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Rev. 0

Key Words:Diffusion
Saltstone
Concrete

Nitrate diffusional releases from the Saltstone Facility, Vault 2, with respect to different concrete wall thicknesses

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Prepared by:

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January, 2005

Westinghouse Savannah River Company
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LIST OF ACRONYMS and ABBREVIATIONS

1-D	One dimensional
2-D	Two dimensional
DOE	U.S. Department of Energy
in	inch
kg	kilogram
L	liters
m	meters
mg	milligram
PA	performance assessment
SA	Special Analysis

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EXECUTIVE SUMMARY

To assist the Saltstone Vault 2 Design Team, an investigation was conducted to evaluate the effectiveness of alternative concrete wall thicknesses in limiting nitrate diffusion away from the planned facility. While the current design calls for 18-inch concrete walls, alternative thicknesses of 12-in, 8-in, and 6-in were evaluated using a simplified 1-D numerical model. To serve as a guide for Saltstone Vault 2 conceptual design, the results of this investigation were applied to Saltstone Vault 4 to determine what the hypothetical limits would be for concrete wall thicknesses thinner than the planned 18-inches. This was accomplished by adjusting the Vault 4 Limits, based on the increased nitrate diffusion rates through the thinner concrete walls, such that the 100-m well limit of 44 mg/L of nitrate as nitrate was not exceeded. The implication of these preliminary results is that as thinner vault walls are implemented there is a larger release of nitrate, thus necessitating optimal vault placement to minimize the number of vaults placed along a single groundwater flow path leading to the discharge zone.

INTRODUCTION

An investigation was conducted to evaluate the effectiveness of alternative concrete wall thicknesses as barriers to diffusion of nitrate from Vault 2 of the Saltstone Disposal Facility. This effectiveness has implications for the selection of the final design concept for future vaults.

The concrete wall thickness of the current vault design is 18-inches. This thickness, along with alternative thicknesses of 12-in., 8-in. and 6-in. were evaluated using a 1-D numerical model extending through the concrete wall, and including saltstone on one side and soil on the outside. 2-D numerical simulations for the Saltstone Vault 4, currently being developed, indicate that nitrate migration through the 18-in. outer wall is dominated by diffusion during the Performance Assessment (PA) evaluation period. This finding was built upon to perform the simplified simulations described herein.

It is anticipated that the results of this scoping evaluation will assist the Saltstone Design Team in selecting a final design concept for future saltstone disposal.

MODEL DEVELOPMENT

Conceptual Model

The diffusion flux of nitrate through different thicknesses of the concrete wall of a saltstone disposal facility was evaluated in this investigation. Nitrate migration through the outer concrete wall has been demonstrated to be dominated by diffusion, rather than advection, in the closure setting of the planned saltstone facilities over the PA period of interest. Using this information, a simplified numerical model was set up to evaluate nitrate diffusion from saltstone material, through concrete wall-material of differing thicknesses, and into soil.

Numerical Model

The mathematical model utilized in this report is provided by the PORFLOW™ simulation package. PC-based PORFLOW™ Version 5.97.0 was used to conduct a series of simulations.

PORFLOW™ is developed and marketed by Analytic & Computational Research, Inc. to solve problems involving transient and steady-state fluid flow, heat and mass transport in multi-phase, variably saturated, porous or fractured media with dynamic phase change. PORFLOW™ has been widely used at the SRS and in the DOE complex to address major issues related to ground water and nuclear waste management.

The governing equation for mass transport of species *k* in the fluid phase is given by

$$\frac{\partial C_k}{\partial t} + \frac{\partial}{\partial x_i}(V_i C_k) = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C_k}{\partial x_j}) + \gamma_k$$

Where

C_k	concentration of species *k*
V_i	fluid velocity in the i^{th} direction
D_{ij}	effective diffusion coefficient for the species
γ_k	net decay of species *k*
i, j	direction index
t	time
x	distance coordinate

This equation is solved within PORFLOW to evaluate transient nitrate diffusive transport through the concrete walls of a hypothetical Saltstone Vault to determine mass flux over time. The mass fluxes through different concrete wall thicknesses were evaluated and compared.

Model Development and Assumptions

The numerical representation of the conceptual model is as a 1-dimensional (1-D) horizontal stack of elements configured to represent the different concrete wall thicknesses, as shown below in Figure 1, a conceptual diagram of the model domain.

Since the nitrate source is dissolved in the pore water, diffusion was allowed to proceed only through the water-saturated portion of the pores. Diffusion was the only transport mechanism simulated in the model and advection was disabled.

