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A Graded Approach to Flow and Transport Modeling to Support Decommissioning Activities at the Savannah River Site, Aiken SC

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ABSTRACT

A graded approach to flow and transport modeling has been used as a cost effective solution to evaluating potential groundwater risk in support of Deactivation and Decommissioning activities at the United States Department of Energy's Savannah River Site. This approach incorporates both simple spreadsheet calculations and complex numerical modeling to evaluate the threat to human health posed by contaminants leaching from decommissioned concrete building slabs. Simple spread sheet calculations were used to produce generic slab concentration limits for a suite of radiological and non-radiological contaminants for a chemical separations area at Savannah River Site. These limits, which are based upon the United States Environmental Protection Agency Soil Screening guidance, were used to eliminate most building slabs from further risk assessment. Of the more than 58 facilities located in the area, to date only one slab has been found to have a contaminant concentration in excess of the area specific slab limit. For this slab, a more rigorous numerical modeling effort was undertaken reducing the conservatisms inherent in the spreadsheet calculations.

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Using the more sophisticated numerical model, it was possible to show that the remaining contaminant of concern would not likely impact groundwater above drinking water standards.

Key words: groundwater; radioactivity, residual; ¹²⁹I; contamination

INTRODUCTION

The U.S. Department of Energy's (DOE) Savannah River Site (SRS) is an 800 km² DOE reservation in southwestern South Carolina. Five nuclear reactors were constructed in the 1950s to produce nuclear materials for national defense, primarily tritium and plutonium-239. Supporting facilities included two chemical separations plants, a heavy water extraction plant, a nuclear fuel and target fabrication facility, a tritium extraction facility, and waste management facilities. Today the SRS is primarily engaged in the processing of legacy nuclear wastes, environmental cleanup, nonproliferation activities, tritium recycling, and deactivation and decommissioning (D&D) of legacy facilities.

D&D is a major emphasis at the SRS with 700,000 m² of radiological and chemical facilities slated for demolition by 2025. Most buildings will be demolished leaving behind only the concrete slab that formed the building foundation. It is necessary to demonstrate that risk-based criteria have been met for the concrete slab end state. Slabs that pose unacceptable risk are subsequently scabbled or removed entirely to reduce or eliminate the associated risk. Typically, the limiting component of the risk assessment is to determine the potential impacts to groundwater from contaminants leaching from the concrete slabs.

SRS has employed a graded approach as a cost effective solution to evaluating potential groundwater impacts which incorporates both simple spreadsheet calculations and complex numerical modeling to cost effectively evaluate the threat to human health posed by potential impact to groundwater. The simple spreadsheet calculations produce generic derived guideline concentration levels (DCGLs), or slab limits, based upon the Environmental Protection Agency's (EPA) soil screening guidance protocol for comparison to subsequent end state verification sampling results. For this analysis, the DCGL may be defined as the maximum allowable contaminant concentration in the concrete that will not exceed the groundwater Safe Drinking Water Act Maximum Contaminant Levels (MCLs) or EPA Region IV preliminary remedial goals (PRGs) within a 1000 y time period.

In most cases, no further analysis is required. However, when concentrations are found that exceed the slab limit for a given analyte, a more rigorous modeling effort is undertaken reducing the conservatism inherent in the simple screening calculation. In most cases, the more rigorous modeling exercise shows risk levels to be acceptable allowing the concrete slab to be left in place.

This paper describes the graded approach employed at SRS and provides an overview of the screening and rigorous methods used to evaluate potential impacts to groundwater. A case study is presented where the graded approach was successfully used to evaluate potential groundwater impacts from a chemical separations facility at SRS.

METHODS

The graded approach to flow and transport modeling used at SRS incorporates both screening level spreadsheet calculations and complex, numerical modeling. The premise of this approach is that simple spreadsheet calculations can be used to eliminate most building slabs from further, more complicated and time consuming analysis. For this analysis, VZCOMML[®] (Rucker 1999 and 2004) was used to develop DCGLs for potential impacts to groundwater from metals, inorganic compounds, volatile organic compounds, and radionuclides leaching from concrete slabs in F-Area of SRS. In the case where a contaminant was found at a concentration in excess of the DCGL established using VZCOMML[®], more detailed analysis was conducted using the PORFLOW[™] simulation package.

VZCOMML[®] is a conservative spreadsheet based model that can be used as a preliminary tool to evaluate the potential for vadose zone contamination to impact groundwater. The model simulates transport in the vadose zone by steady-state one-dimensional flow and represents average flow conditions over the period of interest. The analysis approach employed within the VZCOMML[®] suite is consistent with the approved Contaminant Migration Protocol of the Federal Facility Implementation Management Plan and EPA Soil Screening Guidance (EPA 1996).

