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Revision 0

Radius of Influence Estimates for Injection Wells in Support of Stage B Enhanced Attenuation Remedy for the Hanford Site 300 Area Vadose Zone

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

P.O. Box 1600
Richland, Washington 99352

Approved for Public Release;
Further Dissemination Unlimited

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Terms

3-D	three-dimensional
AMSL	above mean sea level
CHPRC	CH2M HILL Plateau Remediation Company
DOE	U.S. Department of Energy
EA	enhanced attenuation
EAA	enhanced attenuation area
ECF	environmental calculation file
EHM	equivalent homogeneous media
FEP	features, events, and processes
HfSG	Hanford formation sandy gravel
HISI	Hanford Information System Inventory
HSU	hydrostratigraphic unit
IFRC	Integrated Field Research Challenge
MC	Monte Carlo
OU	operable unit
PA	power averaging
PRZ	periodically rewetted zone
ROD	record of decision
ROI	radius of influence
SAP	sampling and analysis plan
STOMP	Subsurface Transport Over Multiple Phases
SZ	saturated zone
TCT	tensorial connectivity-tortuosity
TDS	total dissolved solids
VZ	vadose zone

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1 Purpose

Uranium is identified as a contaminant of concern at the Hanford Site 300 Area. The remediation goal is to sequester uranium in situ by forming and precipitating calcium-polyphosphate minerals in the sediment pores so that the labile uranium is not available for transport through the vadose zone and aquifer. The enhanced attenuation (EA) remedy is being implemented using a phased approach in two sequential stages:

- Stage A covers an area of 3,035 m^2 or 0.30 hectare (0.75 ac).
- Stage B covers the remaining portion of 9,105 m^2 or 0.91 hectare (2.25 ac).

The purpose of this calculation is to provide estimates, along with the supporting basis, of the radius of influence (ROI) created within the vadose zone during the remedial action of injecting polyphosphate bearing solutions into the periodically rewetted zone (PRZ) within the Stage B Enhanced Attenuation Area (EAA).

2 Background

The 300-FF-5 Groundwater Operable Unit (OU) comprises groundwater contaminated by releases from facilities and waste sites associated with past operation of uranium fuel production, research, and development in the 300 Area Industrial Complex. Completion of the cleanup is being accomplished under EPA and DOE, 2013, *Hanford Site 300 Area Record of Decision for 300-FF-2 and 300-FF-5, and Record of Decision Amendment for 300-FF-1*, hereafter referred to as the 300 Area Record of Decision (ROD)/ROD Amendment.

The sampling and analysis plan (SAP) presents the plans for the 300-FF-5 Groundwater OU remedy implementation, performance monitoring, and groundwater monitoring (DOE/RL-2014-42, *300-FF-5 Operable Unit Remedy Implementation Sampling and Analysis Plan*). The SAP is prepared in accordance with the groundwater remedial actions presented in the 300 Area ROD/ROD Amendment (EPA and DOE, 2013). The SAP supplements information provided in DOE/RL-2014-13, *Integrated Remedial Design Report/Remedial Action Work Plan for the 300 Area (300-FF-1, 300-FF-2 & 300-FF-5 Operable Units)*, and DOE/RL-2014-13-ADD2, *Remedial Design Report/Remedial Action Work Plan for the 300 Area Groundwater*.

3 Methodology

A closed-form analytical solution and a three-dimensional (3-D) numerical flow and transport model were used to estimate the ROI for the 300 Area EA Stage B injection wells. Appendix A summaries the analytical solution.

The 3-D flow and transport modeling involves developing a conceptual model by incorporating the important features, events, and processes (FEP) that control the saturated-unsaturated media fluid flow and transport. Sandy gravel is the predominant hydrostratigraphic unit (HSU) at the Stage B EA site. For vadose zone modeling, small core-scale laboratory measurements for hydraulic properties serve as the basis for the predicted behavior at the large macroscopic field scale. For modeling purposes, the heterogeneous sandy gravel unit is conceptualized as an equivalent homogeneous medium (EHM) with macroscopic flow and transport properties. With the heterogeneous unit assigned its upscaled or effective hydraulic properties, the simulated flow fields represent the bulk or mean flow behavior at the field scale. Thus, the upscaling process accounts for the differences in scale between small core-scale measurements and large field-scale modeling.

Field-scale anisotropy (ratio of conductivity parallel to geologic bedding to conductivity perpendicular to bedding) for an EHM can impact the ROI estimates. However, the field-scale anisotropy is not known a priori. Simulation cases with a constant anisotropy of either 1:1 (i.e., isotropic) or 1:10 are, therefore, considered to evaluate its effect on calculated ROI.

In addition to constant anisotropy for saturated hydraulic conductivity, a simulation case considered variable anisotropy for the vadose zone sediments. For this particular simulation, the unsaturated hydraulic conductivity of the EHM is assumed to be anisotropic and moisture (or matric potential or tension) dependent. Tension dependent anisotropy, in essence, provides a framework for upscaling small-scale measurements to the effective (upscaled) properties for the large-scale, macroscopic vadose zone. A tensorial connectivity-tortuosity (TCT) model combined with power averaging (PA) (Zhang et al., 2003, *A Tensorial Connectivity – Tortuosity Concept to Describe the Unsaturated Hydraulic Properties of Anisotropic Soils*) is used to evaluate and apply tension dependent anisotropy for the sandy gravel HSU at the Stage B site. The PA-TCT model has the advantage because its data requirements are less stringent, and it has unrestricted application over the entire range of saturation or tension expected at the Stage B site. Furthermore, an evaluation of the PA-TCT model using a controlled Hanford database has been performed and documented elsewhere (Zhang and Khaleel, 2010, "Simulating field-scale moisture flow using a combined power-averaging and tensorial connectivity-tortuosity approach;" PNNL-23711, *Physical, Hydraulic, and Transport Properties of Sediments and Engineered Materials Associated with Hanford Immobilized Low-Activity Waste*).

The flow and transport simulator (Subsurface Transport Over Multiple Phases [STOMP])©[1] was used to model the 3-D vadose zone flow and transport (PNNL-15782, *STOMP Subsurface Transport Over Multiple Phases Version 4.0 User's Guide*). The porous media continuum assumption, an extended form of the Darcy-Buckingham Law for vadose zone applications, soil relative permeability/saturation/capillary pressure relations, and the advective-dispersive transport equation provide the basis for STOMP calculations (Appendix B).

In generating the STOMP files, information for the following cards are included for each run:

- Simulation title
- Solution control
- Grid
- Inactive nodes
- Rock/soil zonation
- Source
- Boundary condition
- Mechanical properties
- Hydraulic properties
- Saturation function
- Aqueous relative permeability
- Solute/fluid interaction
- Solute/porous media interaction
- Output option

4 Assumptions and Inputs

A pair of sequential STOMP simulations was used to determine the ROI. The purpose of the first simulation run was to achieve, by simulating for an arbitrarily long time, equilibrium (steady state) condition for the moisture regime within the modeling domain. The second simulation run solved for

[1] Battelle Memorial Institute (Battelle) retains copyright on all versions, revisions, and operational modes of the Subsurface Transport Over Multiple Phases (STOMP) software simulator, as permitted by the U.S. Department of Energy. STOMP is used here under a limited government use license.

water flow and polyphosphate transport; the moisture regime (matric potential field) derived from the first simulation was used as the initial condition for the second simulation.

Inputs to STOMP models and supporting assumptions are divided into the following categories:

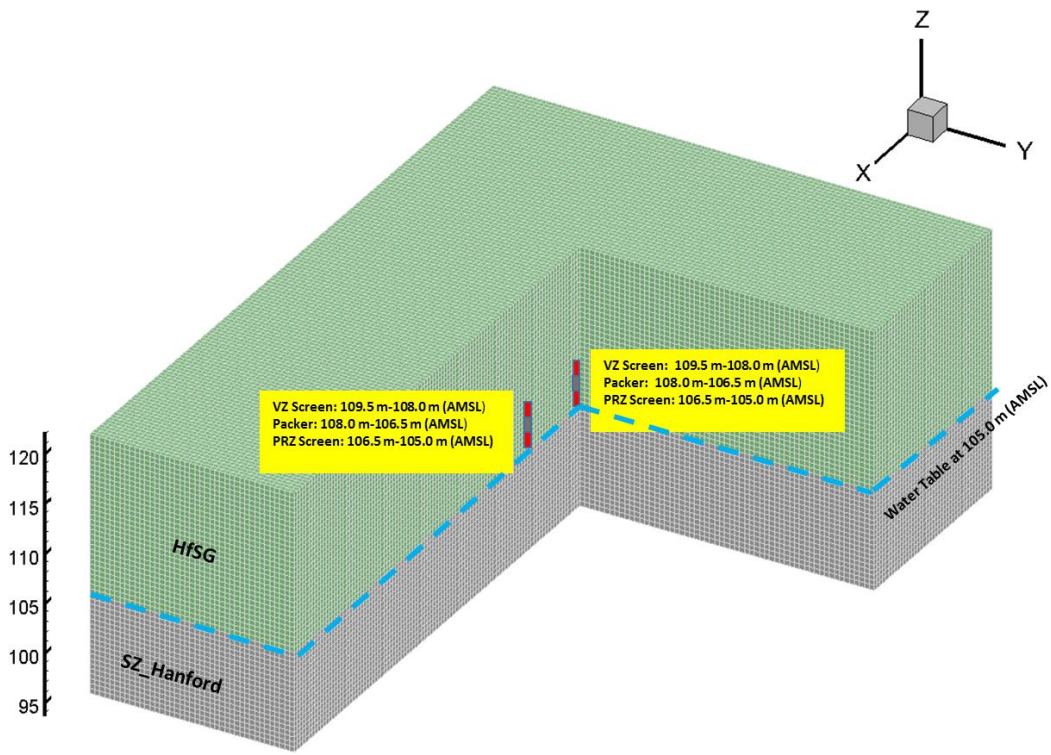
- Hydrostratigraphic framework
- Model domain
- Boundary conditions
- Hydraulic parameters
- Transport parameters

4.1 Hydrostratigraphic Framework

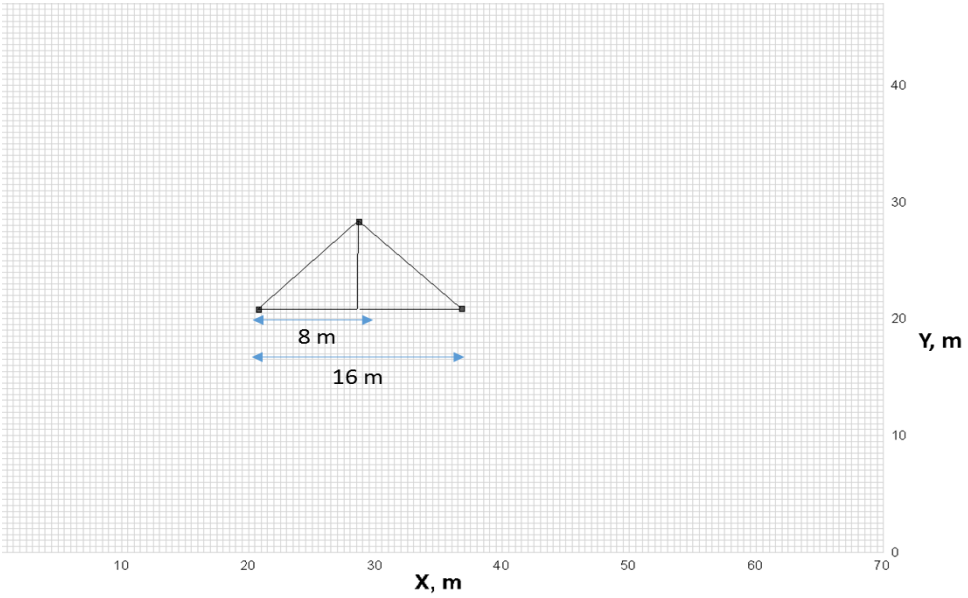
Hanford formation sandy gravel is the predominant HSU at the Stage B EA site (ECF-HANFORD-13-0029, *Development of the Hanford South Geologic Framework Model, Hanford Site, Washington*). For modeling, the heterogeneous sandy gravel unit is conceptualized as an EHM with macroscopic flow and transport properties. For the bulk EHM, a macroscopic anisotropy, assumed either as constant or variable, accounts for the heterogeneities present within the sandy gravel unit.

4.2 Model Domain

For the STOMP 3-D model, a 70-m (X-direction [east-west]) by 50-m (Y-direction [north-south]) model grid was used. In the vertical direction, the model extends from the ground surface through the upper 5 m of the saturated Hanford formation. The water table elevation is at 105 m (NAVD88, *North American Vertical Datum of 1988*). The grid spacing was chosen to be 0.5 m in all three directions. Figure 1(a) shows a cut-away view of the model domain, while Figure 1(b) shows an areal view of the model domain with location of the three injection wells used in the simulation.



(a)



(b)

AMSL	=	above mean sea level	HfSG	=	Hanford formation sandy gravel
SZ	=	saturated zone	VZ	=	vadose zone

Figure 1. Model Domain with Injection Well Locations

4.3 Boundary Conditions

The boundary conditions for the flow and transport model domain are described in this section. Steady state flow conditions are simulated prior to injection.

Figure 2(a) shows the boundary condition used for the steady state flow model for the 3-D integrated unsaturated-saturated media. A Neumann-type (specified flux) boundary condition was applied at the top surface to simulate an estimated recharge of 55 mm/yr (ECF-300FF5-16-0091, *Uranium Transport Modeling in Support of the Stage A Enhanced Attenuation Remedy at 300-FF-5 Operable Unit*) throughout the simulation period. A hydraulic gradient of 3.33E-4 m/m (ECF-300FF5-16-0091) was specified to induce lateral flow for the saturated media. The eastern and western boundaries of the aquifer (top 5 m thickness) were assigned hydraulic gradient type boundary condition.

Figure 2(b) shows the boundary condition used for the polyphosphate flow and transport model. To conserve simulation time, the saturated zone in the transport model was kept inactive since the focus of the simulation was to calculate the ROI within the vadose zone. The bottom boundary of the modeling domain was assigned an atmospheric pressure (101325 Pa) condition. A Dirichlet type outflow boundary condition was used to allow solute mass to flow in and out of the system. To verify use of such an approach for the outflow boundary condition, a separate STOMP flow and transport simulation was performed (Case S9 in Chapter 7). Because it included the saturated zone as part of the STOMP active modeling domain, Case S9 required a much longer computational time, compared to the inactive saturated zone run. The STOMP modeling results, presented later in Chapter 7 with the active and inactive saturated zones, suggest that the simulated polyphosphate plumes for both cases are alike, and a simplified treatment of the water table as an outflow boundary is acceptable.

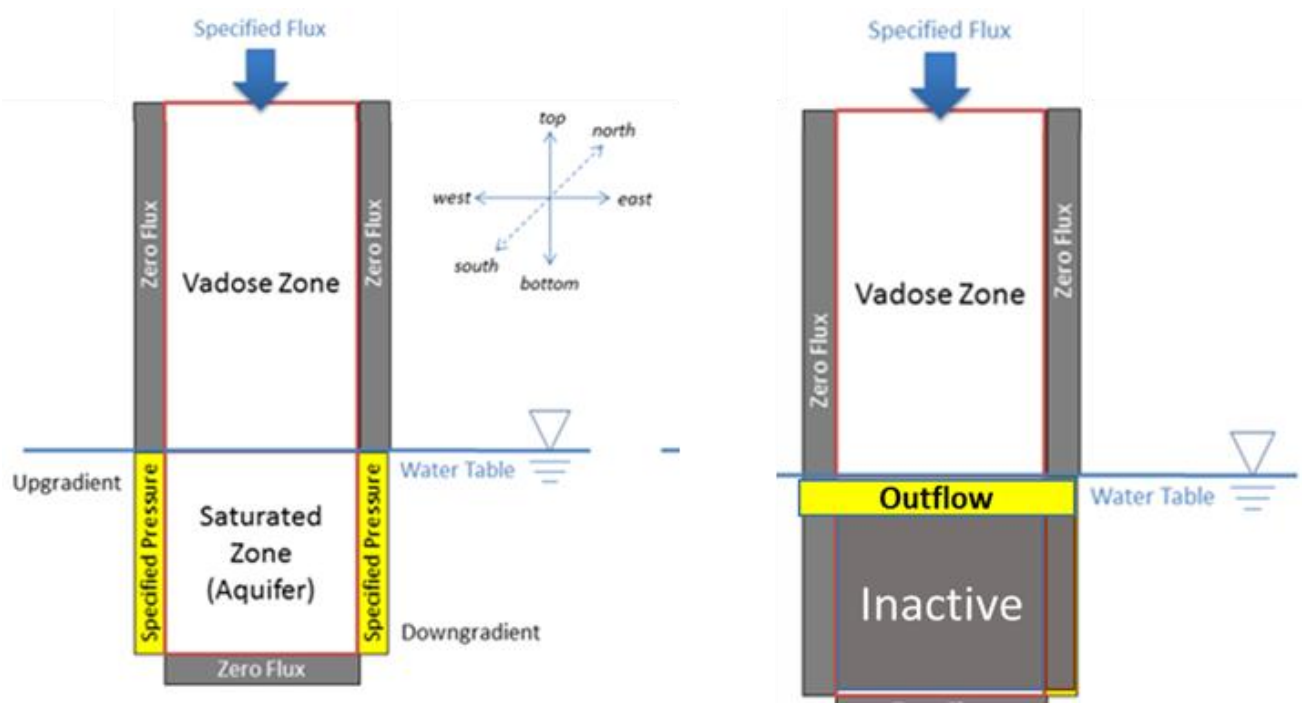


Figure 2. Boundary Conditions for Steady State Flow Model (a) and Boundary Conditions Used in the Polyphosphate Flow and Transport Model (b)

For the steady state simulation, an arbitrary pressure head field (STOMP restart file) was assigned as the initial pressure head field for each simulation case. The final pressure head field (STOMP restart file) from the steady state simulation was used as the initial pressure head field for the polyphosphate flow and transport simulations. The solute concentration was introduced in the model via the STOMP source card along with the injected water.

