1 of 1

**USE OF A COMPREHENSIVE CALCULATION "GAUNTLET"
APPROACH FOR IMPROVED CONTAMINANTS TRANSPORT
MODELING AT THE F AND H AREA SEEPAGE BASINS (U)**

by

B. B. Looney

Westinghouse Savannah River Company
Savannah River Site
Aiken, South Carolina 29808

J. S. Haselow, WSRC

W. W. Pidcoe, WSRC

C. M. Lewis, WSRC

P. F. Anderson, GeoTrans, Inc.

C. P. Spalding, GeoTrans Inc.

DOE Contract No. **DE-AC09-89SR18035**

This paper was prepared in connection with work done under the above contract number with the U. S. Department of Energy. By acceptance of this paper, the publisher and/or recipient acknowledges the U. S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering this paper, along with the right to reproduce and to authorize others to reproduce all or part of the copyrighted paper.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

**USE OF A COMPREHENSIVE CALIBRATION "GAUNTLET" APPROACH
FOR IMPROVED CONTAMINANT TRANSPORT MODELING AT THE
F AND H AREA SEEPAGE BASINS (U)**

by

^{BBL}
B. B. Looney¹, J. S. Haselow¹, W. W. Pidcoe¹, C. M. Lewis¹, P. F. Anderson², and
C. P. Spalding²

¹ Westinghouse Savannah River Company
Savannah River Site
Aiken SC 29808

² GeoTrans Inc
46050 Manekin Plaza, Suite 100
Sterling VA 20166

The information contained in this article was developed during the course of work under Contract No. DE-AC09-88SR18035 with the U.S. Department of Energy. By acceptance of this paper, the publisher and/or recipient acknowledges the U.S. Government's right to retain a nonexclusive, royalty free license in and to any copyright covering this paper along with the right to reproduce, and to authorize others to reproduce all or part of the copyrighted paper.

Use of a Comprehensive Calibration "Gauntlet" Approach for Improved Contaminant Transport Modeling at the F and H-Area Seepage Basins

B. B. Looney*, J. S. Haselow*, W. W. Pidcoe*, C. M. Lewis*, P. F. Andersen**, and C. P. Spalding**

*Westinghouse Savannah River Company, Aiken, SC

**GeoTrans Inc., Sterling, VA

Abstract

Many types of facility and monitoring data have been collected to support operation, closure and environmental restoration of the F and H-Area Seepage Basins at the Savannah River Site. Based on the various types of data, we developed contaminant transport models to allow projection of contaminant releases and comparison of restoration alternatives. The modeling was performed in the following three stages:

1. postulation of a conceptual model of the flow and transport system
2. development of a simplified analytical model based on a transfer function
3. development of a numerical model

A key feature of the work was use of both traditional data sources and calibration targets such as heads, geological data and pump test results, and non-traditional data sources and calibration targets, such as plume arrival times and shapes, contaminant release rates, and surface water concentrations. Throughout the process, the intermediate and final results were compared to all of the various data types and the earlier modeling stages. The result was a calibration "gauntlet" with explicit criteria for refinement and acceptance of the final model. Failure to match at any step within the gauntlet necessitated appropriate reformulation or modification of the model and rechecking for acceptable matches.

This modeling approach successfully produced a clear and concise description of the flow and transport (the conceptual model), an intuitive tool that was useful for rapid scoping calculations (the transfer function model), and a robust numerical model that allowed evaluation of a wide range of potential groundwater remediations. Using stepwise development, incorporating all available data, and using appropriate acceptance criteria, resulted in a high level of internal consistency and overall defensibility.

Introduction

The F and H-Area Seepage Basins received large volumes of dilute aqueous wastes from the 1950s through 1988. Over the years, the relatively mobile constituents in the wastewater migrated into the water table and then downgradient to Four Mile Branch. Breakthrough of tritium and nitrate was measured in the downgradient stream in the early 1960s. The shape of the plumes as they evolved, the shape of the arrival front, and the average transit time (i.e., the magnitude of radioactive decay during flow) all indicated the presence of large-scale preferential flow paths in the downgradient system. Sediment cores beneath the basins and groundwater/mineralogy data provided information about the magnitude of sorption and transport of the various contaminants.

In the baseline case, water enters the system from infiltration (and formerly the basins) and exits to the downgradient wetlands along Four Mile Branch. Site-specific studies of rainfall, runoff, and evapotranspiration were used to estimate the magnitude of water flow and the approximate size range of a postulated remediation system.