The conceptual model for the spreadsheet calculations assumes that complex building geometries and contaminant distributions can be represented as simple slabs with uniformly distributed contamination. The general conceptual

model for VZCOMML[®] is presented in Figure 1. The model allows up to four layers to describe the vadose zone in addition to the source layer and aquifer layer. Thickness, porosity (total and effective), and hydraulic conductivity are specific for each layer.

The spreadsheet model 1) estimates the theoretical peak groundwater concentration for an analyte at the surface of the water table and 2) predicts the time to maximum groundwater concentration at a down gradient receptor by application of a dilution factor. The nature of the input data and the analytical model assumptions are such that the estimated groundwater concentrations are conservative. Analytes with maximum concentrations predicted to occur within 1000 y are then compared to the MCL or PRG. A time limit of 1,000 y is used to determine if constituents have the potential to pose a future leachability risk based upon the SRS Contaminant Migration Protocol.

There are several simplifying assumptions associated with the model. The most significant is that the concrete slab may be represented as soil. This is a conservative assumption because concrete would be expected to delay the release of contaminants to the environment due to its low hydraulic conductivity and diffusion coefficient compared to most soils. Other assumptions include the contaminants are homogeneously distributed throughout the subsurface, the system is at equilibrium, and soil/water partitioning is reversible, instantaneous, and linear in the contaminated zone. VZCOMML[®] assumes that the receptor well is located at the edge of the source and screened within the plume. Dispersion is not

incorporated into the vadose zone flow estimate because in most cases it minimally affects the maximum groundwater concentration.

Lithologic data from F-Area was used to establish the four vadose zone layers allowed by VZCOMML[®]. Table 1 lists the inputs for the vadose zone layers used in the model setup. The parameters used to describe the saturated zone (i.e. water table aquifer) are given in Table 2.

¹²⁹I PORFLOWTM Analysis

Of the more than 58 facilities in F-Area, only one building slab has been found to have a contaminant concentration in excess of the area specific slab limit determined using VZCOMML[®]. The contaminant of concern for this slab was ¹²⁹I. For this slab and contaminant, a more detailed analysis was conducted using the PORFLOWTM simulation package (ACRI, 2000). PORFLOWTM is a numerical code used 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. PORFLOWTM has been widely used at the SRS and in the DOE complex to address major issues related to the groundwater and nuclear waste management.

PORFLOWTM Version 5.97.0 was chosen for the more rigorous simulation of flow and transport in the vadose zone for the F-Area ¹²⁹I analysis. Several conservative assumptions inherent to VZCOMML[®] were eliminated using the more sophisticated PORFLOWTM model. Facility specific input parameters were used including building geometry, slab thickness, material properties, and depth to water table. Unlike with VZCOMML[®], in PORFLOWTM,

the source layer was represented as concrete and the main mechanism for contaminant transport from the slab was diffusion rather than advection.

The conceptual model for the F-Area PORFLOWTM analysis considered the movement of water and contaminants through the facility and vadose zone in two dimensions. The two dimensional model represents a transverse slice through the facility and surrounding porous media (Fig. 2).

The selection of appropriate physical and chemical parameters is an important step in the process of simulating the movement of water and contaminants through the vadose zone. For most parameters, a wide range of applicable values are reported in the literature with only limited SRS specific data available. In general, a conservative but realistic approach was used in the selection of input parameters for this analysis. Material properties and parameter values used in the PORFLOWTM vadose zone flow and transport model are listed in Tables 3 and 4.

PORFLOWTM requires that boundary conditions be defined in order to solve the equations for flow. The top of the model domain was established as a constant flux boundary. Because the model domain extends laterally beyond the facility, a portion of the upper boundary is concrete and the remainder is soil. PORFLOWTM can accommodate variable flux assignments to boundary elements and two infiltration rates were used to define the flux for this boundary. The bottom of the model domain was established as a constant head boundary maintained by the presence of the water table. The left and right boundaries were set as no flow boundaries.

Boundary conditions for the mass transport simulations were set as follows for the model domain. The left and right boundaries were established as no flux boundaries consistent with the no flow boundaries used in the flow simulations. For the upper boundary, the infiltrating water was assumed to have a concentration of zero. For the bottom boundary, the concentration gradient normal to the boundary was set to zero. This boundary condition sets the diffusive flux across the boundary equal to zero and allows contaminant mass to be removed from the model domain by advection only.

RESULTS

VZCOMML[®] was used to calculate DCGLs for 96 contaminants including 41 radionuclides. Of these contaminants, only ¹²⁹I has been measured in a F-Area slab at concentration exceeding the screening level DCGL of 0.035 Bq g⁻¹. This slab was further evaluated using the PORFLOW[™] simulation package.