4.4 Hydraulic Parameters

The purpose of this study was to find a range for the ROI for Stage B polyphosphate injection. Data on hydraulic properties from several sources were used.

The 300 Area Stage B EAA sandy gravel sediments were assumed to follow the van Genuchten, 1980, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," moisture retention constitutive relation and the Mualem-van Genuchten relative permeability constitutive relation (Mualem, 1976, "A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media"), thus requiring the following values to be specified in STOMP:

- K_s, saturated hydraulic conductivity (LT^{-1})
- n_T, total porosity (L^3L^{-3})
- θ_s, saturated volumetric water content, called diffusive porosity n_D in STOMP (L^3L^{-3})
- s_r, residual saturation (dimensionless), equal to the residual water content (volumetric) θ_r divided by the saturated water content (volumetric) θ_s
- α, van Genuchten fitting parameter (L^{-1}), proportional to the inverse of the air entry matric potential
- n, van Genuchten exponential fitting parameter (dimensionless)

The van Genuchten (1980) m parameter was kept fixed and equal to $(n - 1)/n$, and the Mualem (1976) β exponent was fixed at 0.5 (RPP-20621, *Far-Field Hydrology Data Package for the Integrated Disposal Facility Performance Assessment*).

Tables 1 and 2 list the hydraulic parameters used for STOMP simulations. The saturated media Hanford formation properties are based on ECF-300FF5-16-0091.

4.5 Transport Parameters

The following contaminant transport parameters are required by STOMP:

- Particle density
- Macrodispersivity
- Molecular diffusion coefficient
- Distribution coefficient for polyphosphate

Table 3 lists the transport parameters used in STOMP modeling. Since the saturated zone is considered inactive in the transport model, the saturated zone properties are not included in Table 3 for Cases S1 through S7 (Chapter 6).

Table 1. Hydraulic Properties for STOMP Simulation Cases S1 through S6, S8, and S9

Simulation Case (Chapter 6)	HSU	Ks (X) (cm/s)	Ks (Y) (cm/s)	Ks (Z) (cm/s)	K Anisotropy (Kz/Kx or Kz/Ky)	Saturated Volumetric Moisture Content θ_s (cm^3/cm^3)	Residual Volumetric Moisture Content θ_r (cm^3/cm^3)	van Genuchten Inverse Air Entry Head Fitting Parameter α (1/cm)	van Genuchten Fitting Parameter n	Residual Saturation (θ_r/θ_s) S_r
S1	HfSG	2.83E-03[a]	2.83E-03[a]	2.83E-04[a]	1:10	0.152[a]	0[a]	0.0388[a]	1.3776[a]	0[a]
S2	HfSG	2.83E-04[a]	2.83E-04[a]	2.83E-04[a]	1:1	0.152[a]	0[a]	0.0388[a]	1.3776[a]	0[a]
S3	HfSG	3.72E-02[b]	3.72E-02[b]	3.72E-03[b]	1:10	0.285[b]	0[b]	0.2286[b]	1.2691[b]	0[b]
S4	HfSG	3.72E-03[b]	3.72E-03[b]	3.72E-03[b]	1:1	0.285[b]	0[b]	0.2286[b]	1.2691[b]	0[b]
S5	HfSG	3.30E-03[c]	3.30E-03[c]	3.30E-04[c]	1:10	0.167[c]	0.022[c]	0.017[c]	1.725[c]	0.1317[c]
S6	HfSG	3.30E-04[c]	3.30E-04[c]	3.30E-04[c]	1:1	0.167[c]	0.022[c]	0.017[c]	1.725[c]	0.1317[c]
S8	HfSG	3.30E-03[c]	3.30E-03[c]	3.30E-04[c]	1:10	0.167[c]	0.022[c]	0.017[c]	1.725[c]	0.1317[c]
	SZ_Hanford	4.62[d]	4.62[d]	0.462[d]	1:10	0.167[d]	0.025[d]	0.082[d]	2.093[d]	0.152[d]
S9	HfSG	3.30E-03[c]	3.30E-03[c]	3.30E-04[c]	1:10	0.167[c]	0.022[c]	0.017[c]	1.725[c]	0.1317[c]
	SZ_Hanford	4.62[d]	4.62[d]	0.462[d]	1:10	0.167[d]	0.025[d]	0.082[d]	2.093[d]	0.152[d]

a. From PNNL-22886, *System-Scale Model of Aquifer, Vadose Zone, and River Interactions for the Hanford 300 Area – Application to Uranium Reactive Transport* (Table A.2, Sample C6186, 18.4-19.4).

b. From PNNL-22886 (Table A.2, Sample C6203, 20-21).

c. PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments* (Table 4.5).

d. From ECF-300FF5-16-0091, *Uranium Transport Modeling in Support of the Stage A Enhanced Attenuation Remedy at 300-FF-5 Operable Unit* (Table 7.1).

HfSG = Hanford formation sandy gravel

HSU = hydrostratigraphic unit

SZ = saturated zone

Table 2. Hydraulic Properties for STOMP Simulation Case S7 (Chapter 6)

Vadose Zone Parameter	HfSG
K_{sat} (cm/s) vertical	7.714×10^{-3}
K_{sat} (cm/s) horizontal	4.671×10^{-2}
Saturated moisture content, Θ_s	0.174
Residual moisture content, Θ_r	0.0038
van Genuchten α (1/cm)	0.08859
van Genuchten n	1.271
Residual saturation, s_r	0.02184
X, Y pore scale parameter, L	0.637
Z pore scale parameter, L	-0.225

Reference: van Genuchten, 1980, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils."

Note: Values in second column are from PNNL-23711, *Physical, Hydraulic, and Transport Properties of Sediments and Engineered Materials Associated with Hanford Immobilized Low-Activity Waste*.

HfSG = Hanford formation sandy gravel

Table 3. Transport Parameters Used for STOMP Simulation Cases S1 through S9

Simulation Case (Chapter 6)	HSU	Particle Density ρ_s (g/cm^3)	Longitudinal Dispersivity (m)	Transverse Dispersivity (m)	Specific Storage (1/m)	Molecular Diffusion Coefficient (m^2/s)	Partitioning Coefficient K_d (mL/g)
S1	HfSG	2.71[a]	0.05	0.005	1.E-04	2.50E-11	0
S2	HfSG	2.71[a]	0.05	0.005	1.E-04	2.50E-11	0
S3	HfSG	2.71[b]	0.05	0.005	1.E-04	2.50E-11	0
S4	HfSG	2.71[b]	0.05	0.005	1.E-04	2.50E-11	0
S5	HfSG	2.32[c]	0.05	0.005	1.E-04	2.50E-11	0
S6	HfSG	2.32[c]	0.05	0.005	1.E-04	2.50E-11	0
S7	HfSG	2.53[d]	0.05	0.005	1.E-04	2.50E-11	0
S8	HfSG	2.32[c]	0.05	0.005	1.E-04	2.50E-11	0
	SZ_Hanford	2.63[e]	0.5	0.05	1.E-04	2.50E-11	0.2

Table 3. Transport Parameters Used for STOMP Simulation Cases S1 through S9

Simulation Case (Chapter 6)	HSU	Particle Density ρ_s (g/cm^3)	Longitudinal Dispersivity (m)	Transverse Dispersivity (m)	Specific Storage (1/m)	Molecular Diffusion Coefficient (m^2/s)	Partitioning Coefficient K_d (mL/g)
S9	HfSG	2.32[c]	0.05	0.005	1.E-04	2.50E-11	0
	SZ_Hanford	2.63[e]	0.5	0.05	1.E-04	2.50E-11	0.2

a. PNNL-22886, *System-Scale Model of Aquifer, Vadose Zone, and River Interactions for the Hanford 300 Area – Application to Uranium Reactive Transport* (Table A.2, C6186, 18.4-19.4).

b. PNNL-22886 (Table A.2, C6203, 20-21).

c. PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments* (Table 4.5).

d. PNNL-23711, *Physical, Hydraulic, and Transport Properties of Sediments and Engineered Materials Associated with Hanford Immobilized Low-Activity Waste*.

e. PNNL-14702 (Table 4.6).

HfSG = Hanford formation sandy gravel

SZ = saturated zone

5 Software Applications

STOMP (PNNL-12030, 2000, *STOMP Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide*; PNNL-15782; PNNL-11216, *STOMP Subsurface Transport Over Multiple Phases Application Guide*) was the primary software used for this calculation, and the required information is provided in this chapter. A commercial graphics software package (Tecplot®[2]) was used for graphical display of results.

5.1 Description

The vadose zone fate and transport calculations are performed using CH2M HILL Plateau Remediation Company (CHPRC) Build 4 of the STOMP software, registered in the Hanford Information System Inventory (HISI) under identification number 2471. STOMP use by CHPRC is managed under the following software lifecycle documents: CHPRC-00222, *STOMP Functional Requirements Document*; CHPRC-00176, *STOMP Software Management Plan*; CHPRC-00211, *STOMP Software Test Plan*; CHPRC-00515, *STOMP Acceptance Test Report*; and CHPRC-00269, *STOMP Requirements Traceability Matrix*.

- Software Title: STOMP
- Software Version: CHPRC Build 4 (executable `stomp-w-cgst-chprc04i.x`, MD5 hash (`6c25051016db2fe1f883a7caaaab1e97`)
- HISI Identification Number: 2471

[2] Tecplot is a registered trademark of Tecplot, Inc., Bellevue, Washington.

- Workstation type and property number (from which software is run): STOMP was executed on the GREEN Linux cluster (owned and operated by INTERA, Incorporated at its Richland, Washington office). As given by the command "uname -a", the operating system details for these compute nodes are: Linux green 3.2.0-65-generic #98-Ubuntu SMP Wed Jun 11 20:27:07 UTC 2014 x86_64 GNU/Linux

5.2 Software Installation and Checkout

A copy of the Software Installation and Checkout Form for the STOMP installation used for this calculation is provided in Appendix C.

5.3 Statement of Valid Software Application

DOE/RL-2011-50, *Regulatory Basis and Implementation of a Graded Approach to Evaluation of Groundwater Protection*, contains a summary of the main model attributes and code selection criteria that serve as the basis for the demonstration of the adequacy of the STOMP code for use in vadose zone modeling at the Hanford Site. Results of the evaluation in DOE/RL-2011-50 show that the STOMP code is capable of meeting or exceeding the identified attributes and criteria. Comparison of the code selection criteria to the STOMP code capabilities indicates that the STOMP code is capable of simulating all of the necessary FEPs, and STOMP meets all of the other required code selection criteria. Section 6.4.1 of DOE/RL-2011-50 addresses code selection criteria, including quality assurance documentation of verification studies for specific model attributes (e.g., unsaturated flow, solute transport, infiltration, and drainage) and a discussion of other code related criteria (i.e., intercode comparisons, hardware requirements, solution methodology, dimensionality, and output capability).

The results of CHPRC acceptance testing (CHPRC-00515) demonstrate that the STOMP software is acceptable for its intended use by the CHPRC. Installations of the software are operating correctly, as demonstrated by the GREEN Linux Cluster system producing the same results as those presented for selected problems from the STOMP application guide (PNNL-11216) in accordance with the software test plan (CHPRC-00211).

6 Calculation

The calculation details are presented in this chapter, which includes an analytical solution and numerical modeling with variable hydraulic properties.

6.1 Analytical Solution

As described in Appendix A, the sharp wetting front approximation (also referred to as the Green and Ampt model) and mass balance considerations serve as the basis for the simplified analytical solution (Warrick, 2003, *Soil Water Dynamics*). Appendix A provides a detailed derivation of Equation A-10, which is used to compute the steady state value for the ROI, r_f (Equation A-10) during injection.

The Stage B EA site injection wells are planned to be 15.24 cm (6 in.) in diameter. An effective well radius is defined as the horizontal distance from the axis of a well to the outside of the gravel pack. For an assumed effective well radius (r_o) = 0.25 m for injection wells, an injection volume (Q) = 90.84 m^3 (50 gal/min for 8 hours), an initial moisture content (θ_{dry}) = 0.05 (volumetric) ahead of the wetting front, and a saturated moisture content (θ_{wet}) = 0.152 (volumetric) behind the wetting front (Figure A-1), the estimated ROI, r_f = 5.97 m (Equation A-10). Changing the saturated moisture content value behind the wetting front from 0.152 to 0.302, and keeping all other values the same results in a r_f = 4.41 m. The values being used for θ_{dry} and θ_{wet} are representative of dry and wet moisture content data for

300 Area soils (PNNL-22886, *System-Scale Model of Aquifer, Vadose Zone, and River Interactions for the Hanford 300 Area – Application to Uranium Reactive Transport*, Table A.2).

6.2 Numerical Solution (STOMP Models)

As stated earlier, for STOMP vadose zone modeling, small core-scale laboratory measurements for hydraulic properties serve as the basis for the predicted behavior at the large macroscopic field scale. Sandy gravel is the predominant HSU at the Stage B EA site. For modeling purposes, the heterogeneous sandy gravel unit is conceptualized as an EHM with macroscopic flow and transport properties.

Nine different STOMP simulation cases were run to obtain a range of ROI estimates. The STOMP simulation cases are described in the following subsections.

6.2.1 Case S1 (Low θ_s, Constant Anisotropy)

Moisture characteristic data for 10 intact core samples from the 300 Area Integrated Field Research Challenge (IFRC) site (adjacent to Stage B EA site) are cataloged in PNNL-22886 (Table A.2). The van Genuchten-Mualem parameters representing these samples are assumed to be representative of hydraulic properties of Stage B EA site sandy gravel sediments (Table 1).

For Case S1, hydraulic properties having the minimum moisture holding capacity (i.e., lower saturated moisture content), among the 10 IFRC samples, were chosen (i.e., sample C6186 [18.4 to 19.4 ft]) (Table 1). The sandy gravel HSU at the Stage B EA site was treated as an EHM; a vertical to horizontal saturated hydraulic conductivity anisotropy of 1:10 was used for the STOMP modeling.

6.2.2 Case S2 (Low θ_s, Isotropic)

Case S2 uses the same properties as S1, except the saturated hydraulic conductivity is assumed to be isotropic. Similar to S1, the sandy gravel HSU at the Stage B EA site was treated as EHM but considered isotropic for the STOMP modeling.

6.2.3 Case S3 (High θ_s, Constant Anisotropy)

For Case S3, the 300 Area IFRC hydraulic properties data set having the maximum moisture holding capacity (i.e., higher saturated moisture content θ_s) was chosen (sample C6203, 20-21 ft) (Table 1). The sandy gravel HSU at the Stage B EA site was treated as EHM; a vertical to horizontal saturated hydraulic conductivity anisotropy of 1:10 was used for the STOMP modeling.

6.2.4 Case S4 (High θ_s, Isotropic)

Case S4 uses the same properties as S3, except the saturated hydraulic conductivity is assumed to be isotropic. Similar to S3, the sandy gravel HSU at the Stage B EA site was treated as EHM but considered isotropic for the STOMP modeling.

6.2.5 Case S5 (High θ_r, Constant Anisotropy)

Case S5 uses the sandy gravel hydraulic properties for a different data set described elsewhere (PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments*) (Table 1). The sandy gravel HSU at the Stage B EA site was treated as EHM; a vertical to horizontal saturated hydraulic conductivity anisotropy of 1:10 was used for the STOMP modeling.

6.2.6 Case S6 (High θ_r, Isotropic)

Case S6 uses the same properties as S5, except the saturated hydraulic conductivity is assumed to be isotropic. Similar to S5, the sandy gravel HSU at the Stage B EA site was treated as EHM but considered isotropic for the STOMP modeling.

6.2.7 Case S7 (Variable Moisture-Dependent Anisotropy)

Unlike other cases which considered a constant anisotropy, the unsaturated hydraulic conductivity of the EHM based sandy gravel HSU at the Stage B EA site is assumed to be variably anisotropic (i.e., anisotropy depends on the spatial variability of matric potential or tension or moisture content) for Case S7 (Table 2).

As stated earlier, tension dependent anisotropy provides a framework for upscaling small-scale measurements to the effective (upscaled) properties for the large-scale, macroscopic vadose zone. A TCT model combined with PA (Zhang et al., 2003) is used to evaluate and apply tension dependent anisotropy for the sandy gravel HSU at the Stage B site.

6.2.8 Case S8 (High Saturated Hydraulic Conductivity K_s for the PRZ, Constant Anisotropy)

Case S8 uses a saturated hydraulic conductivity of 4,000 m/d for the PRZ (105 to 107.5 m elevation) with a vertical to horizontal anisotropy of 1:10 (Table 1). Case S8 is unlike Cases S1 through S7, whose saturated conductivity values are based on small-scale laboratory measurements that are orders of magnitude lower.