At this point, preliminary numerical models and a transfer function model were generated to facilitate a more quantitative evaluation of potential remediations. The transfer function approach assumes that the flow system may be entirely described using a mathematical equation to transform the contaminant input record into a contaminant output prediction. Such models typically simplify complex flow and transport processes into a function that has only a few

parameters. The parameters are estimated using a period of record for inputs and outputs. High quality measurements of tritium input to the F and H-Area Basins every year of operation are available; similar measurements of output to Four Mile Branch beginning in 1958 (H Area) and 1967 (F Area) are also available. The transfer function model was useful for modeling relatively simple remediation scenarios.

A numerical model, consistent with the conceptual and analytical models, was developed to allow quantitative assessment of more complex remediation schemes. In particular, the numerical simulation was needed to simulate the effect of upgradient or downgradient barriers, and for placement of recovery wells to maximize recovery and minimize wetland impacts.

Geology and Hydrology

As shown on Figure 1, the F and H Area Seepage Basins are located in the center of SRS between two streams, Upper Three Runs to the north and Fourmile Branch to the south. Recharge to the groundwater in this area is primarily due to infiltration of rainwater (rainfall minus runoff and evapotranspiration). Groundwater moves downward and laterally, draining to the nearby streams. As expected, there is a groundwater divide in the shallow water-bearing zones. North of the divide, flow is toward Upper Three Runs and its tributaries and south of the divide, flow is toward Fourmile Branch and its tributaries. In the vicinity of the basins, the shallow groundwater discharges to Fourmile Branch.

Measurements (e.g., flow and contaminant concentrations) in surface waters and in groundwater downgradient of these facilities have been performed from the 1950s through the present. Additionally, examination of cores from drilling and boring and geological descriptions of the area have been performed during this period. Most of the flow to Fourmile branch occurs in the upper two water-bearing layers, a water table zone and a semiconfined zone. A leaky aquitard (clayey zone) is present between these zones. Within these zones, there are areas with higher and lower permeability. This structure controls the water flow rates, the contaminant plume shape, and the contaminant arrival times and locations in the downgradient surface water. As expected, vertical water flow in these plumes follows a curved path downward near the source and then upward into the draining surface water. Surface water monitoring stations in the vicinity of these facilities have been used to determine the groundwater and contaminant flux to Fourmile Branch and to associate the fluxes in the various stream reaches to the upgradient facilities.

Operational History/Conceptual Model

The F and H Area Seepage Basins received large volumes of dilute aqueous wastes from the late 1950s through 1988. The primary dissolved constituents in the wastewater were hydrogen ions (low pH), nitrate, and sodium. The wastewater also contained relatively low concentrations of other chemical constituents (e.g., mercury, cadmium, and lead). The radioactive constituent with the highest activity in the wastewater was tritium; other relatively mobile radionuclides in the wastewater included ⁹⁰Strontium, ⁹⁹Technetium, and ¹²⁹Iodine. A large amount of operational data, geology studies, groundwater and plume chemistry data, ecology characterizations, hydrology and modeling studies are available to support decision-making for these facilities. Observations in the sediments, groundwater, wetlands, and streams underlying and downgradient of the F and H-Area Seepage Basins are indicative of the behavior of contaminants under the substantively perturbed conditions during basin operations (see Fenimore and Horton 1968 & 1972; Christensen and Gordon 1983; Killian et al. 1987a & 1987b; Looney et al. 1988; Haselow et al. 1990; Corbo et al. 1985; Dixon and Rogers 1992):

- During basin operations, relatively large volumes of water were added to the subsurface, maximizing the driving force to move contaminants through the underlying sediments into the groundwater and to the downgradient hydrologic boundary (primarily Fourmile Branch).
- Breakthrough of tritium and nitrate was measured in the downgradient wetlands in the early 1960s.