Flow and transport simulations were conducted using the PORFLOW[™] simulation package to refine the DCGL for ¹²⁹I. The steady state saturation profile and groundwater velocity fields are given in Figures 3 and 4. These figures show that the movement of water through the model domain is consistent with the boundary conditions selected. Flow near the left and right model boundaries is essentially vertical as controlled by the no horizontal flow boundary conditions for each scenario. The saturation profile (Fig. 3) shows that the facility is partially filled with water due to a small amount of infiltration through the vault cap as well as a small amount of seepage through the sides of the vault. The water level in the facility is approximately 5.5 m at steady state. The velocity

vectors through the model domain are consistent with the boundary conditions and material types (Figure 4). The vector field clearly shows that advective flow through the facility is minimal. Outside the facility, the velocity vectors are parallel to the concrete structure but the vectors bend tightly around the corner at the bottom. Flow at this point accelerates and sweeps along the bottom of the vault bending downwards toward the water table. This figure shows that contaminant release from the slab will be predominantly the result of diffusion and that once this contaminant reaches the soil beneath the facility it will be transported to the water table via advection by infiltrating rain water.

A total of five concrete samples were collected from the facility slab and analyzed for ^{129}I . The measured concentrations were used to determine an area weighted average concentration of ^{129}I of 0.039 Bq g^{-1} for input into the mass transport simulations. The mass transport simulations were run for a 2000 y time period based upon the steady state flow field from the flow simulations. Results from the analysis showed the maximum ^{129}I concentration in a down gradient receptor well to be 0.025 Bq L^{-1} which is below the MCL of 0.037 Bq L^{-1} . The screening level DCGL of 0.035 Bq g^{-1} is increased to 0.059 Bq g^{-1} when impacts to groundwater are based on the more rigorous PORFLOWTM analysis, thereby yielding no potential impacts to groundwater for the contaminated slab.

CONCLUSION

In the graded approach to flow and transport modeling, the VZCOMML[©] model is used to establish screening level conservative slab limits for comparison to measured concentrations of contaminants of concern. If the measured

concentration of a contaminant exceeds the slab limit, a more sophisticated numerical model such as PORFLOWTM can be used and often demonstrates that there is no potential impact to groundwater above drinking water standards. The graded approach to assessing groundwater risk due to contaminants leaching from concrete slabs has been successfully used at SRS to reduce costs and to accelerate the decommissioning schedule.

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Table 1. Vadose zone parameters used in VZCOMML[®] for F-Area calculations.

	Thickness, m	Effective Porosity (Looney et al. 1987)	Total Porosity (McDowell- Boyer 2000)	Hydraulic Conductivity, m y ⁻¹
Source	0.15 ^a	0.18	0.18	5 ^b
Layer 1	6	0.2	0.4	26
Layer 2	11	0.2	0.4	40
Layer 3	5	0.2	0.4	540
Layer 4	3	0.2	0.4	40

^aA source layer thickness of 0.05 m was used for radionuclides (except tritium).

^bThe hydraulic conductivity of clay was used for the source layer, which was the lowest available conductivity in VZCOMML[®] Version 3.01.

Table 2. Aquifer parameters used in VZCOMML[®] for F-Area calculations.

Parameter	Value	Source
Slab length parallel to groundwater flow, m	20.7	Site ArcGIS coverage
Infiltration rate, m y ⁻¹	0.38	Looney et al. 1987
Aquifer hydraulic conductivity, m y ⁻¹	835	Flach and Harris 1999; Flach 2004
Aquifer thickness, m	8.2	Flach and Harris 1999; Flach 2004
Hydraulic gradient, m m ⁻¹	0.0047	Hiergesell 2003

Table 3. Material Properties used in the Facility Specific PORFLOW™ Vadose Zone Flow and Transport Simulations.

Parameter	Concrete	Gravel	Native Soil	Units
Saturated hydraulic conductivity, $K_{xx}=K_{yy}$	1.0×10^{-10}	1.0×10^{-2}	1.0×10^{-5}	cm sec ⁻¹
Porosity, η	0.18	0.38	0.42	fraction
Particle density, ρ_s	2.65	2.65	2.65	g cm ⁻³

Table 4. Parameter Values used in the Facility Specific PORFLOW™ Vadose Zone Flow and Transport Model.