6.2.9 Case S9 (Active Saturated Zone for the Modeling Domain)

For Cases S1 through S8, a Dirichlet type outflow boundary condition was used to allow solute mass flow in and out of the system. Case S9 was run to verify use of such an approach for the outflow boundary condition; it included the saturated zone as part of the STOMP active modeling domain.

For each preceding STOMP simulation cases, the following steps were used:

1. First, STOMP was executed for an arbitrary period of time to achieve an equilibrium steady state flow condition. The simulated matric potential and volumetric water content values were examined to ensure that the flow regime reached equilibrium. Steady state simulation results provided an initial pressure head field for the subsequent simulation, which solved for flow and polyphosphate transport.

2. For the PRZ injection, all three wells were screened between 106.5 to 105.0 m (349 to 345 ft) elevation, with packers located between 108.0 to 106.5 m (354 to 349 ft) elevation. For the lower vadose zone injection, all three wells were screened between 109.5 to 108.0 m (359 to 354 ft) elevation (DOE/RL-2014-42-ADD1, *300-FF-5 Operable Unit Remedy Implementation Sampling and Analysis Plan Addendum 1 for Stage B Uranium Sequestration*).

3. Each well was set up to inject 50 gal/min for 8 hours within the PRZ followed by 8 hours of lower vadose zone injection at the same well and at the same rate.

4. For modeling purposes, an initial concentration of 8,280 mg/L of polyphosphate was injected (STOMP source card) as solute along with water injections for both PRZ and lower vadose zone wells.

5. For each simulation, STOMP plot files were created at the end of each hour during the injection period.

6. All plot files were converted to Tecplot data file format by running “PlotTo.pl”.

7. Data files were imported using Tecplot and the output concentrations were normalized based on the initial concentration (8,280 mg/L).

8. ROI was calculated as the distance from the injection point to the horizontal location where the maximum concentration is about 20% of the injected concentration.

7 Results/Conclusions

This chapter provides the results of the analyses described in Chapter 6.

7.1 Analytical Solution

As described in Section 6.1, the calculated ROI (r_f), via Equation A-10, varies between 4.41 and 5.97 m, depending on the saturated moisture content and initial moisture content estimates. Because it is based on a sharp wetting front approximation, Equation A-10 assumes a complete absorption or imbibition of the available pore volume. In reality, the imbibition process is uneven and incomplete, so the preceding r_f values are underestimated. The computed r_f values are for a steady state moisture plume and are expected to be different from the STOMP based contaminant plume calculations described in this chapter. Unlike the analytical solution, STOMP can account for transient flow as well as mass transport (i.e., advection, diffusion, and dispersion) processes. Unlike the analytical solution, STOMP can also model macroscopic, field-scale variable state-dependent (i.e., moisture-dependent) anisotropy. Consideration of these processes will lead to considerably larger r_f estimates, compared to the approximate analytical solution.

7.2 Numerical Solution (STOMP Models)

This section presents results for the STOMP simulation cases described in Chapter 6. Figure 3 shows the cross-section location (red line) where the STOMP modeling results for the polyphosphate plume are presented. Intermediate results (moisture content and matric potential distributions) are available for all STOMP simulations; such results are presented only for STOMP simulation Cases S1 and S3.

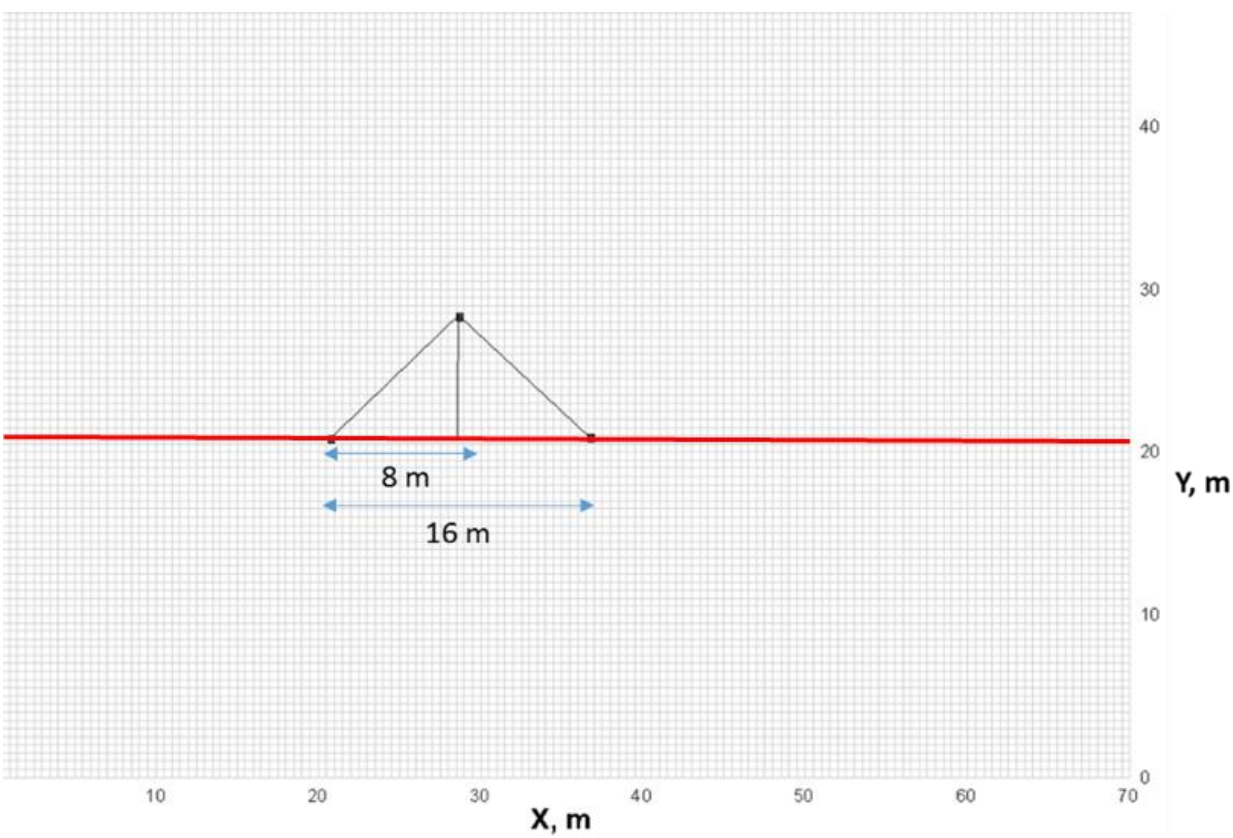


Figure 3. Location of Cross-Section of All STOMP Simulation Cases for the Observed Concentration

7.2.1 Case S1 (Low θ_s, Constant Anisotropy)

Figure 4(a) shows the moisture content distribution after 8 hours of PRZ injection. Figure 4(b) shows the moisture content distribution after 16 hours (8 hours of injection within the PRZ and the subsequent 8 hours of injection within the lower vadose zone). Figure 4(c) and Figure 4(d) illustrate, respectively, the corresponding matric potential distribution at 8 hours and 16 hours. As expected, the simulated moisture content and matric potential values for the injection domain (Figure 4) reflect the saturated moisture regime for Case S1 (Table 1).

Figure 5 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 7 m. The ROI increased to 8.5 m after 16 hours. Figure 6(a) and Figure 6(b) show, respectively, the normalized polyphosphate concentration plumes at 8 hours and 16 hours.

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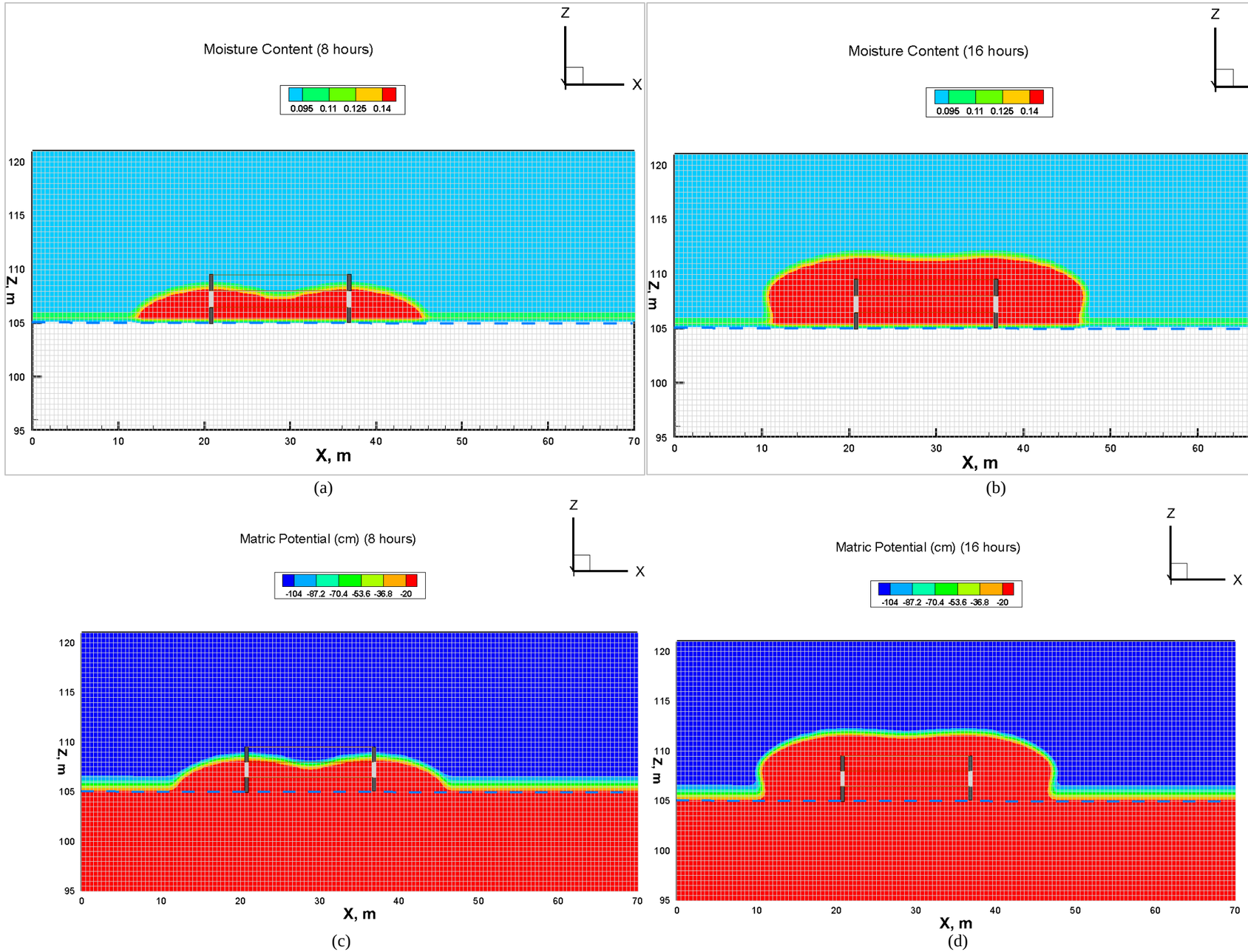

Figure 4. Vertical Distribution of Moisture Content (Volumetric) and Matric Potential for Case S1

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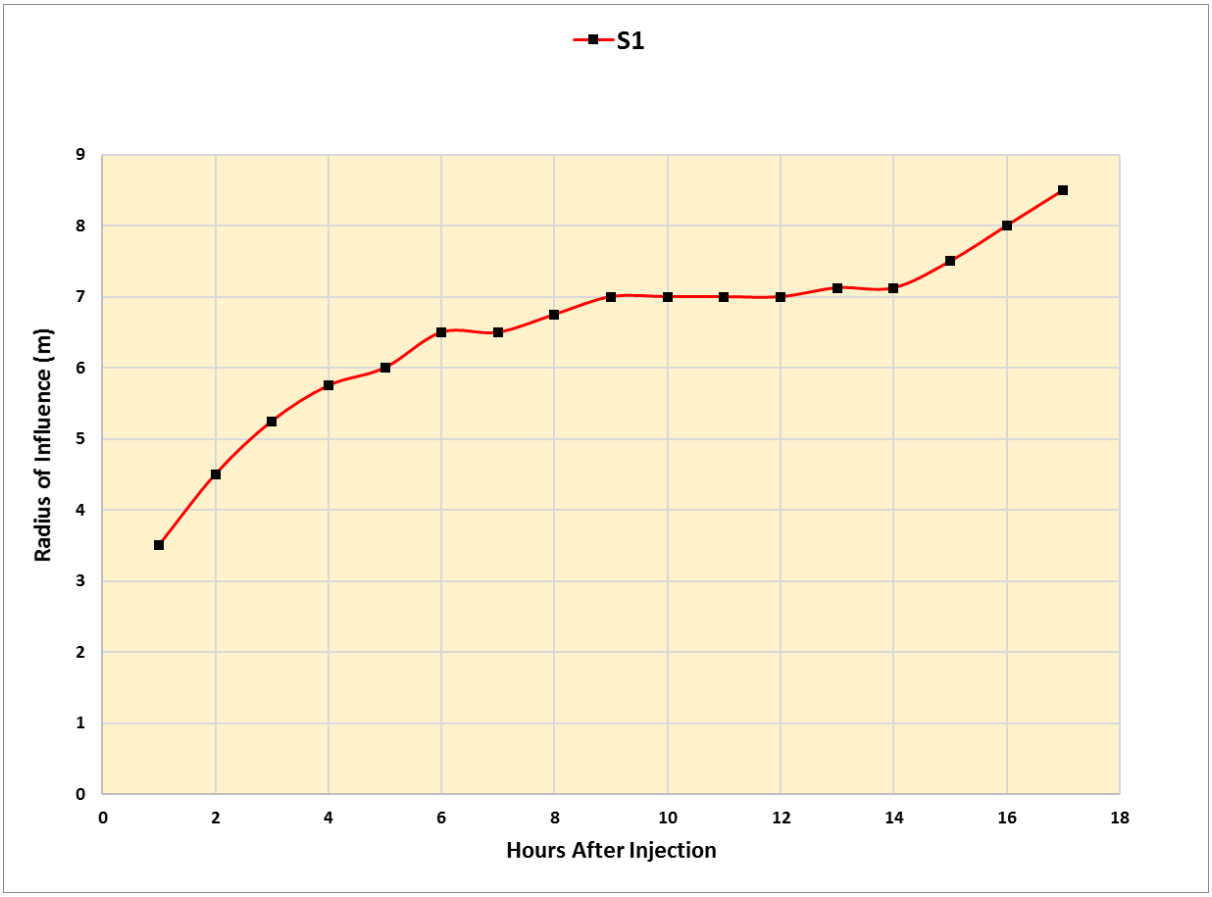
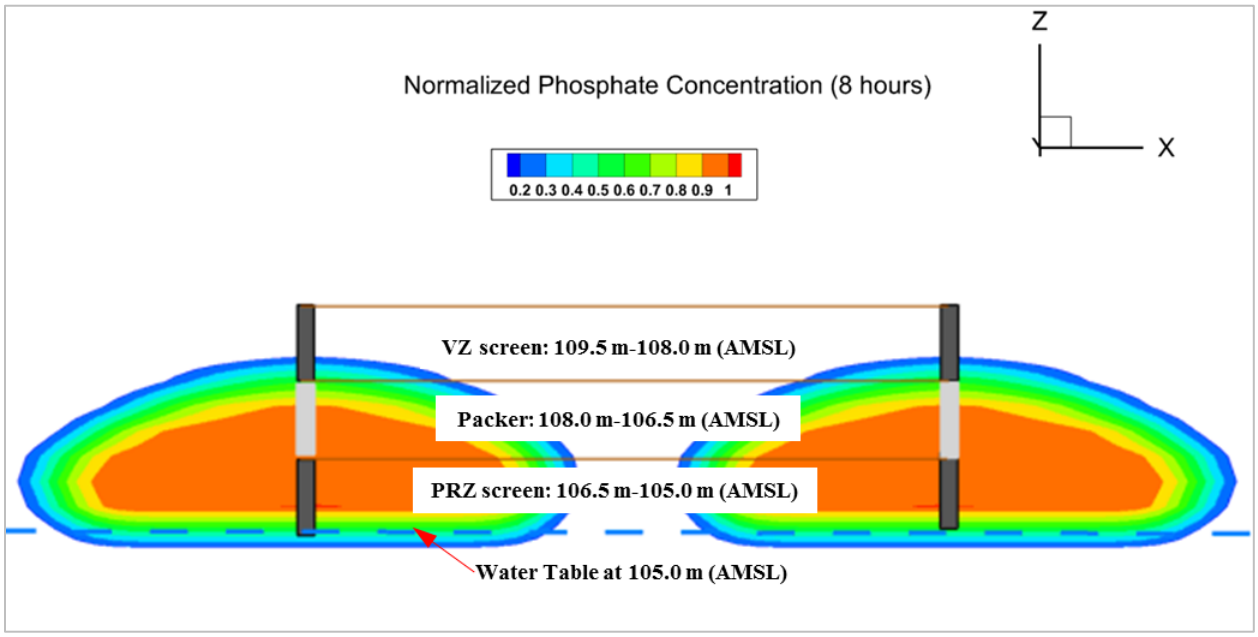
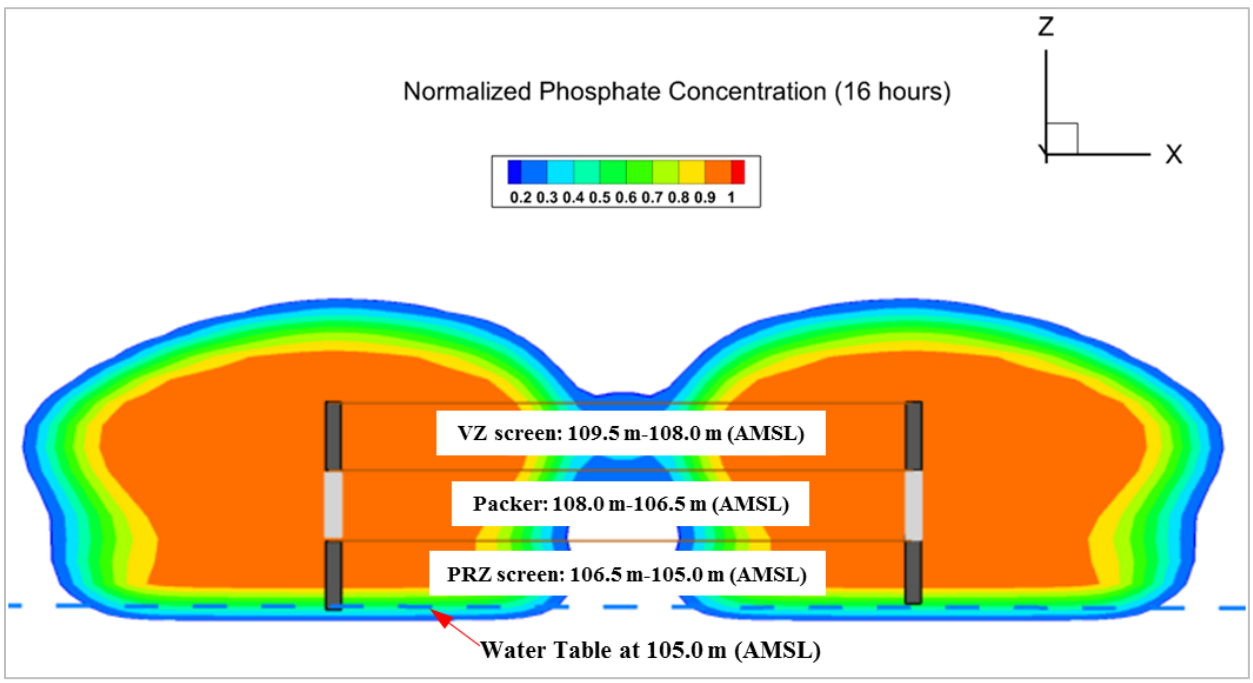


