within GoldSim such that the results could easily be compared. Dose was calculated as a function of groundwater concentration at the compliance point, a hypothetical well located 100 m down gradient. The results indicate that the GoldSim peaks arrive sooner than the PorFlow.

Results are shown for 4 radionuclides, C-14, I-129, Tc-99 and Np-237, which represent two non-retarded species and two retarded species. PORFLOW results (dashed lines) are plotted against GoldSim results (solid lines). The radionuclide peaks for all 4 radionuclides are in general conformance with respect to timing and magnitude but the degree of conformance is significantly better for the non-retarded species, C-14 and I-129.

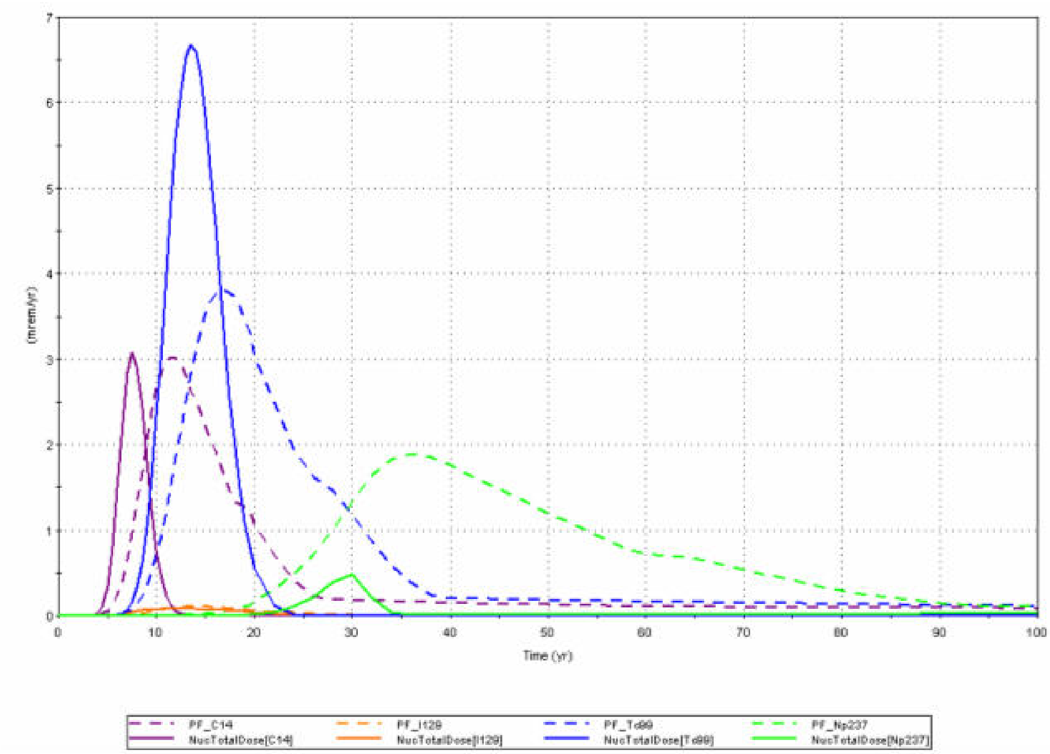

Figure 2. Results of Slit Trench 5 model in deterministic mode

The difference in timing and magnitude of the peaks for the sorbing radionuclides can arise from several causes, primarily differences in the effective retardation and the size of the selected time steps. A time step sensitivity/comparison between the two models was not made in the initial investigation although this was addressed later in the F-Area Tank Farm uncertainty analysis, as were differences in effective retardation.

The results of the Slit Trench 5 probabilistic uncertainty analysis is shown in Figure 3. The results are expressed as All Pathways over the 1000-year PA compliance period. The performance measure for the All Pathways is 0.25 mSv/yr (25 mrem/yr) and is indicated by the horizontal red line. The PORFLOW deterministic results are shown with the dark blue line while the "calibrated" probabilistic model results, e.g. the mean, median and 95% confidence level are also plotted. The shape of these curves are quite similar, however the deterministic peak is significantly earlier. The cause for the difference could be an artifact of the calibration process or, alternatively, could be related to how the PDFs are defined for the selected parameters. This issue was addressed further in the F-Area Tank Farm PA uncertainty analysis.