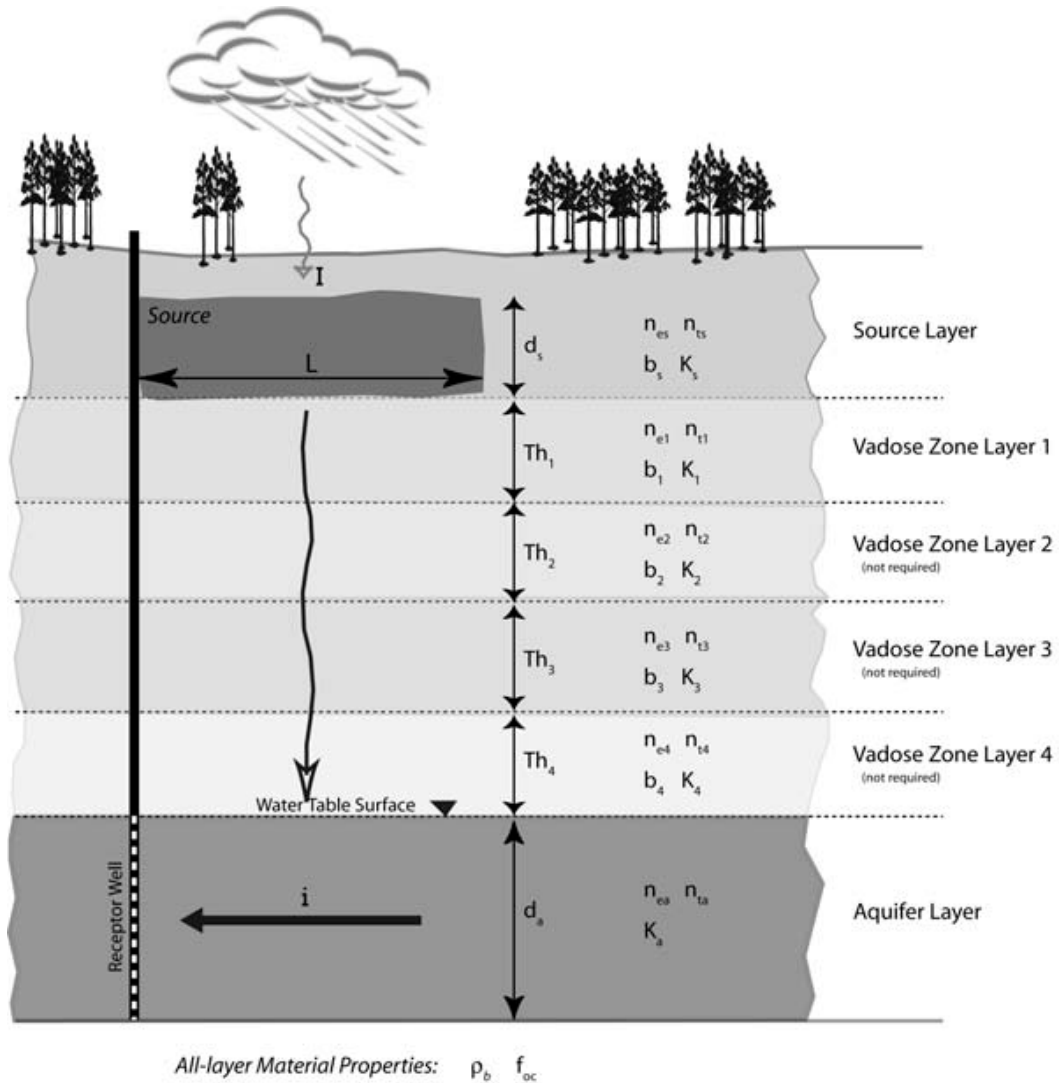
Parameter	Concrete	Units
Slab Apparent diffusion coefficient, D_a	5.01×10^{-8}	$\text{cm}^2 \text{sec}^{-1}$
Soil Apparent diffusion coefficient, D_a	5.01×10^{-6}	$\text{cm}^2 \text{sec}^{-1}$
Longitudinal dispersivity, α_L	0	cm
Transverse dispersivity, α_T	0	cm
Distribution coefficient (K_d) for the native soil material type	0.6	ml g^{-1}
Distribution coefficient (K_d) for the concrete material type	2	ml g^{-1}
Dilution Attenuation Factor (DAF)	2.93	Unitless
^{129}I half life	1.6×10^7	y
Infiltration rate over soil	0.457	m y^{-1}
Infiltration rate over concrete	0.086	cm y^{-1}
MCL	1.0	$\mu\text{g L}^{-1}$

Table 5. Results from the Facility Specific PORFLOW™ ^{129}I Transport Simulation for a Water Table Receptor Well.