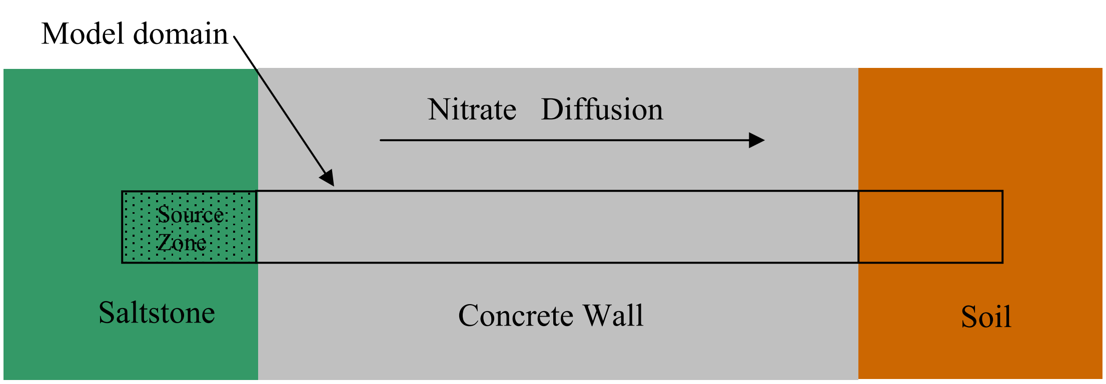

Figure 1. Conceptual diagram of model domain

The boundary and initial conditions imposed on the model domain included:

- No-flux designation was specified for nitrate along sides and bottom.
- Nitrate concentration set to 0 at the outer edge of the soil material zone.
- A unit nitrate source term was introduced and uniformly distributed within in the saltstone material zone.

Simulations were conducted in transient mode for diffusive transport, with results being obtained over 10,125 years at the outer edge of the soil material zone. This simulation length was selected to account for 25 years of facility operation, 100 years of institutional control and a 10,000-year performance period. A set of consistent units were employed in the simulations for length, mass and time, these being meters, grams and years, respectively.

The model grid was constructed as a node mesh 3 nodes tall, and laterally by a differing number of nodes, ranging from 21 to 27, depending thickness of the concrete wall being evaluated. These nodal meshes create element stacks that ranged from 19 to 25 model elements.

Material zones

The model domain was divided into three zones, the saltstone waste zone, the soil zone and the concrete zone that separates the two. The saltstone and soil zones were established at 0.5 m thick while the concrete zones were evaluated for thicknesses of 6-in., 8-in., 12-in. and 18-in.

Material zone properties and other input parameters

Material properties utilized within the 1-D numerical model were specified for the 3 material zones defined in the model. Each material zone was assigned values for total porosity, residual saturation, water-filled porosity, matrix density, water density and an effective nitrate molecular diffusion coefficient. The rock (matrix) density was selected based on the density of quartz, and is regarded to be representative of the materials selected in this simulation.

Values for total porosity and long-term residual saturation for saltstone and concrete were obtained from vadose zone 2-D simulations conducted to evaluate the groundwater pathway for Saltstone Vault 4 study currently being conducted. Saltstone, concrete and soil porosities were established at 0.42, 0.18 and 0.31, respectively, in that analysis. The steady-state residual saturations were obtained from representative nodes in the simulation domain. The effective nitrate molecular diffusion coefficients for each of the radionuclides evaluated were based on values selected for this parameter in the Saltstone Vault 4 study. A summary of the values of porosity, long-term residual saturation, water-filled porosity and effective NO_3 diffusion coefficients are listed for each material type in Table 1.

Table 1 Porosity, residual saturation and water-filled porosity values

Layer Material	Representative Porosity	Long-term Residual Saturation	Water-Filled Porosity	Effective NO_3 Diffusion Coefficient
				(m^2/yr)
Soil	0.31	0.5	1.55E-01	1.58E-02
Concrete	0.18	0.99	1.78E-01	3.15E-05
Saltstone	0.42	0.99	4.16E-01	1.58E-05

A value for the density of water was obtained from the Bolz, R.E., et. al., CRC Handbook of Tables for Applied Engineering Science.

MODEL RESULTS

Model simulations were conducted to evaluate the peak nitrate flux and cumulative nitrate flux over time for each of the concrete wall thicknesses. Results were reported in Kg/yr for the peak instantaneous flux (assuming the initial inventory was 1 Kg.) and as a percentage of the initial inventory for cumulative flux. The simulation results (i.e. peak fluxes and time peak occurs) are tabulated below in Table 2 and shown graphically in Figures 2 and 3. In Figure 2 it is apparent that the effect of thinning the concrete wall results in shortening the time until the peak instantaneous flux occurs and increases the magnitude of the peak flux. The magnitude of the instantaneous peak fluxes for the 12-in. 8-in. and 6-in. concrete walls are higher than the 18-in. base case by factors of 1.48, 2.18 and 2.86, respectively.