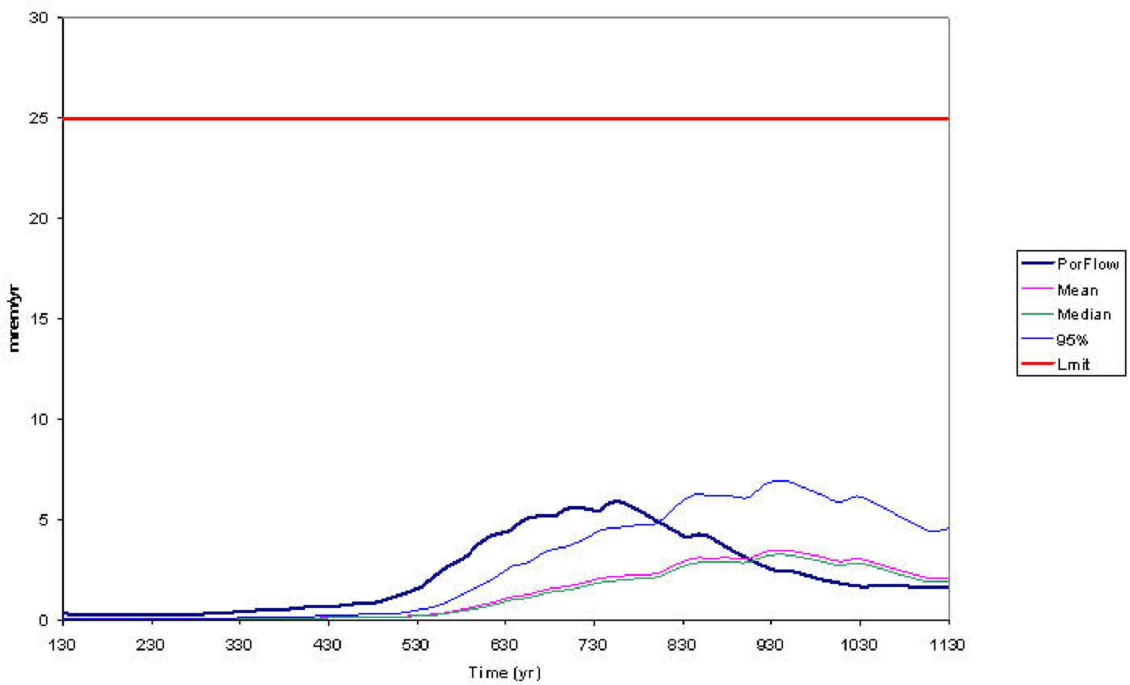

Figure 3. Results of Slit Trench 5 model in probabilistic mode

Results of the vadose zone calibration part of the F-Area Tank Farm uncertainty analysis are presented in Figure 4. These results are plotted in terms of flux from the vadose zone to the water table in terms of moles/year versus time for PORFLOW and GoldSim model results for the abbreviated Pu-239 decay chain, which also includes U-235, Pa-231 and Ac-227. These are all radionuclides that are retarded (partitioning coefficients ranged from 270 ml/g for Pu to 0.6 ml/g for Pa) and yet, there is a much improved adherence of the deterministic PORFLOW results with the deterministic GoldSim model results. This refined comparison is a significant improvement over the degree of adherence achieved in the Slit Trench 5 analysis. Calibration is still in progress for the saturated zone, but it is expected to produce results equally as good. Upon completion of that part of the deterministic GoldSim model, the calibrated model will then be used in probabilistic mode to evaluate uncertainty.

The initial departure of the curves for U and Pa in Figure 4 are an artifact of the PORFLOW code which does not have the ability to allow a certain boundary condition to be established on the interior of the model domain. In this case, the deterministic GoldSim model is more true to the conceptual model upon which both models are based.