Location	Time to Peak (y)	Peak Concentration (Bq L^{-1})	DCGL (Bq g^{-1})
Water Table Boundary	273	0.074	0.0195
Receptor Well	273	0.025	0.059

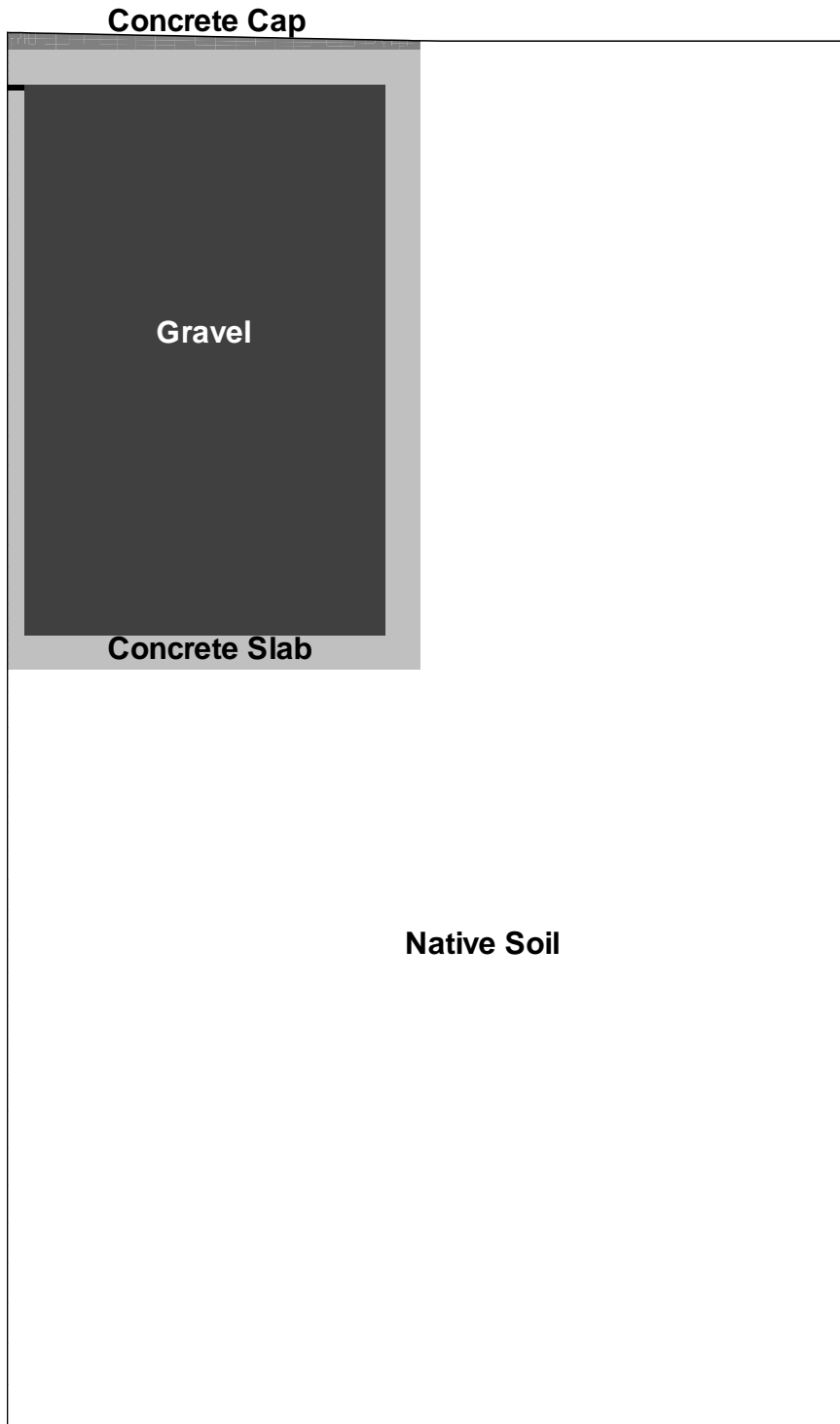