- The shapes of the groundwater plumes indicate that there are permeable sediments or large scale heterogeneities (or both) in the downgradient system that result in relatively rapid flow.
- The bulk chemistry in the contaminant plume has been altered (increases ionic strength, reduced pH, etc.). This tends to reduce the partitioning of metal ions to the soil because of competition with hydrogen ion for exchange sites. Also, the perturbation in bulk chemistry results in a more aggressive solution chemistry and enhances the leaching of constituents from the sediments in the flow path. The chemical shift would also tend to generate and stabilize colloidal solids that are a documented transport vector for small amounts of a normally sorbed contaminant.
- Sediment cores from the basins indicated that a large fraction of the contaminants normally assumed to have relatively high distribution coefficients are held up in the sediments above the water table, despite the bulk chemistry of the plume.
- Following basin closure, mobile contaminant fluxes (e.g., tritium) to the seep line have begun to decline as these contaminants flush from the system.

The facility installation and operation records and the environmental monitoring data form the basis for the modeling activities. The modeling was performed in the following three stages:

1. postulation of a conceptual model of the flow and transport system
2. development of a simplified analytical model based on a transfer function
3. development of a numerical model

The conceptual model is outlined in the listing above; the subsequent modeling activities are addressed below.

Transfer Function Modeling

To facilitate quantitative projection of tritium fluxes and to provide initial estimates of the impacts of corrective action implementation, a straightforward analytical model of contaminant transport from the seepage basins to the downgradient stream was developed. The approach used in the model is an intuitive "transfer function" similar to that developed by Jury (1982) for describing transport of agricultural contaminants. The transfer function model assumes that the flow system, in this case the flow path between the basins and the seep line, may be entirely described using a mathematical equation to transform the contaminant input record into a contaminant output prediction. The mathematical transformation used is selected based on its consistency with measured data and the assumed governing chemical and physical processes. Such models typically simplify the complex processes governing transport into a function that has only a few parameters. Specific flow and dispersion relationships and permeability variations caused by channels or barriers are not explicitly described. Instead, the transfer function model estimates the average and extreme behavior of the contaminant based on the field measured distribution of travel times. Such models are good predictive tools if the following occurs:

- sufficient historical data on input and output flux are available
- historical input and output can be simply related
- perturbations to the system are describable and relatively small

Measurements of tritium input to the F and H-Area Seepage Basins every year of operation are available; similar measurements of tritium flux to Fourmile Branch beginning in 1958 (H Area) and 1967 (F Area) are also available. As discussed below, a log normal transit time assumption appears reasonable for both areas, providing a simple mathematical function. Applying the model to relatively simple scenarios as a screening tool provides results that are useful to project fluxes into the future. Additionally, the transfer function model results were compared to updated numerical modeling of these areas, calibrated using all of the historical flux, plume shape, geology, and water level data to provide documentation of final corrective action decisions. The

numerical model was used to refine tritium flux projections and to extend the analysis to more complex remediation system analysis.

In the transfer function model for the F and H-Area Seepage Basins, each year's tritium flux to the basins is allowed to reach the seep line as described by a probability density function. The flux contribution from a particular year (t) to the seepage line in a future year ($t+dt$) is equal to the original input flux times the value of the transfer function for a time shift of dt . The total area under the probability density function is 1.0 (for nondecaying contaminants) so that all of the contaminant input to the system in any year leaves the system over time. By superposition, the predicted contaminant output history is simply the sum of all of the various years' contributions. For radioactive constituents, the radioactive decay constant is incorporated into the transfer function to account for contaminant loss during the transit. A large number of investigators have examined subsurface hydraulic conductivity and flow variations (Jury et al. 1982 & 1987; White et al. 1984 & 1986; Molz et al. 1986; Nielson et al. 1973; Van de Pol et al. 1977; Biggar and Nielson 1976; Sharma et al. 1980; Smith et al. 1985). These studies suggest that the appropriate transfer function is a log normal distribution. This distribution has a peak (near the ln mean transit time) and is skewed to the right. As shown below, the distribution as a function of time is entirely defined by the μ and σ .

$$F_t = \frac{1}{\sigma\sqrt{2\pi}} \exp \left(-0.5 \left(\frac{\ln(t) - \mu}{\sigma} \right)^2 \right)$$

Figure 2 shows an example transfer function generated by the model. Both of the curves shown (with and without decay) are calculated for each run. This provides a quality assurance check and documents the amount of contaminant lost by radioactive decay during transit. As described above, the flux of contaminant to the stream in any year is simply the sum of the estimated contributions from all of the previous years disposals to the facility.

$$\text{stream flux (year } j) = \sum_{i=1957}^j \text{basin flux (year } i) \times F_{j-i}$$