Figure 5. Change of ROI with Injection Period for Case S1



(a)



(b)

Figure 6. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S1

7.2.2 Case S2 (Low θ_s, Isotropic)

Figure 7 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 4.25 m. The ROI increased to 6 m after 16 hours (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). As expected, the calculated ROI for the isotropic condition is lower than that for the anisotropic Case S1. Figure 8(a) and Figure 8(b) illustrate, respectively, the normalized polyphosphate concentration plumes at 8 hours and 16 hours.

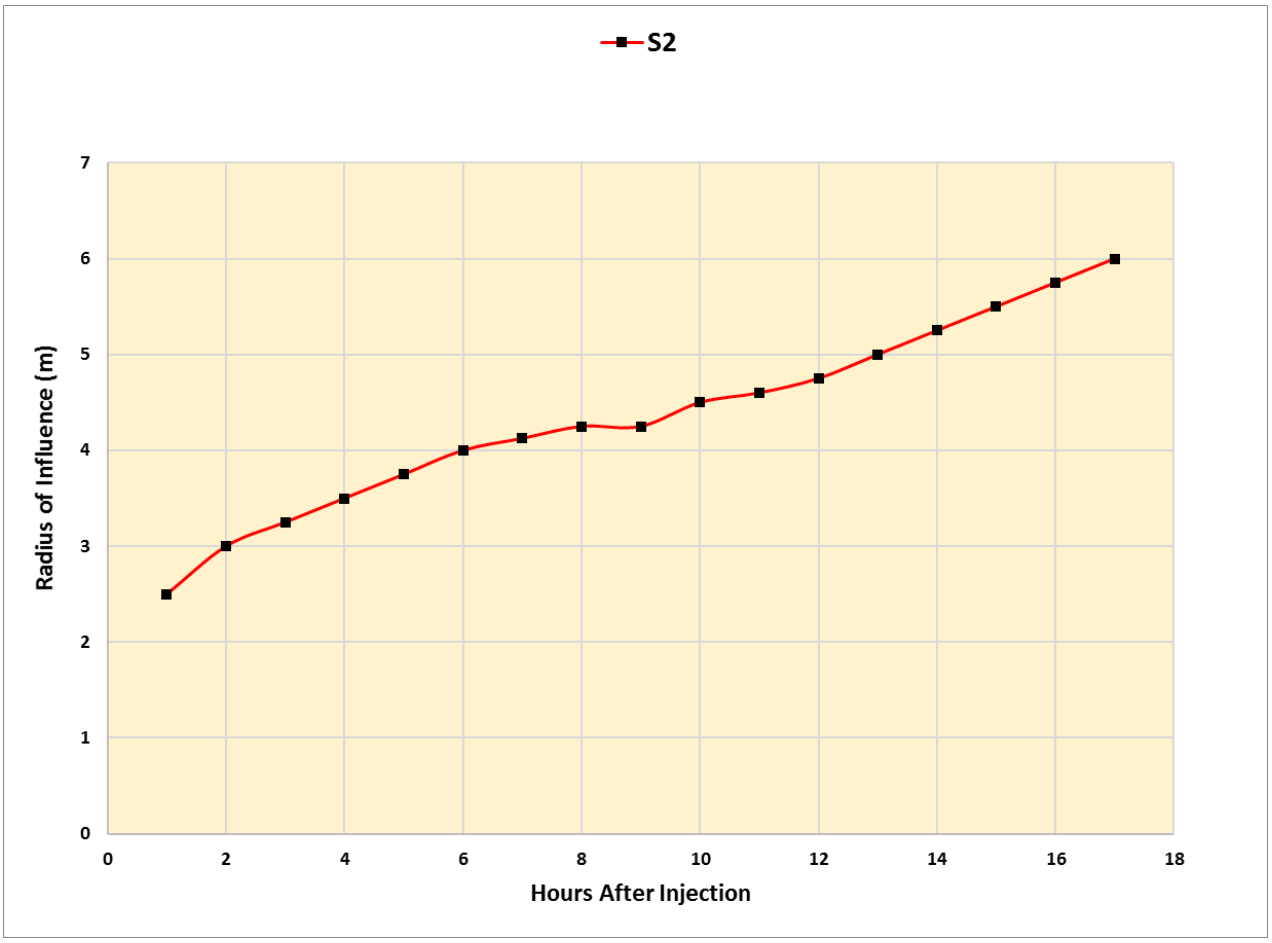
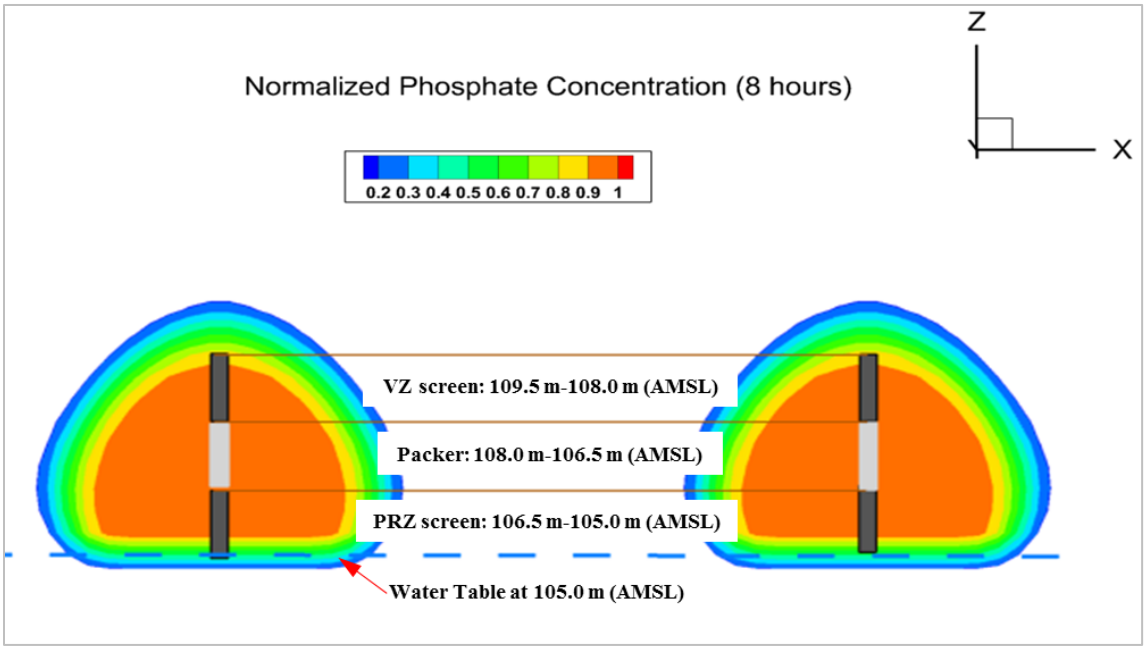
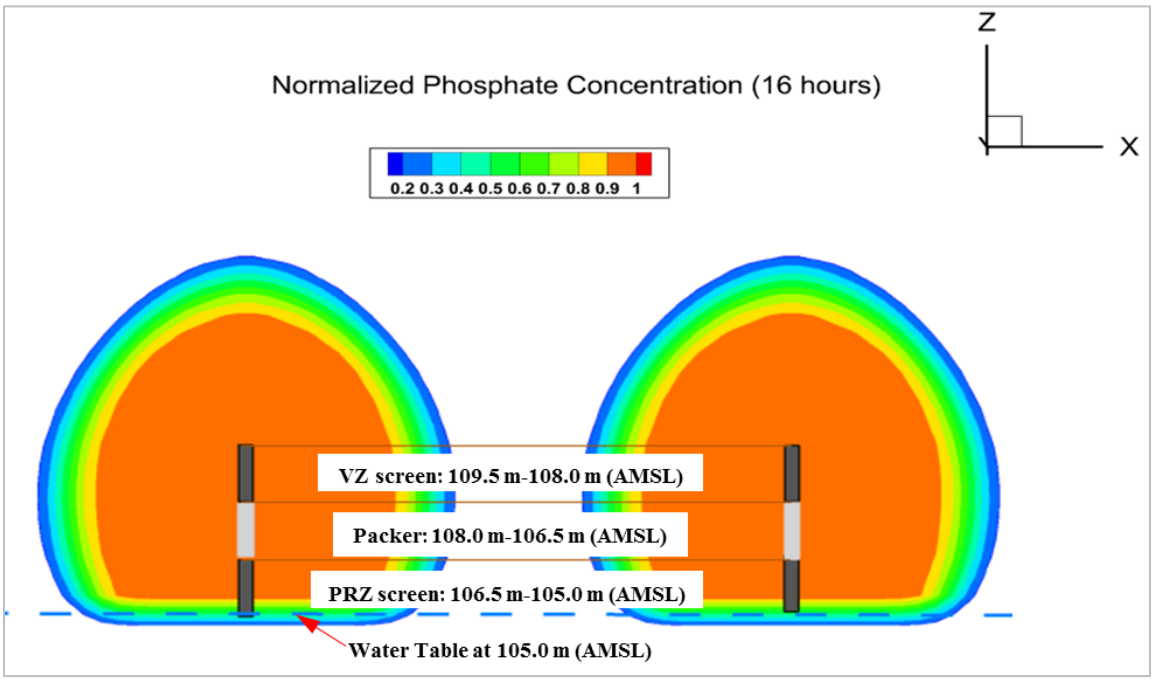


Figure 7. Change of ROI with Injection Period for Case S2



(a)



(b)

Figure 8. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S2

7.2.3 Case S3 (High θ_s, Constant Anisotropy)

Figure 9(a) shows the moisture content distribution after 8 hours of PRZ injection. Figure 9(b) shows the moisture content distribution after 16 hours (8 hours of injection within the PRZ and the subsequent 8 hours of injection within the lower vadose zone). Figure 9(c) and Figure 9(d) illustrate, respectively, the corresponding matric potential distribution at 8 and 16 hours. As expected, the simulated moisture content and matric potential values for the injection domain reflect the saturated moisture regime data for Case S3 (Table 1).

Figure 10 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 4.5 m. The ROI increased to 4.75 m after 16 hours. Figure 11(a) and Figure 11(b) illustrate, respectively, the normalized polyphosphate concentration plumes at 8 hours and 16 hours.

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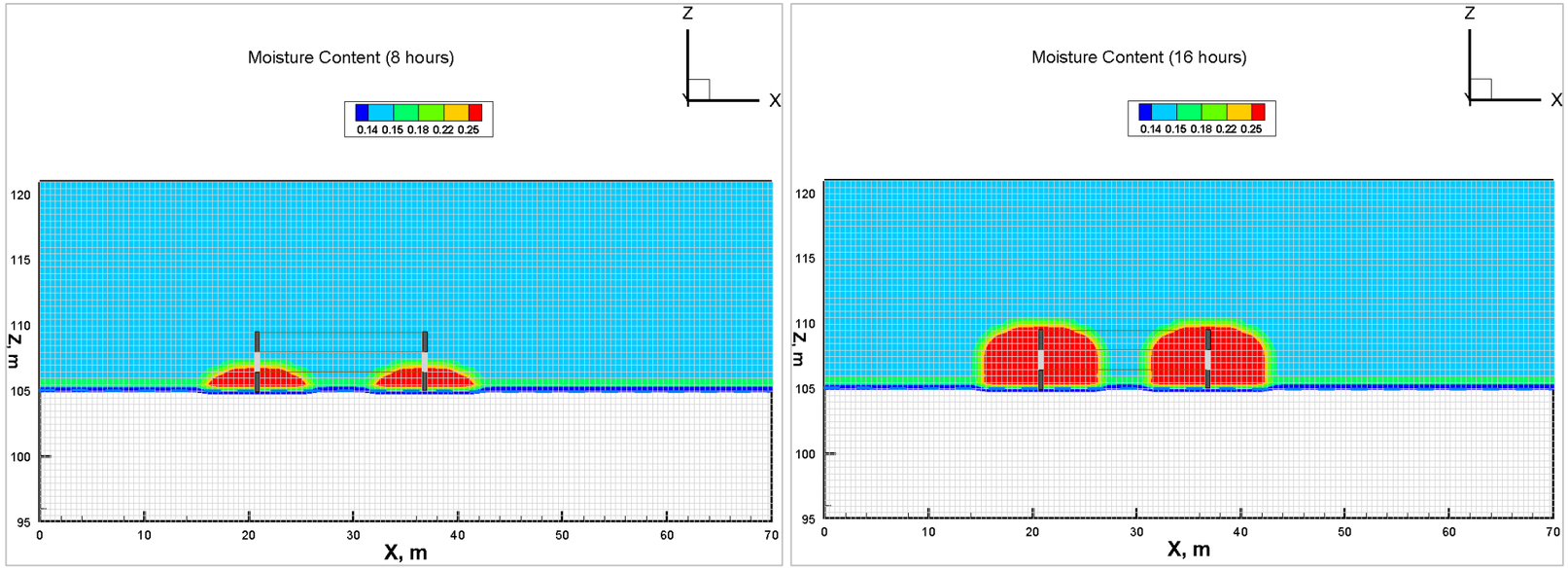
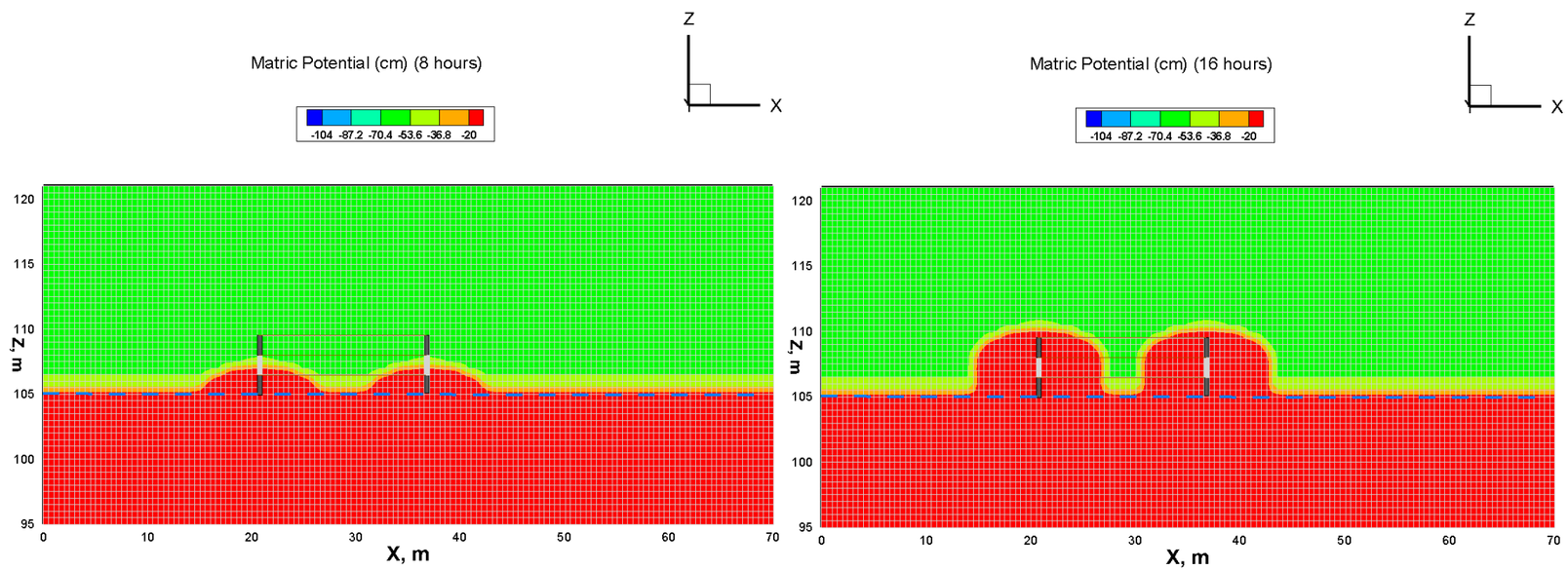