VZCOMML[®] Conceptual Model

Dixon – Fig. 1



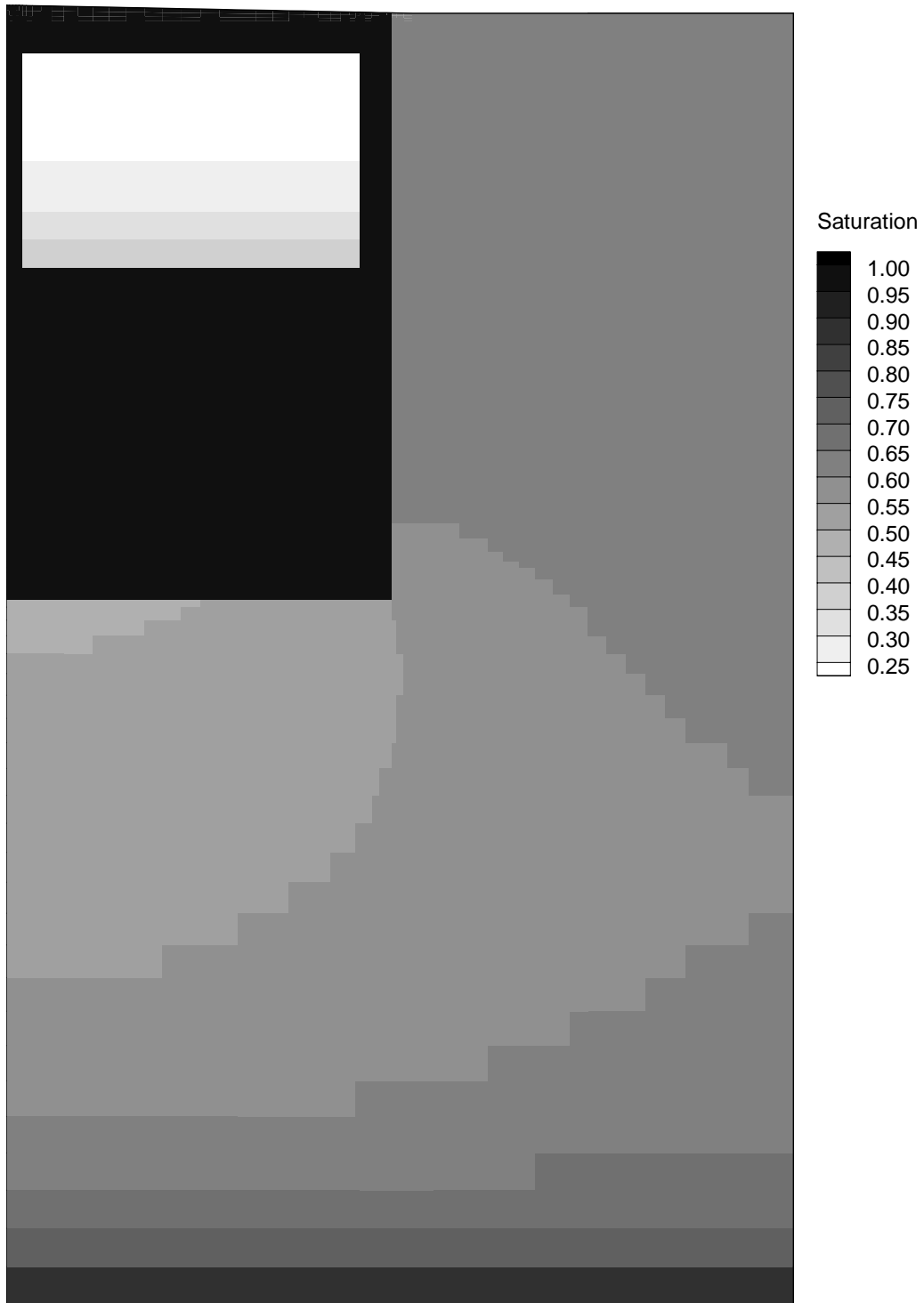
Conceptual Model used in the Facility Specific PORFLOW™ Analysis