The historical tritium input measurements to the F and H-Area Seepage Basins and the historical tritium flux measurements to Fourmile Branch downgradient of these basins are shown in Table 1. The values in Table 1 serve as the calibration targets for estimating μ and σ for each area. Based on minimizing the sum of the squares of the differences between model predictions and the measurements, the following transfer function parameters were selected (t in years):

H Area: $\mu = 2.0$ and $\sigma = 2.0$
 F Area: $\mu = 2.6$ and $\sigma = 0.8$

Figure 3 shows an example calibration for H Area. Overall, the transfer function models reasonably matched the conceptual model (facility operation and site monitoring data). Further, the approach was judged to be adequate for simple contaminant release projections, remediation scenario evaluation, and to assist in numerical model development.

Numerical Modeling

A numerical model, consistent with the conceptual and analytical models, was developed to allow quantitative assessment of more complex remediation schemes. In particular, the numerical simulation was needed to simulate the effect of upgradient or downgradient barriers, and for placement of recovery wells to maximize recovery and minimize wetland impacts.

During the generation of the numerical model, the final calibration gauntlet was generated (Figure 4). A key feature of this approach was use of both traditional and nontraditional calibration targets. Traditional targets included groundwater levels from 382 monitoring wells, observed mounding data during basin operation, groundwater discharge measurements, and others. Nontraditional targets included plume arrival times and shapes, levels of contamination in a lower aquifer, and contaminant flux rate to Fourmile Branch. Throughout the process, the intermediate and final

results were compared to the various data types and earlier modeling stages. The resulting calibration gauntlet had explicit criteria for acceptance. Failure to match at any step within the gauntlet necessitated appropriate reformulation or modification of the model and rechecking for acceptable matches through the entire gauntlet. As an example, Figure 5 shows the calculated tritium flux from the H-Area Seepage Basin to Fourmile Branch for the numerical model and transfer function model. The resulting calibrated numerical model was used to evaluate a wide range of corrective action scenarios, including infiltration reduction, groundwater pump-treat-reinjection, and upgradient or downgradient barriers. The model was also used to optimize pumping rates and recovery/reinjection well placement for the pump-and-treat scenarios.

Conclusion

Using stepwise development, incorporating all available data, and using appropriate acceptance criteria resulted in a high level of internal consistency and overall defensibility. This approach successfully produced a clear and concise description of the flow and transport (the conceptual model), an intuitive tool that was useful for rapid scoping calculations (the transfer function model), and a robust numerical model that allowed evaluation of a wide range of potential groundwater remediations. Based on the results, we recommend early development of a calibration gauntlet (including all types of available site-specific data) to help assure the quality of groundwater and contaminant transport modeling activities.

Acknowledgement

The information contained in this article was developed by Westinghouse Savannah River Company during the course of work under contract No. DE-AC09-89SR18035 with the U. S. Department of Energy.

References

- Biggar, J. W. and D. R. Nielson, 1987. Spatial variability of the leaching characteristics of a field soil, *Water Resources Research*, 23, 1876-1886.
- Corbo, P., M. V. Kantello, and C. B. Fliermans, 1985. Basin Characterization Summary: Analytical Results, Database Management, and Quality Assurance Results for Analysis of Soil Cores from the F- and H-Area Seepage Basins, DPST-85-921, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Christensen, E. J. and D. E. Gordon, 1983. Technical Summary of Groundwater Quality Protection Program at the Savannah River Plant, DPST-83-829, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Dixon, K. L. and V. A. Rogers, 1992. Results of the First Quarter Tritium Survey of the F and H-Area Seepines: May 1992. WSRC-TR-92-304, Westinghouse Savannah River Company, Aiken, SC 29808.
- Fenimore, J. W. and J. H. Horton, Jr., 1968. Influence of High Level Waste Salts on Movement of Strontium and Cesium in Savannah River Plant Soil, DP-1124, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Fenimore, J. W. and J. H. Horton, Jr., 1972. Operating History and Environmental Effects of Seepage Basins in Chemical Separations Areas of the Savannah River Plant, DPST-72-548, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Haselow, J. S., M. Harris, B. B. Looney, N. V. Halverson, and J. B. Gladden, 1990. Analysis of Soil and Water at the Four Mile Creek Seepine near the F & H Areas of SRS WSRC-RP-90-0591, Westinghouse Savannah River Company, Savannah River Laboratory, Aiken, SC 29808.
- Jury, W. A., 1982. Simulation of solute transport using a transfer function model, *Water Resources Research*, 18, 363-368.