(a)

(b)



(b) (d)

Figure 9. Vertical Distribution of Moisture Content (Volumetric) and Matric Potential for Case S3

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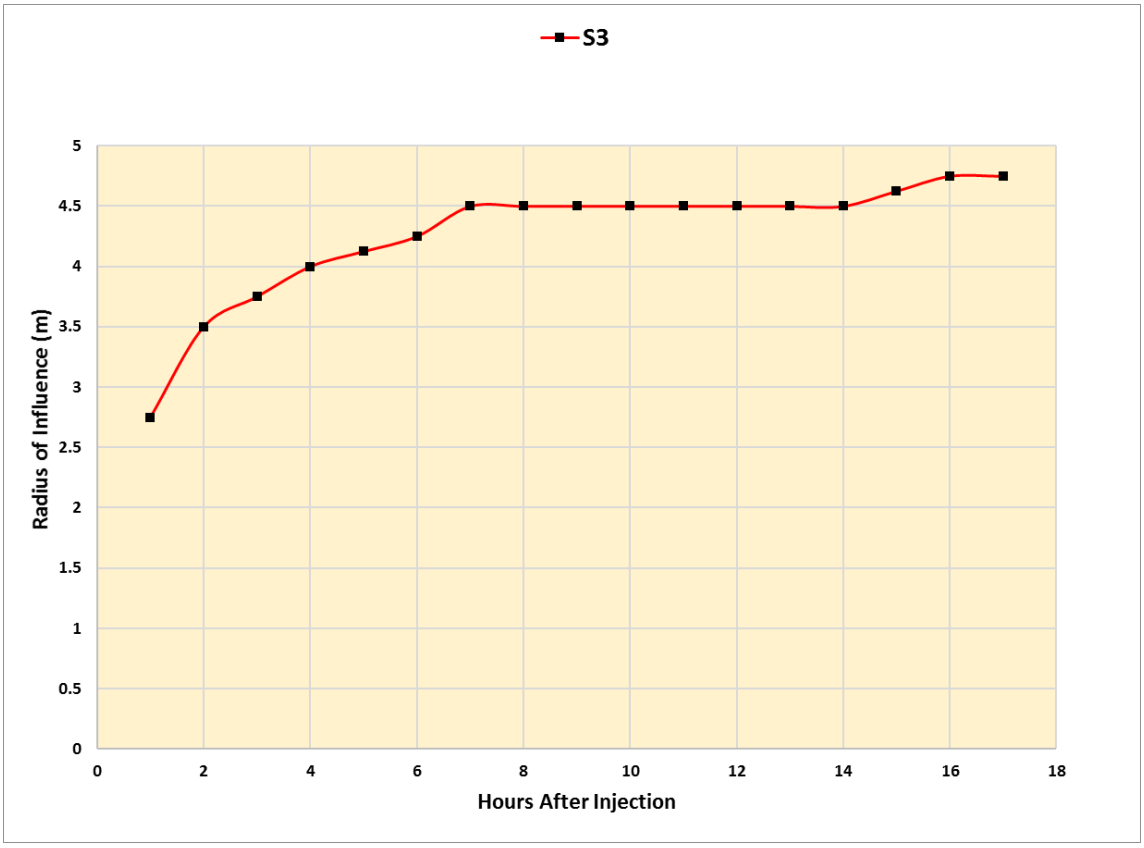
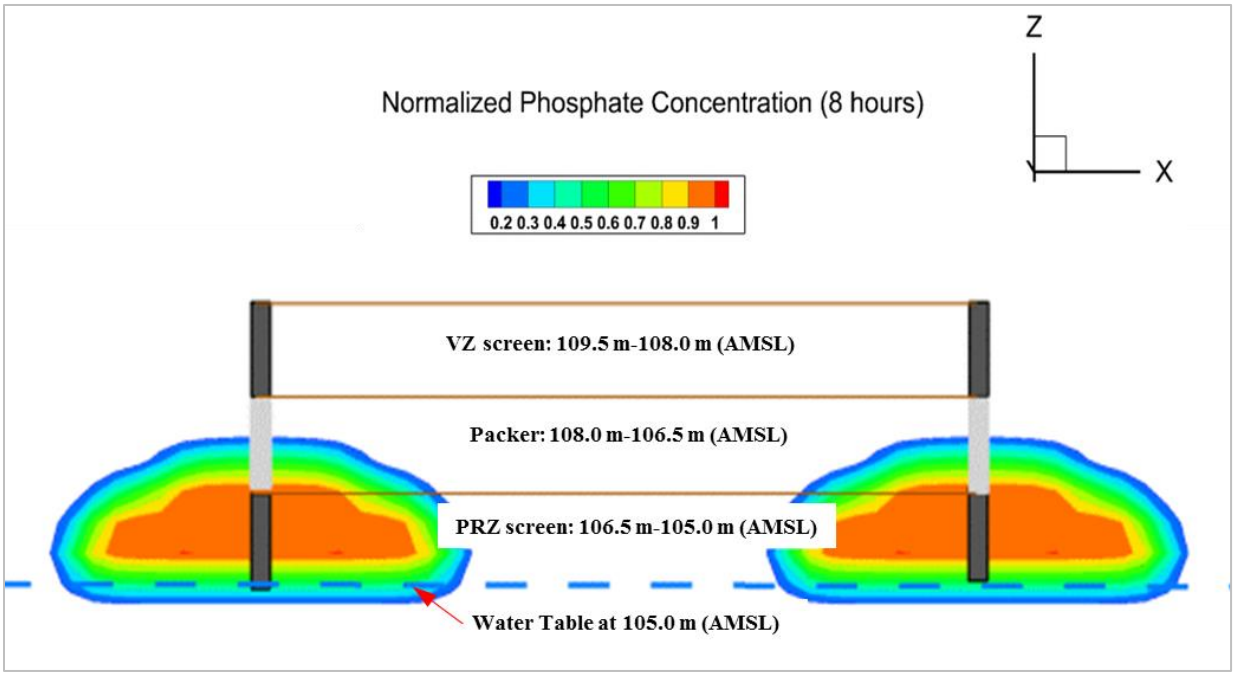
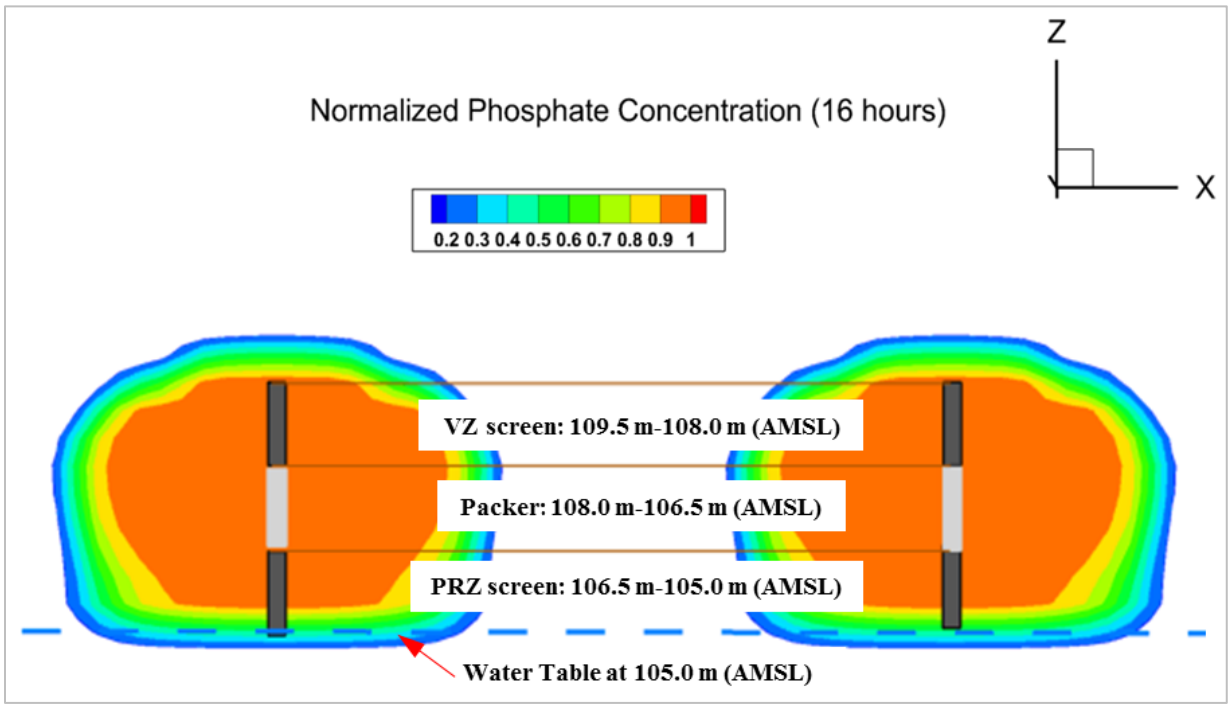


Figure 10. Change of ROI with Injection Period for Case S3



(a)



(b)

Figure 11. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S3

7.2.4 Case S4 (High θ_s, Isotropic)

Figure 12 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 3.25 m. The ROI increased to 4.25 m after 16 hours (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). Once again, as expected, the calculated ROI for the isotropic condition is lower than that for the anisotropic Case S3. Figure 13(a) and Figure 13(b) illustrate, respectively, the normalized polyphosphate concentration plumes at 8 hours and 16 hours.

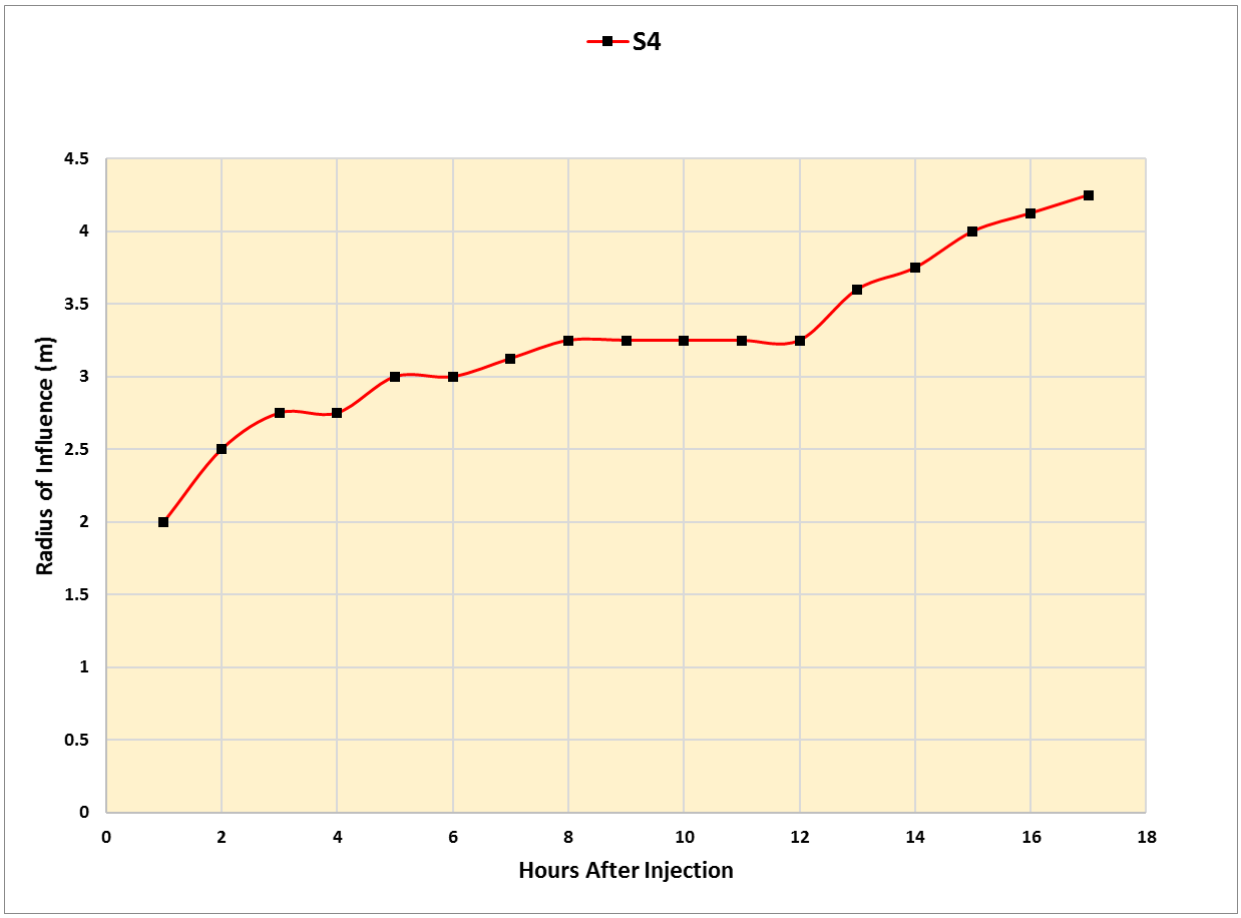
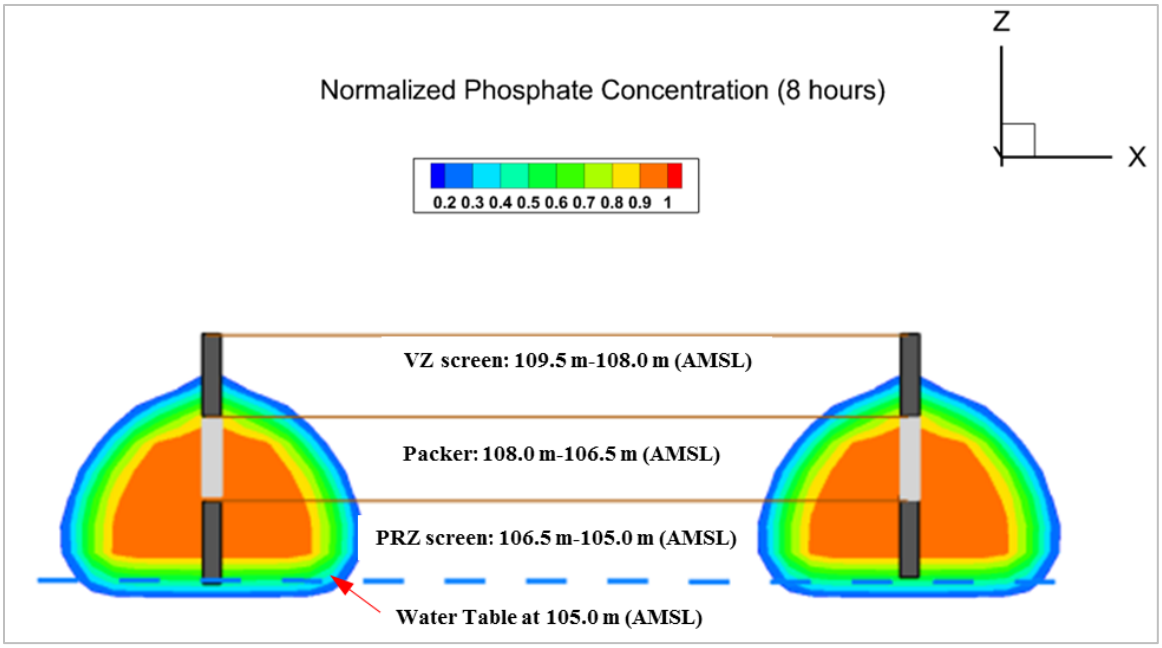
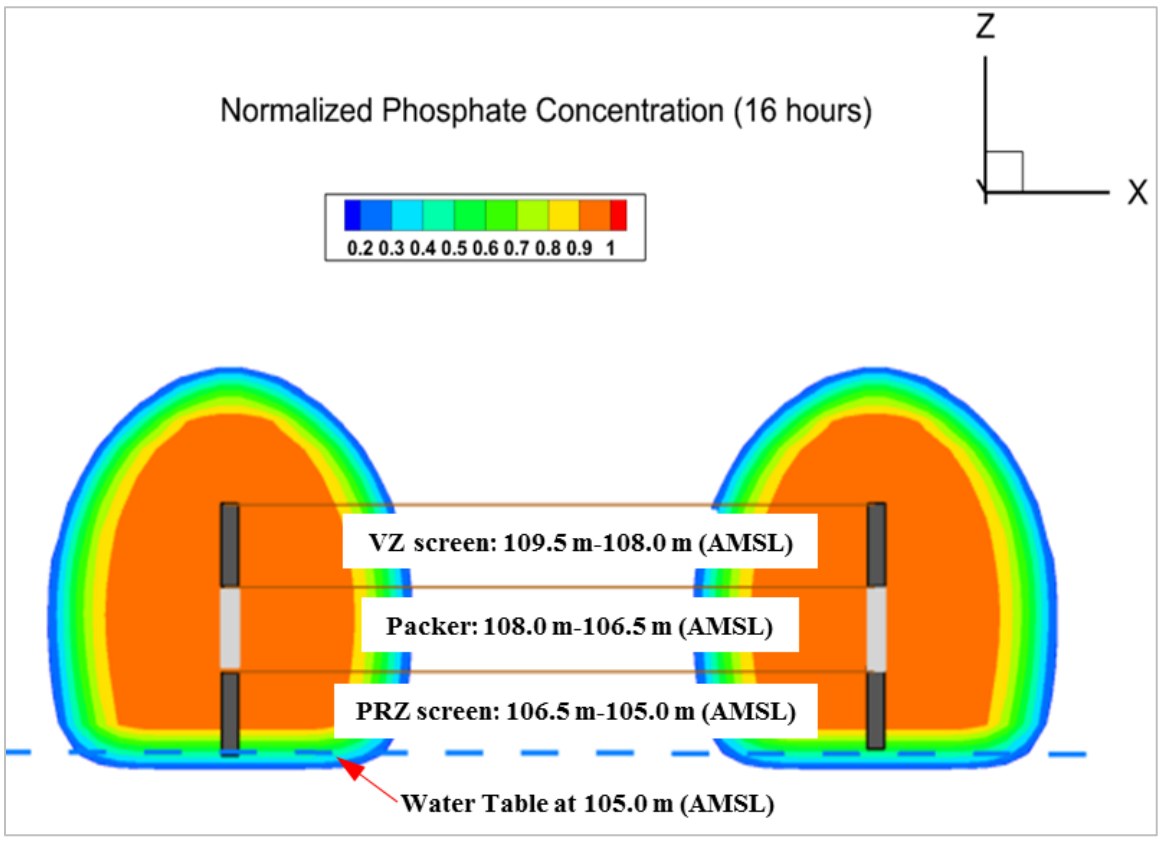