Dixon – Fig. 2



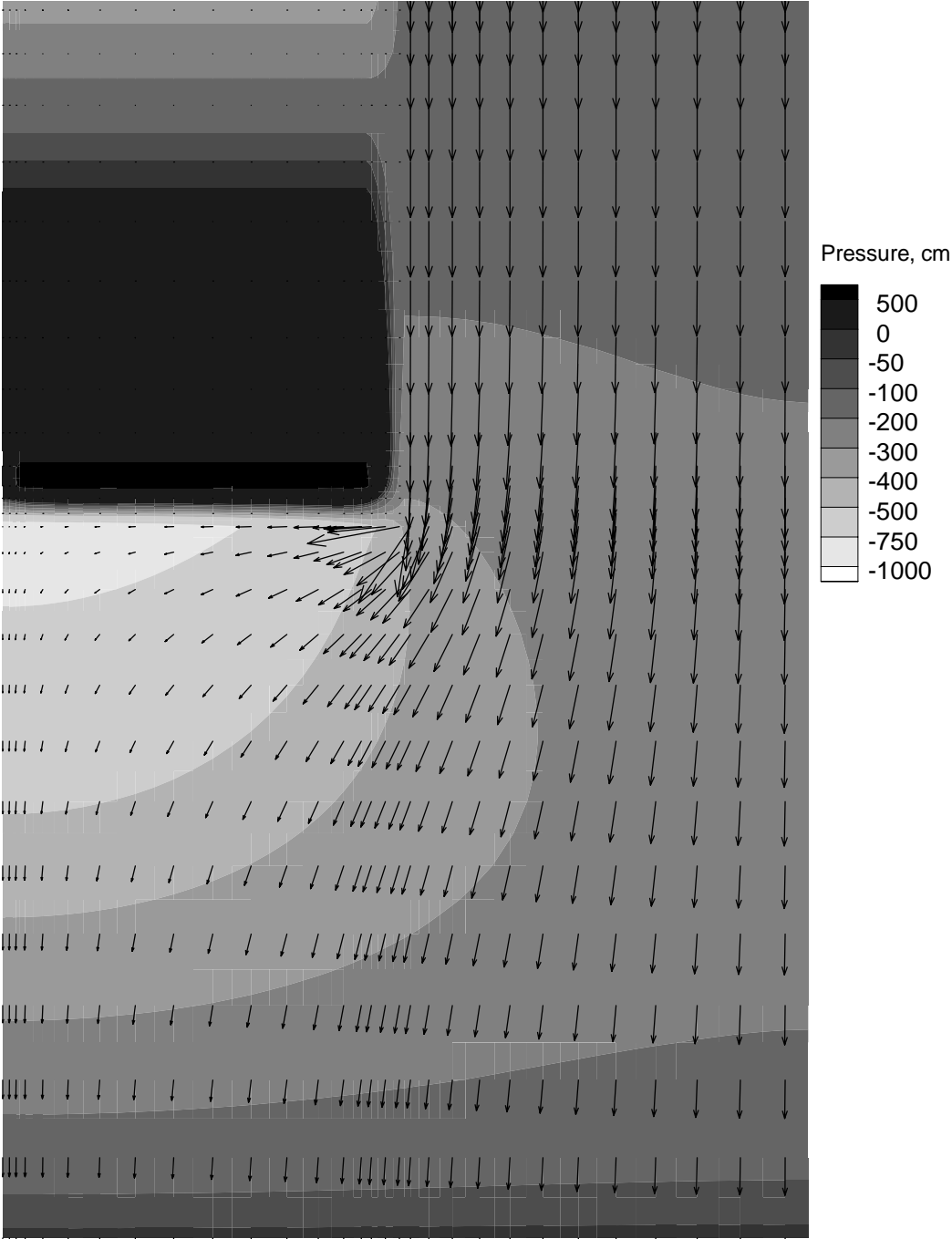
Steady State Water Saturation for the Facility Specific PORFLOW™ Analysis

Dixon – Fig. 3



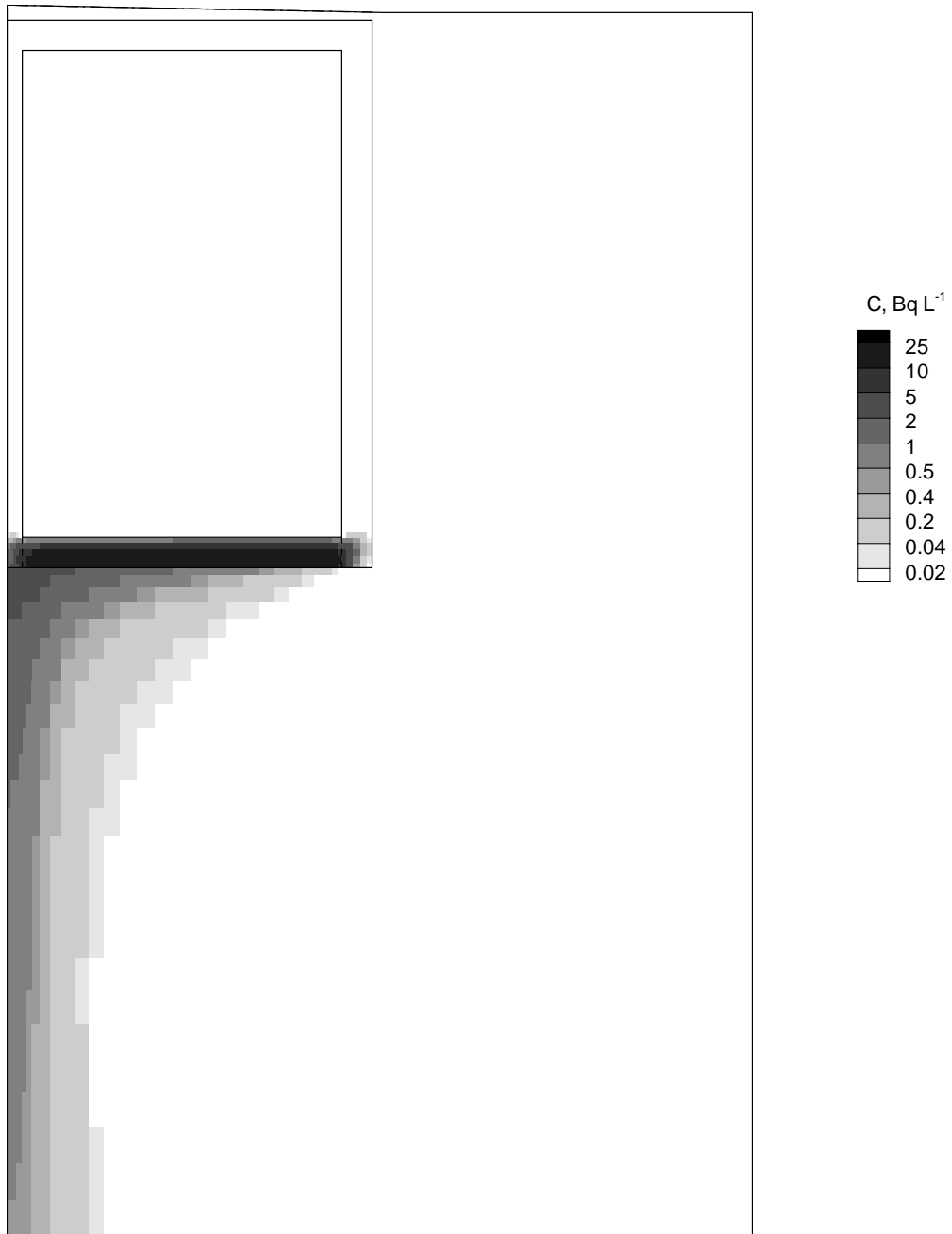
Steady State Flow Field for the Facility Specific PORFLOW™ Analysis