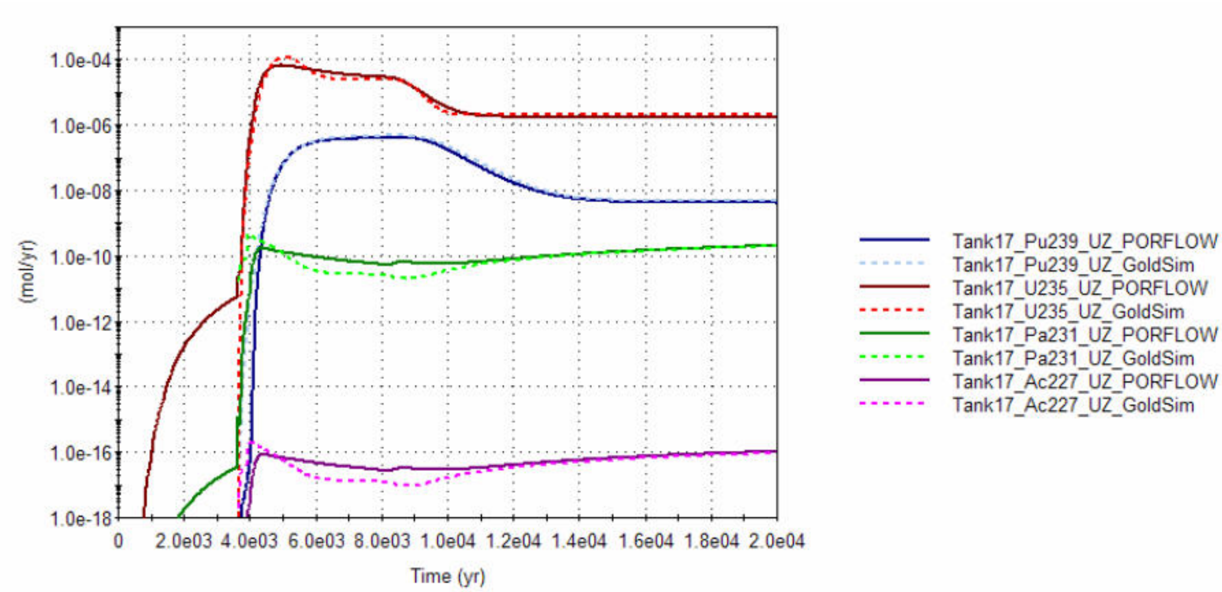

Figure 4. F-Area Tank Farm model benchmarking comparison

CONCLUSIONS

A significant effort has recently been initiated to address probabilistic issues within PA's conducted at the SRS. This effort is considered to be part of a continual process, as is the program of PA analysis and maintenance across the DOE complex. At SRS, findings in the initial probabilistic analysis of the Slit Trenches in the E-Area PA were built upon and improved in the later development of the probabilistic model for the F-Area Tank Farm.

The major challenge in performing this probabilistic analysis was to abstract, or up-scale, the information from the detailed multi-dimensional PORFLOW [1] model to the 1-D GoldSim [2] model. The E-Area model reflects the initial attempt at this process and the results of that effort were useful but the match between model results was not ideal. Trends and peaks, expressed as doses to individuals, were similar, but not identical. These results were adequate, however, considering the purpose of the probabilistic analysis was not to provide a tool to establish quantitative facility disposal limits, but rather to provide added insight into the release pathway mechanisms, help identify the most important parameters and lend added confidence in the deterministically derived facility disposal limits.

The F-Area Tank Farm probabilistic GoldSim model represents a much improved probabilistic model and is an example of the PA process being one of continual improvement. Much better comparisons were made between the PORFLOW and GoldSim model results. The process of abstracting data from one model into another was better understood and implemented. This process involved an iterative approach in which both the deterministic and probabilistic models were used to inform each other as they were being developed and calibrated. This approach has a distinct advantage in that two models were both based on the same conceptual model, thus at successive levels of development the results could be compared and when the models gave different results both models could be investigated to determine the cause of the discrepancy. This approach resulted in a much better understanding of both models and their results.

The interplay that resulted from the parallel development of both the PORFLOW model and the deterministic GoldSim model of the same flow and transport field was a critical factor in developing a more accurate and complete understanding of the actual system that was simulated. This approach allowed the investigation of subtle response differences between the different codes such that each could be adjusted to more accurately reflect the conceptual model basis, and in some cases to refine the conceptual model itself.

REFERENCES

1. ACRI (Analytical & Computational Research, Inc.). 2002. *PORFLOW User's Manual*, Version 5.0, Rev: 5, Analytical & Computational Research, Inc., Bel Air, CA 90077.

2. GTG (GoldSim Technology Group LLC). 2006. *GOLDSIM Users Guide*, Version 9.20, GoldSim Technology Group LLC, Issaquah, WA 98027-5379.

3. WSRC (Washington Savannah River Company). 2007. *E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment,* WSRC-STI-2007-00306 (in press), Washington Savannah River Company, Aiken, SC 29808.