Figure 12. Change of ROI with Injection Period for Case S4



(a)



(b)

Figure 13. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 (b) Hours for Case S4

7.2.5 Case S5 (High θ_r, Constant Anisotropy)

The selected hydraulic properties for Case S5 were the same as those used earlier for Stage A uranium transport modeling (ECF-300FF5-16-0091). Figure 14 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 6.625 m. The ROI increased to 8 m after 16 hours (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). Figure 15(a) and (b) illustrates, respectively, the normalized polyphosphate concentration plumes at 8 hours and 16 hours.

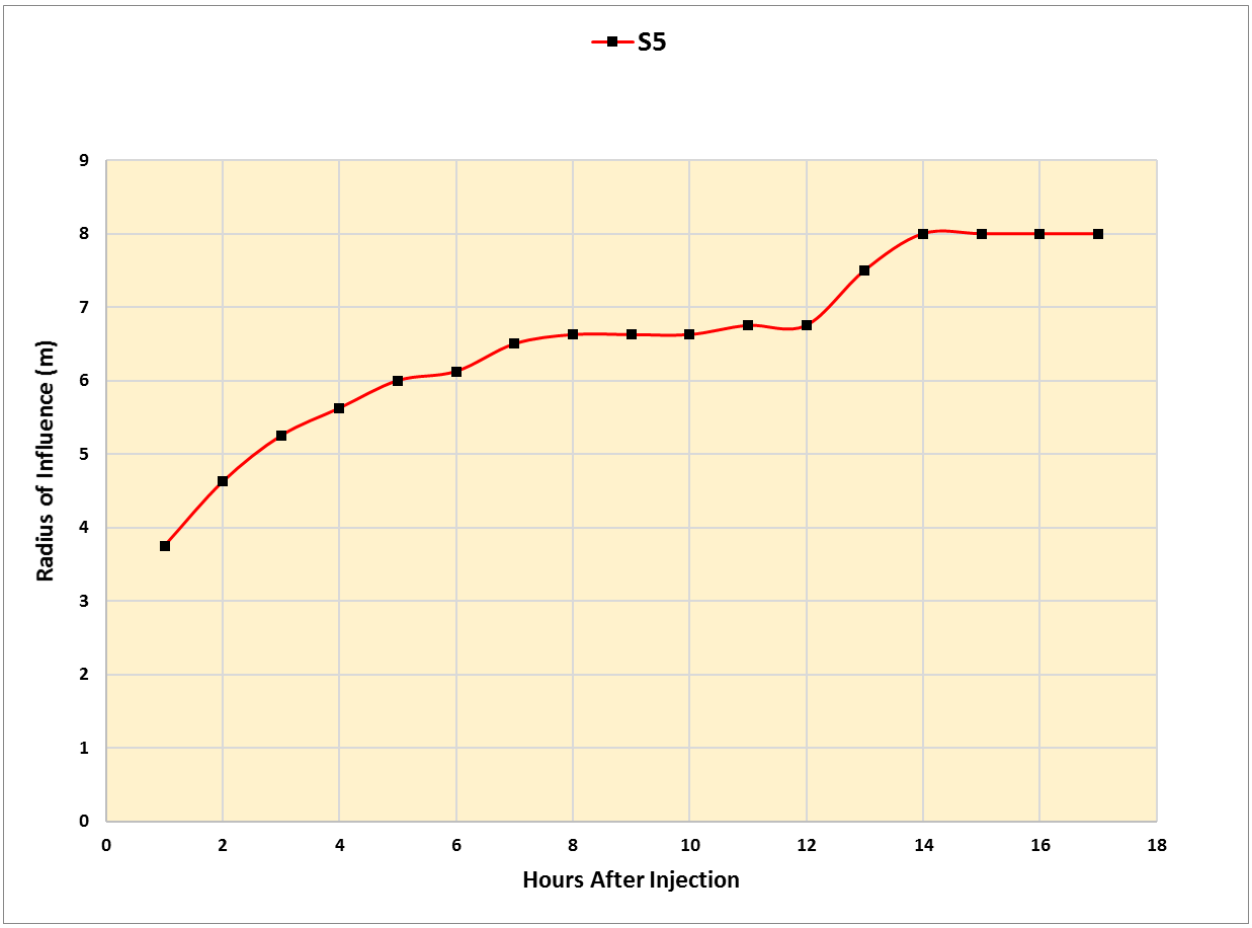
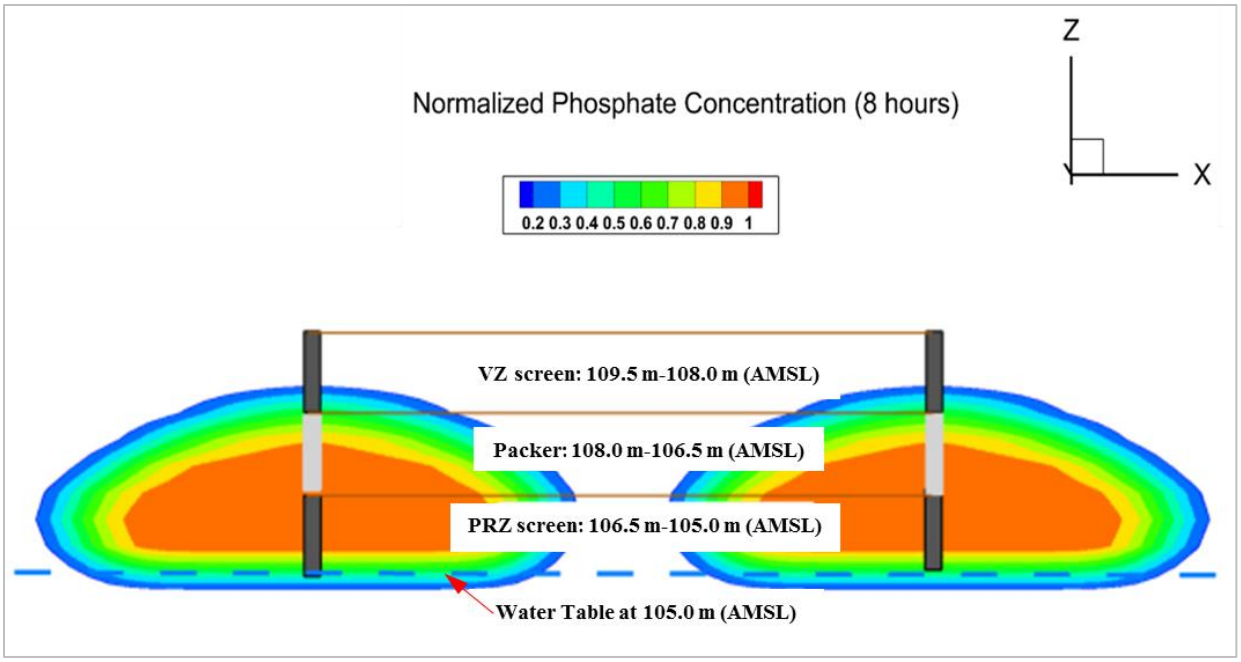
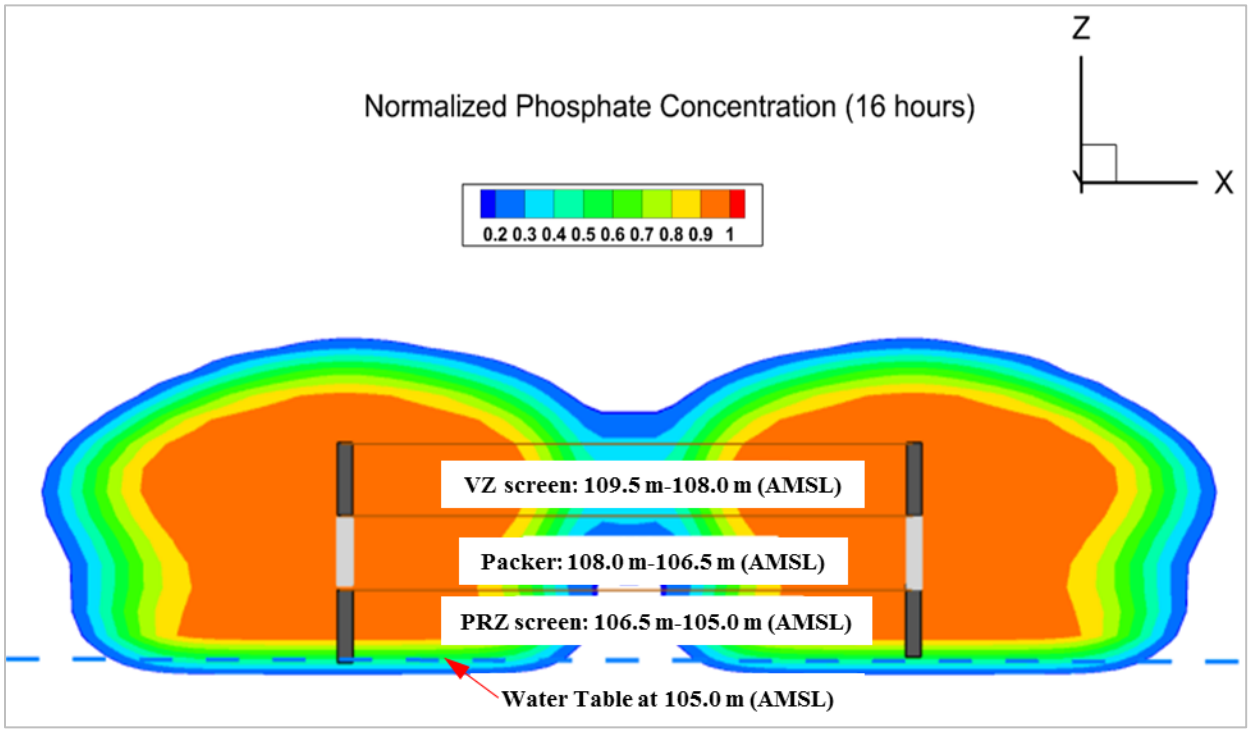


Figure 14. Change of ROI with Injection Period for Case S5



(a)



(b)

Figure 15. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S5

7.2.6 Case S6 (High θ_r, Isotropic)

Figure 16 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 4.25 m. The ROI increased to 6 m after 16 hours (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). Once again, as expected, the calculated ROI for the isotropic condition is lower than that for the anisotropic Case S5. Figure 17 (a and b) illustrates the normalized polyphosphate concentration plumes at 8 hours and 16 hours, respectively.