- Jury, W. A., L. H. Stolzy, and P. Shouse, 1982. A field test of the transfer function model for predicting solute transport, *Water Resources Research*, 22, 243-247.
- Killian, T. H., N. L. Kolb, P. Corbo, and I. W. Marine, 1987b. Environmental Information Document: H-Area Seepage Basins, DPST-85-706, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Looney, B. B., J. E. Cantrell, and J. R. Cook, 1988. Sampling and Analysis of Surface Water in the Vicinity of the F- and H- Area Seepage Basins, DPST-88-229, E. I. du Pont de Nemours and Co., Savannah River Laboratory, Aiken, SC 29808.
- Molz, F. J., O. Guven, J. G. Malville, R. D. Crocker, and K. T. Matteson, 1986. Performance, analysis and simulation of a two well tracer test at the Mobile Site, *Water Resources Research*, 22, 1031-1037.
- Nielson, D. R., J. W. Bigger, and K. T. Erh, 1973. Spatial variability of field measured soil properties, *Hilgardia*, 42, 215-260.
- Sharma, M. L., G. A. Gander, and C. G. Hunt, 1980. Spatial variability of infiltration in a watershed, *Jour. Hydrology*, 45, 101-122.
- Smith, M. S., G. W. Thomas, R. E. White, and D. Ritonga, 1985. Transport of *Escherichia coli* through intact and disturbed columns of soil, *Jour. Environmental Quality*, 14, 87-91.
- Van de Pol, R. M., P. J. Wierenga, and D. R. Nielson, 1977. Solute movement in a field soil, *Soil Science Soc. of America Jour.*, 41, 10-13.
- White, R. E., G. W. Thomas, and M. S. Smith, 1984. Modeling water flow through undisturbed cores using a transfer function model derived from tritium and chloride transport, *Jour. Soil Science*, 35, 159-168.
- White, R. E., J. S. Dyson, R. A. Haigh, W. A. Jury, and G. Sposito, 1986. A transfer function model of solute transport through soil, 2: illustrative applications, *Water Resources Research*, 21, 447-457.

Table 1. Historical Tritium Flux Data for the F and H Area Seepage Basins

year	H Area Basins groundwater system		F Area Basins groundwater system	
	input to basins (Ci)	flux to stream (Ci)	input to basins (Ci)	flux to stream (Ci)
1957	5920	nd	880	nd
1958	5500	400	0	nd
1959	5607	800	5836	nd
1960	4366	1600	8341	nd
1961	11613	2000	10297	nd
1962	12706	1700	18050	nd
1963	8240	2700	17157	nd
1964	6430	4700	21569	nd
1965	13135	5600	16151	nd
1966	17018	4600	19992	nd
1967	7609	3000	11938	2600
1968	20678	2900	14002	2887
1969	11015	3500	11679	2589
1970	21107	4400	10944	2592
1971	14160	9500	4766	2299
1972	15176	5400	7051	3485
1973	19891	6800	11941	4185
1974	8118	5700	7512	3176
1975	10144	6800	3690	2080
1976	15663	4300	6041	2653
1977	8824	4500	3922	3657
1978	8891	5500	4763	3454
1979	7511	6700	5970	2160
1980	8021	5300	5323	1507
1981	13377	4200	7578	1106
1982	9134	4900	4540	2770
1983	12952	6500	7482	2568
1984	11955	8020	9344	2320
1985	12414	4560	9895	2690
1986	26677	7360	10232	1800
1987	13599	5630	13162	2760
1988	9851	3980	3142	3330
1989	0	4600	0	4443
1990	0	1900	0	3570
1991	0	1810	0	5750
1992	0	1500 est	0	4000 est

nd = no data

* MWMF - Mixed Waste Management Facility and the associated Low Level Radioactive Waste Disposal Facility

Figure 1. Map of Study Area

Figure 2. Transfer Function Example - relative flux at seep line from one years input to basins

Figure 3. Example Transfer Function Calibration - H Area Seepage Basins

Figure 4. Final Calibration Gauntlet Used in Study

Figure . Comparison of Measurements, Transfer Function Predictions and Numerical Model

Figure 5. Example Calibration - Comparison of Field Data, Transfer Function Model and Numerical Model

DATE

FILMED

44 / 7 / 94

END