Table 2 Summary of the peak flux rates and time of peak

Concrete Wall Thickness	Peak Instantaneous Flux	Time Peak flux occurs
(inches)	(Kg/yr)	(yrs)
6	1.02E-4	5.20E+2
8	7.80E-5	8.57E+2
12	5.31E-5	1.81E+3
18	3.58E-5	3.30E+3

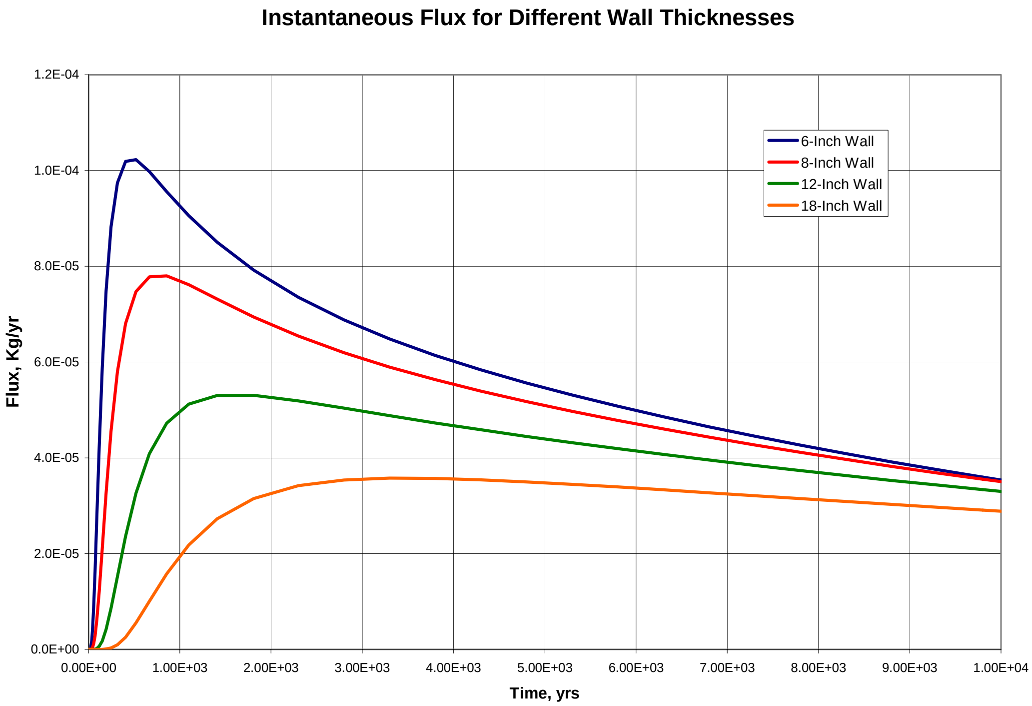

Figure 1. Instantaneous nitrate fluxes vs. time for different wall thicknesses

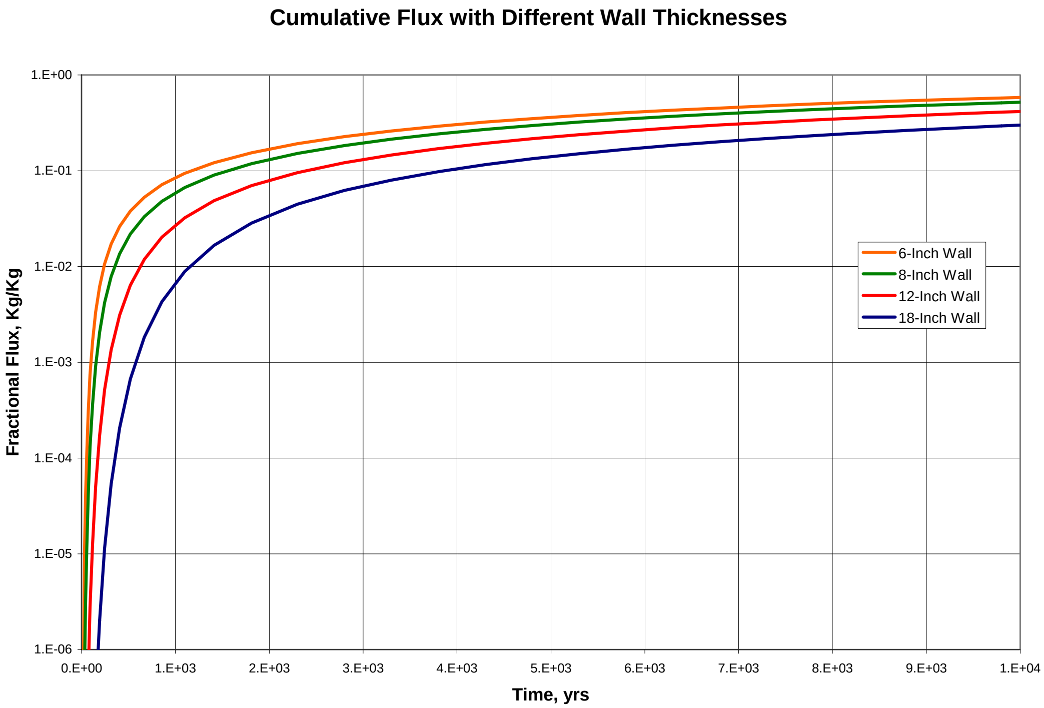

Figure 2. Cumulative fractional nitrate flux vs. time for different wall thicknesses

To serve as a guide for Saltstone Vault 2 conceptual design, the results of this investigation were applied to Saltstone Vault 4 to determine what the hypothetical limits would be for concrete wall thicknesses thinner than the planned 18-inches. This was accomplished by adjusting the Vault 4 Limits, based on the increased nitrate diffusion rates through the thinner concrete walls, such that the 100-m well limit of 44 mg/L of nitrate as nitrate was not exceeded. In Table 3, below, these preliminary Nitrate disposal limits associated with different concrete wall thicknesses for the Vault 4 configuration are indicated.

Table 3. Preliminary Nitrate limits for Vault 4 with different wall thicknesses.

Concrete Thickness (inches)	Nitrate Limit (kg)
18	3.67E+07
12	2.47E+07
8	1.68E+07
6	1.29E+07

The implication of these preliminary results is that as thinner vault walls are implemented there is a larger release of nitrate, thus necessitating optimal vault placement to minimize the number of vaults placed along a single groundwater flow path leading to the discharge zone.

REFERENCES

Bolz, R.E. and G.L. Tuve, (Editors), 1973. *Handbook of tables for APPLIED ENGINEERING SCIENCE, 2'nd Edition*. CRC Press, 18901 Cranwood Parkway, Cleveland, OH.

Design Check Instructions for Saltstone Vault 2 Cement Wall Thickness Evaluations

Files associated with this design check:

BaseCaseResults.xls – "Output" worksheet containing cumulative and instantaneous nitrate diffusional fluxes, "Peaks" worksheet containing a summary of the peak instantaneous diffusive flux and the time of occurrence, two worksheets containing graphs.
WallDiff_Gridding.xls – "Diffusion" worksheet containing calculation of water filled porosity and indicating the Eff. Nitrate Diff. coefs. used for the respective materials, a worksheet indicating the Y-axis gridding associated with each wall thickness.
run18.dat, run12.dat, run8.dat, run6.dat– Porflow input file for evaluating diffusional flux for cement wall thicknesses of 18-in., 12-in., 8-in. and 6-in..
WallThickness.doc - the main documentation of the investigation.

Please review the main text report contained in **WallThickness.doc**

Things to check:

1. Spot check the **run.dat** files to verify that the Y-axis gridding (in **WallDiff_Gridding.xls**) has been correctly represented.

The gridding was checked in each run.dat file and found to be correct.

2. Verify that the nitrate effective diffusion coefficient used in each simulation is the same as the effective diffusion coefficient used in the Saltstone Vault 4 vadose zone simulation(s). Verify these are the values that appear in Table 1 of the report contained in **WallThickness.doc.**

The effective diffusion coefficients were found to be the same as used in the Vault 4 Special Analysis, when converted to m^2/year from cm^2/year

3. Verify that the peak instantaneous fluxes in **BaseCaseResults.xls**, "Output" worksheet correctly identifies the peak instantaneous flux (indicated by cell coloring) and the time the peak occurs. Verify that these are the values listed in the "Peaks" worksheet. Verify that these are the values that appear in Table 2 of the report in **WallThickness.doc.**

The requested entries were checked and all were found to be correct.

4. Verify that the limit calculations in **BaseCaseResults.xls,** "Limits" worksheet are logically correct and calculated correctly.

The limit calculations are logical and were correctly calculated