Dixon – Fig. 4



^{129}I Concentration at 2000 Years for the Facility Specific PORFLOWTM Analysis

Dixon – Fig. 5



I-129 Concentration as Function of Time for a Down Gradient Receptor Well for
the Facility Specific PORFLOW™ Analysis

Dixon – Fig. 6

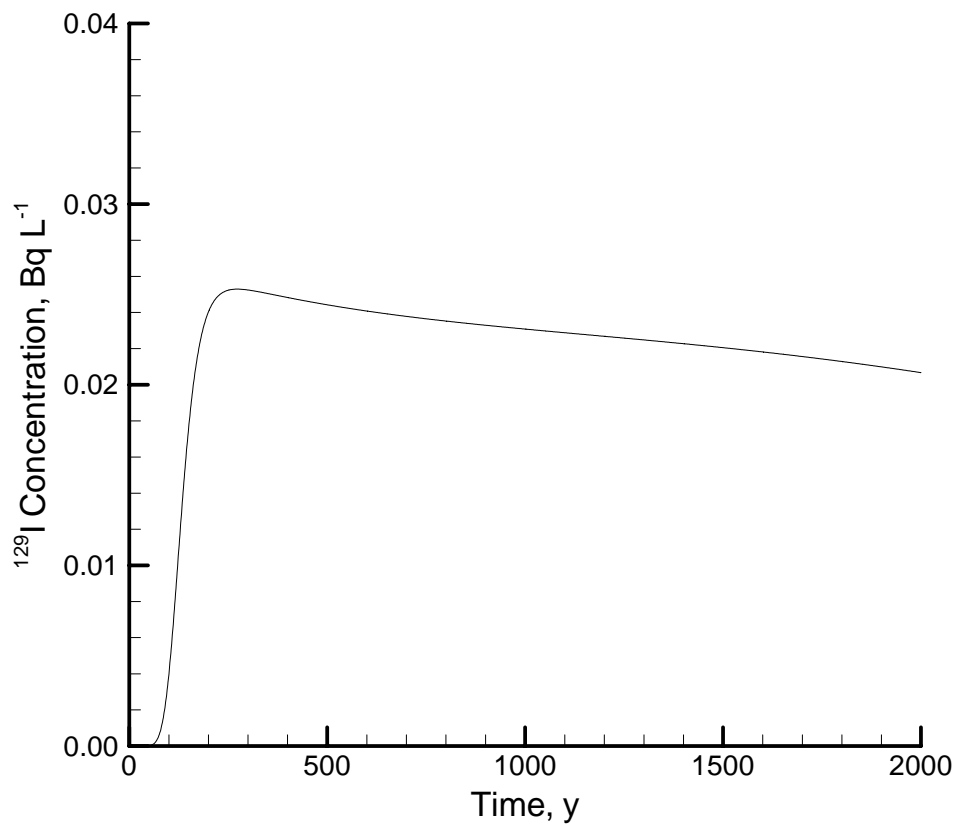


Fig. Captions

- Fig. 1. VZCOMML[®] Conceptual Model
- Fig. 2. PORFLOW Facility Specific Conceptual Model
- Fig. 3. Steady State Water Saturation for the Facility Specific
PORFLOW[™] Analysis
- Fig. 4. Steady State Flow Field for the Facility Specific PORFLOW[™]
Analysis
- Fig. 5. I-129 Concentrations at 2000 Years for the Facility Specific
PORFLOW[™] Analysis
- Fig. 6. I-129 Concentration as a Function of Time for a Down Gradient
Receptor Well for the Facility Specific PORFLOW[™] Analysis