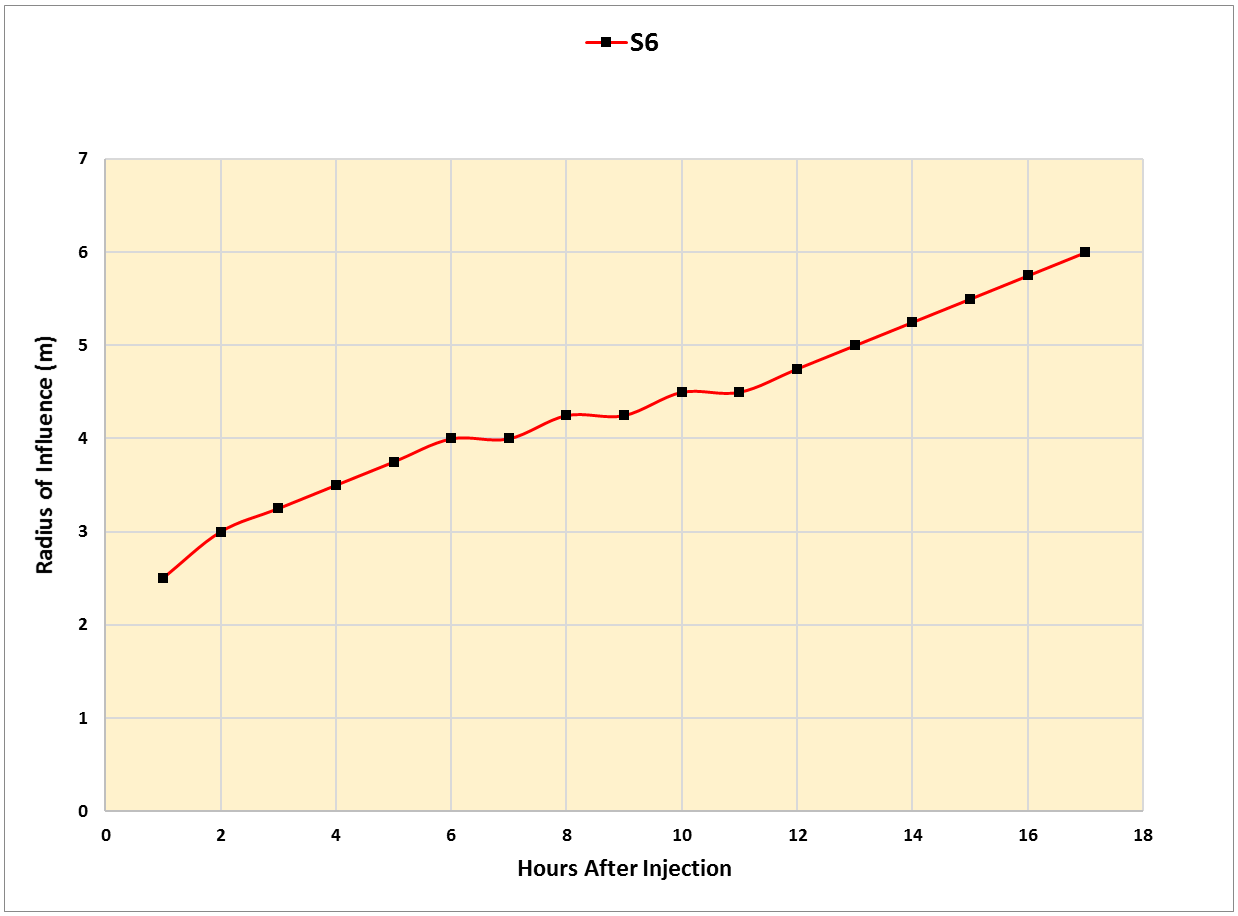
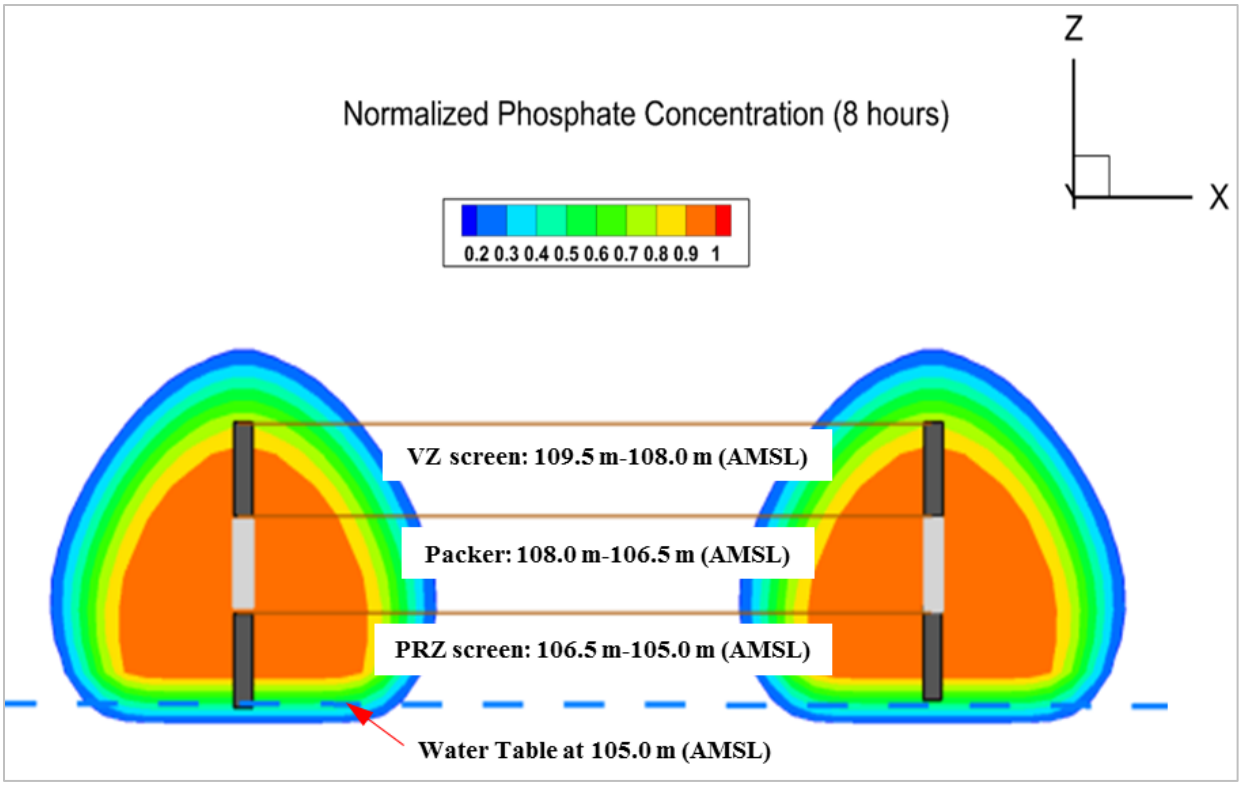
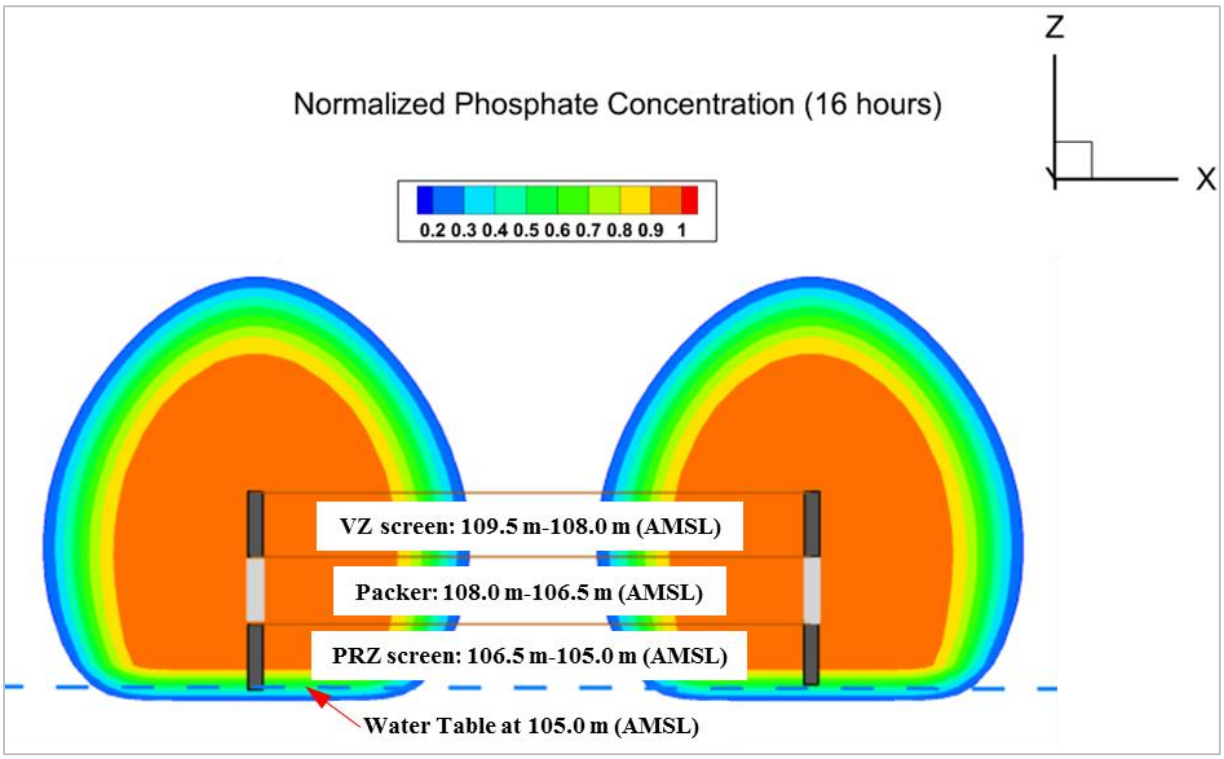


Figure 16. Change of ROI with Injection Period for Case S6



(a)



(b)

Figure 17. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S6

7.2.7 Case S7 (Variable Moisture-Dependent Anisotropy)

A TCT model was developed for Case S7. As stated earlier, unlike the constant anisotropy assumed for Cases S1 though S6, the TCT model simulates the macroscopic, field-scale variable moisture dependent anisotropy (PNNL-23711).

Figure 18 shows the calculated ROI as a function of time since the injections started. After 8 hours of injection within the PRZ, the ROI is 4 m. The ROI increased to 4.75 m after 16 hours (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). Figure 19 (a and b) illustrates the normalized polyphosphate concentration plumes at 8 hours and 16 hours, respectively.

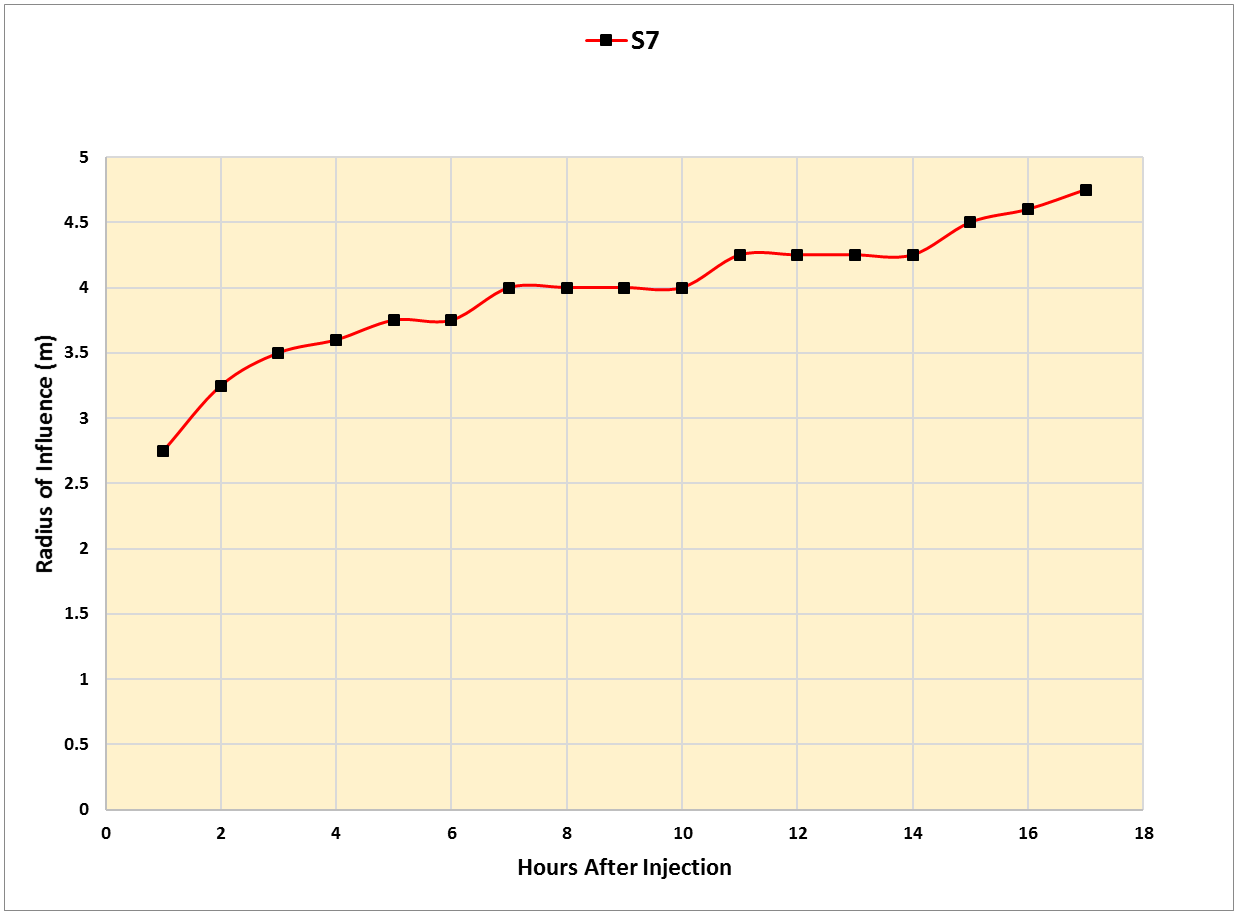
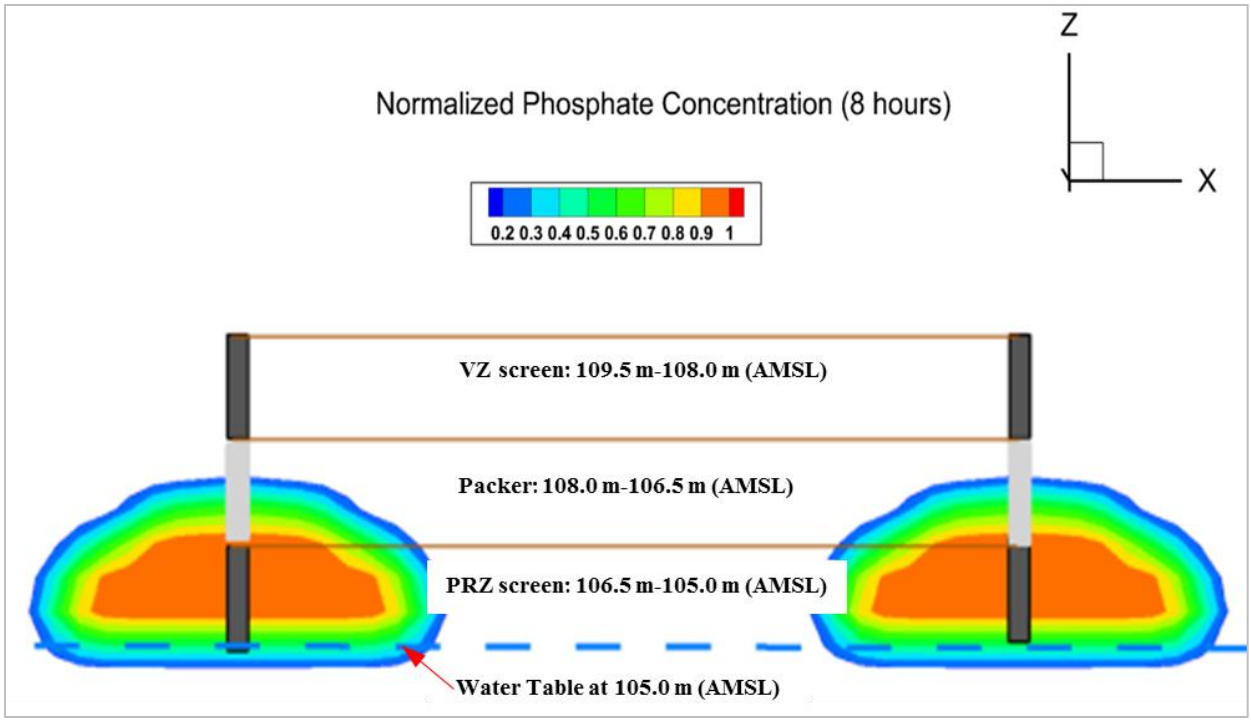
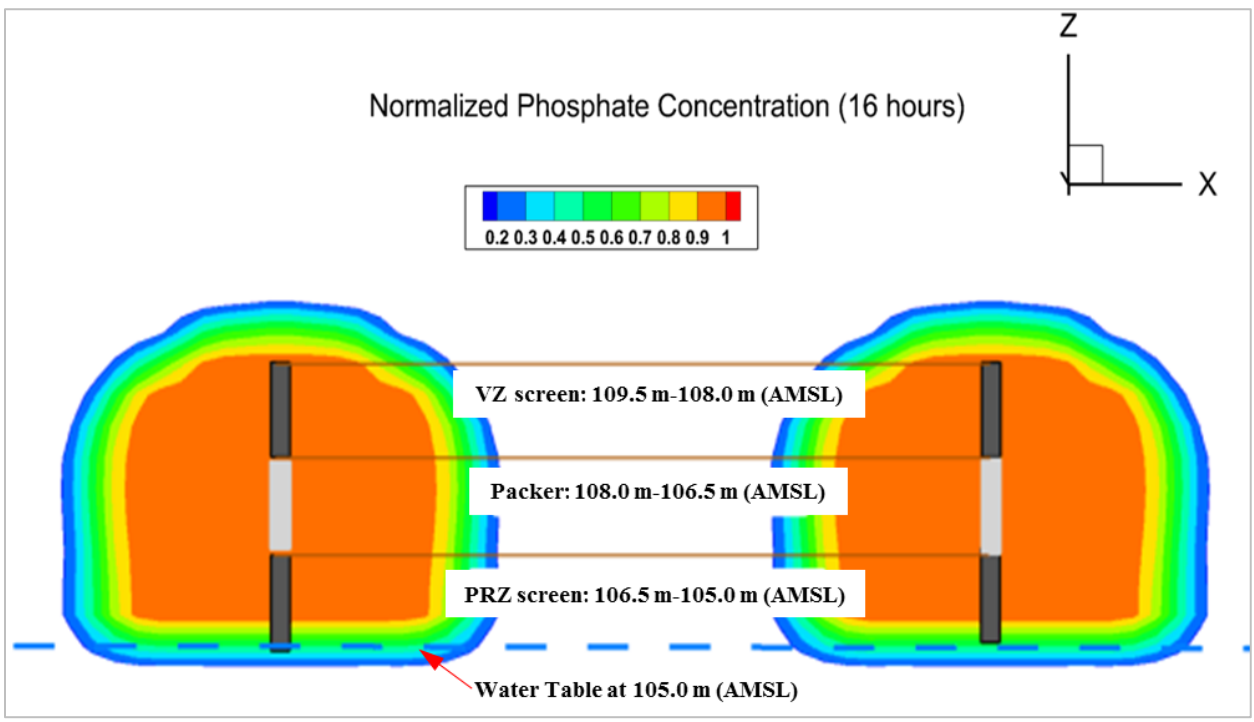


Figure 18. Change of ROI with Injection Period for Case S7



(a)



(b)

Figure 19. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S7

7.2.8 Case S8 (High Saturated Hydraulic Conductivity K_s for the PRZ, Constant Anisotropy)

Case S8 uses a saturated conductivity of 4,000 m/d for the PRZ with a vertical to horizontal anisotropy of 1:10. Figure 20 shows the calculated ROI as a function of time since the injections started. Figure 21 (a and b) illustrates the normalized polyphosphate concentration plumes after 8 hours and 16 hours, respectively (8 hours of injection within the PRZ followed by 8 hours of injection within the lower vadose zone). As expected, because of the use of a PRZ saturated hydraulic conductivity that is orders of magnitude larger than the lower vadose zone saturated hydraulic conductivity, the polyphosphate plume at 16 hours has a smaller (4 m) ROI within the PRZ; the ROI within the lower vadose zone is 8 m.

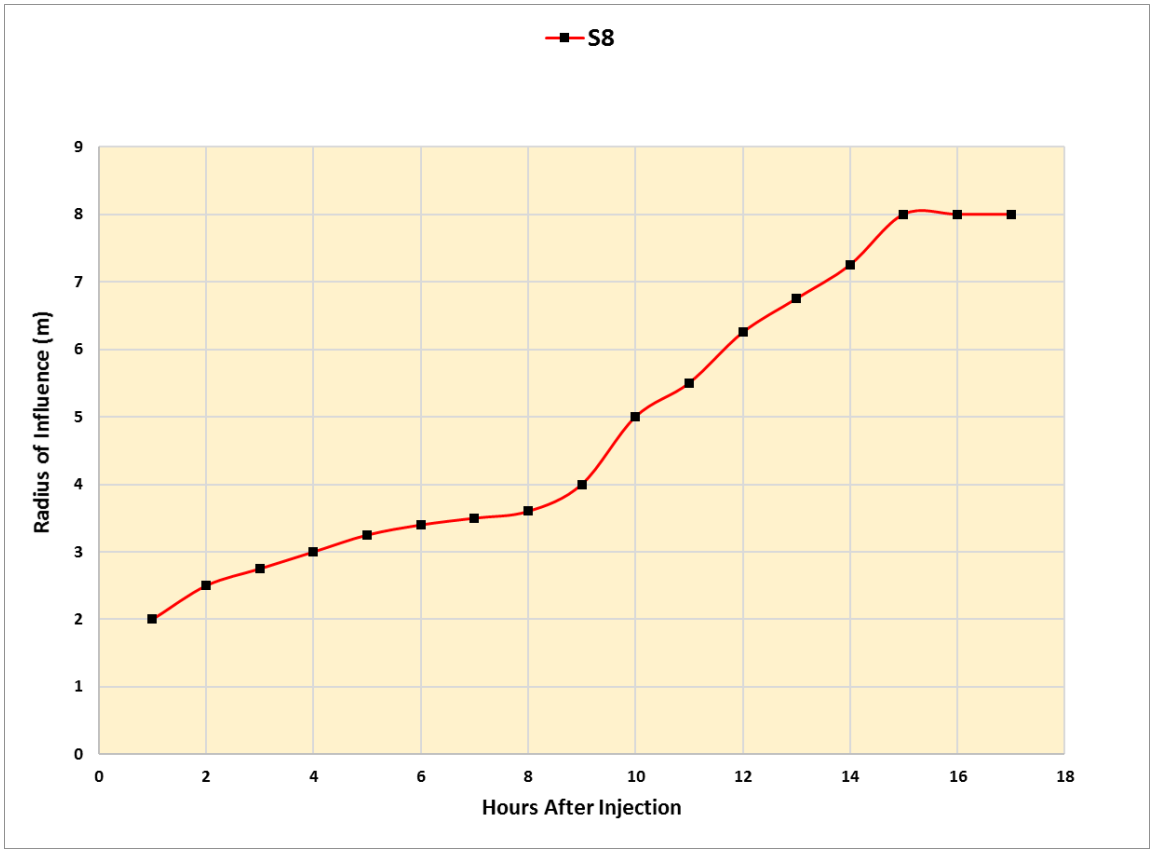
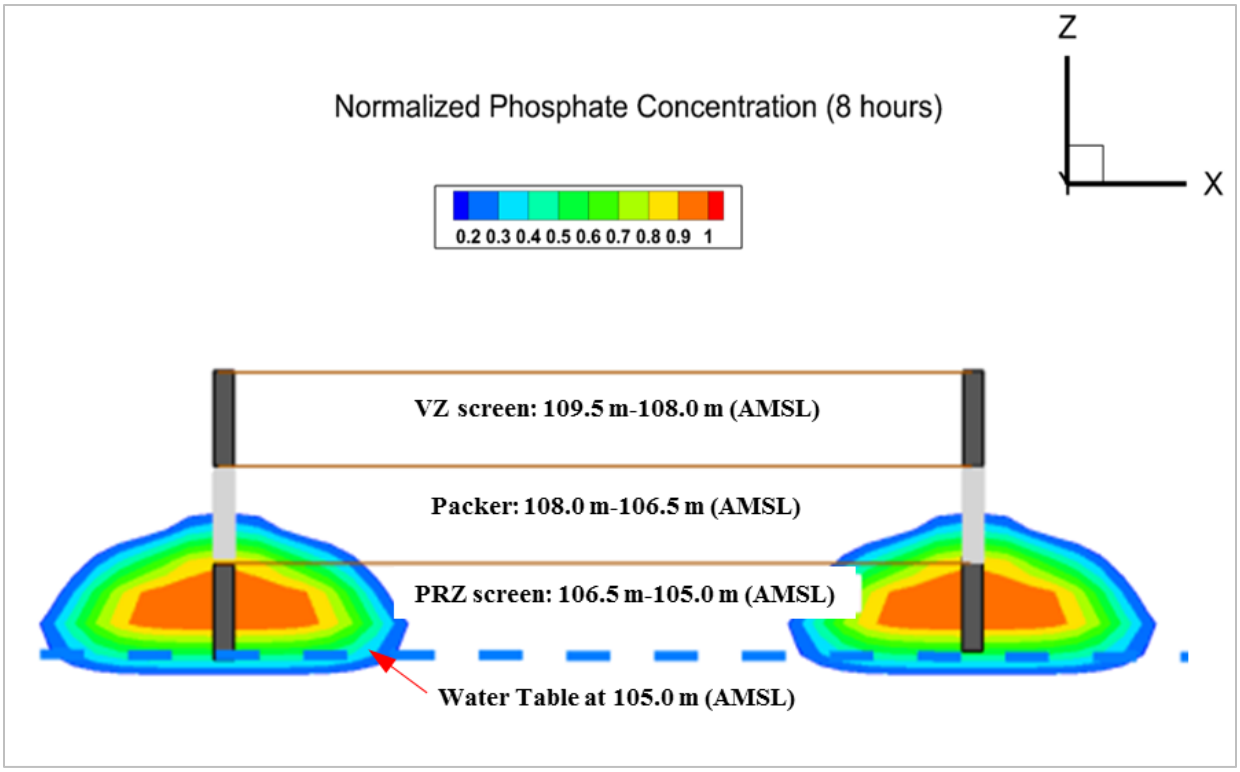
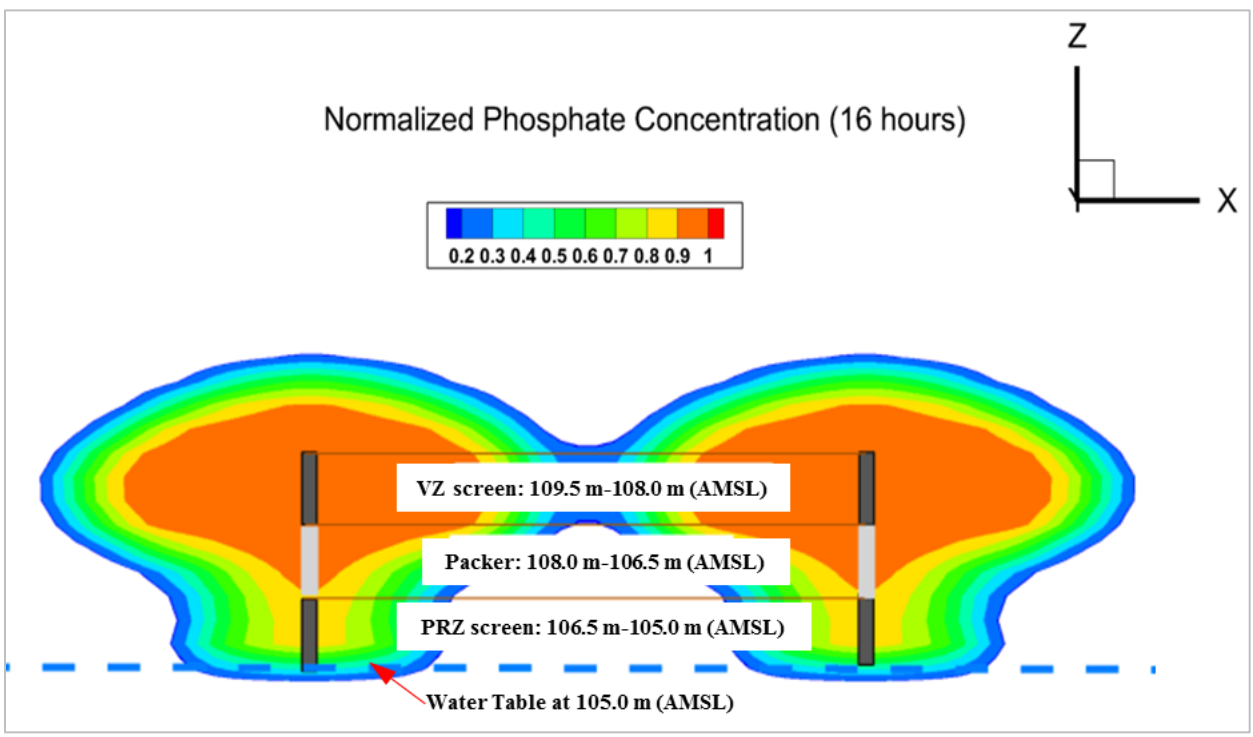


Figure 20. Change of ROI with Injection Period for Case S8



(a)



(b)

Figure 21. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes at 8 Hours (a) and 16 Hours (b) for Case S8

7.2.9 Case S9 (Active Saturated Zone for Modeling Domain)

For Cases S1-S8, a Dirichlet type outflow boundary condition was used to allow solute mass to flow in and out of the system. Case S9 was run to verify use of such an approach for the outflow boundary condition. Case 9 included the saturated zone as part of the STOMP active modeling domain and all other properties were kept the same as those for Case S5. Figure 22 shows the calculated ROI as a function of time since the injections started; the results are same as those for Case S5 (Figure 14). Figure 23 (a and b) shows the normalized polyphosphate concentration plumes after 8 hours of injection with active and inactive saturated zones, respectively. Similarly, Figure 23 (c and d) shows the normalized polyphosphate concentration plumes after 16 hours of injection with active and inactive saturated zones, respectively. Overall, Figure 23 suggests that the simulated polyphosphate plumes for both cases are comparable and the simplified treatment of water table as an outflow boundary is acceptable. The estimated ROI values for cases with active (Figure 22) and inactive (Figure 14) saturated media are almost equal.

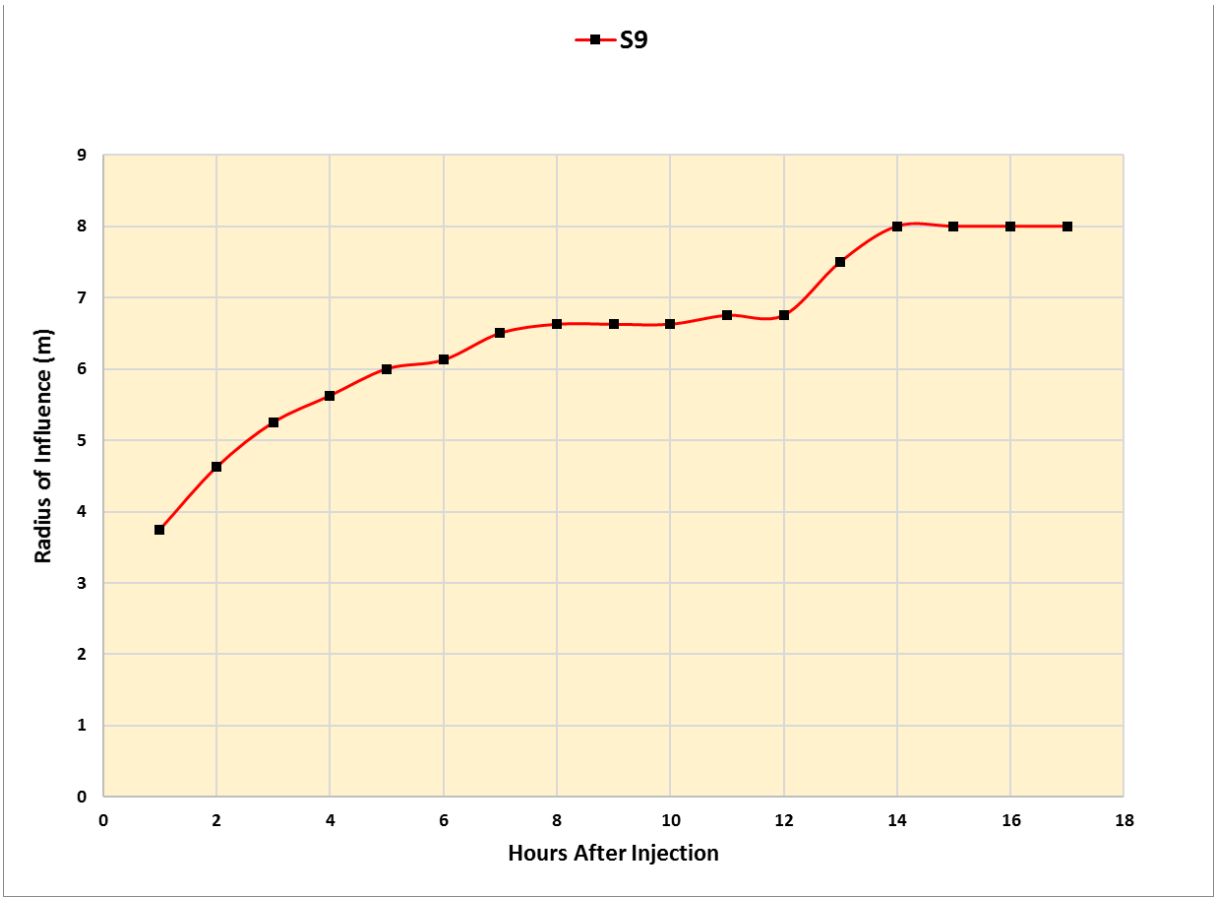


Figure 22. Change of ROI with Injection Period for Case S9

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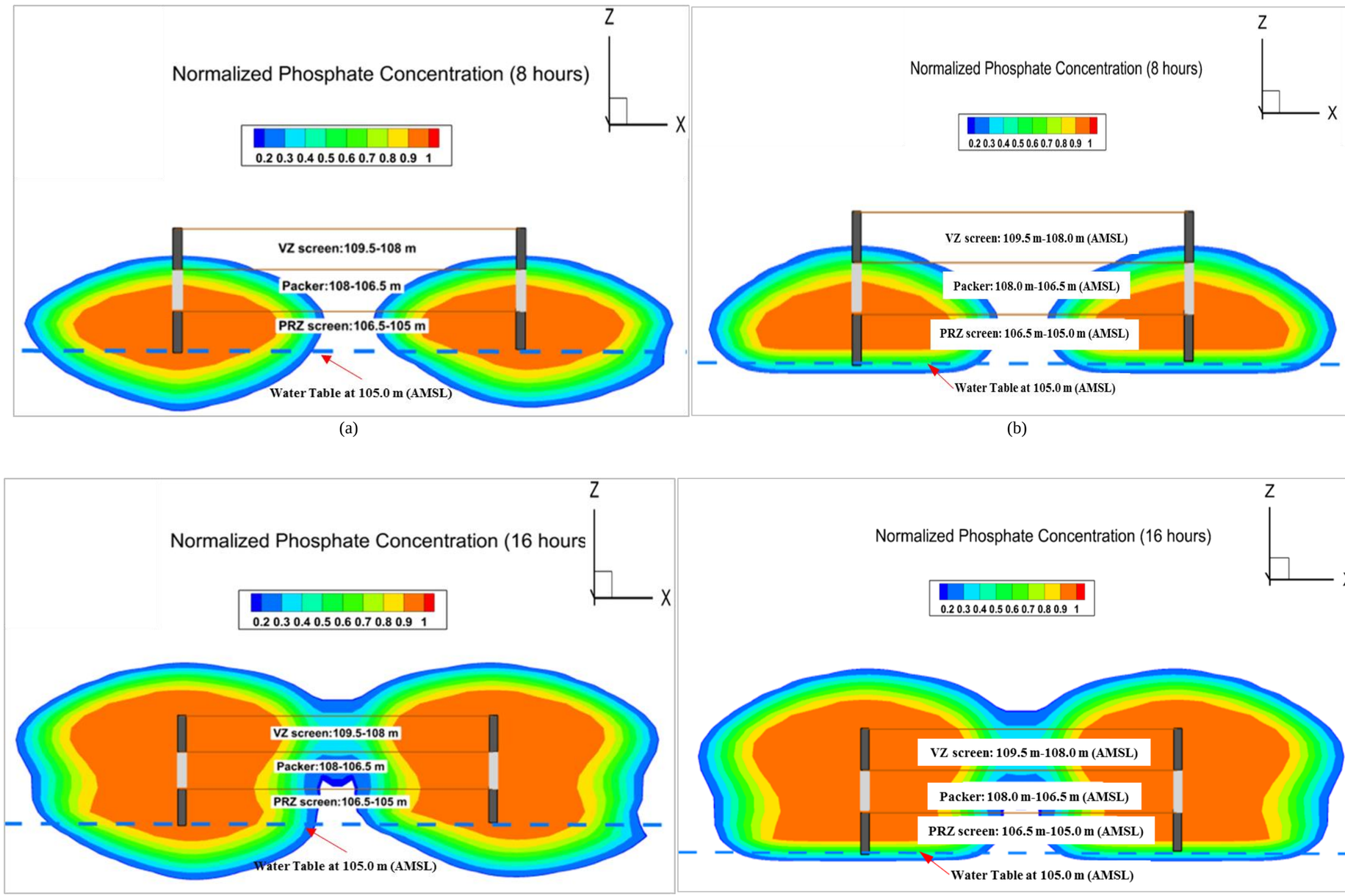

Figure 23. Vertical Cross-Sectional View of Normalized Polyphosphate Concentration Plumes

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8 Summary and Concluding Remarks

Figure 24 shows the change of calculated ROI as a function of time since the injections commenced for the STOMP simulation cases (S1 through S9). Table 4 lists the calculated ROI values following 8 hours and 16 hours of injection for Cases S1 though S9. For identical injection periods and injection rates for the PRZ and the lower vadose zone, the ROI varies from as low as 3.25 m to as high as 8.5 m. The analytical solution based ROI ranges from 4.4 to 6 m.

As expected, the inherent variability of hydraulic properties for the 300 Area heterogeneous sandy gravel sediments exerts considerable impact on the calculated ROI. For modeling, the heterogeneous sandy gravel unit is conceptualized as EHM with macroscopic flow and transport properties. For the field-scale modeling domain, a macroscopic anisotropy is, in effect, induced by the media heterogeneities. However, the field-scale anisotropy at the 300 Area Stage B site is not known a priori. Therefore, to obtain a range of ROI estimates, several cases are considered which include a constant as well as a variable, moisture-dependent anisotropy.

The mass balance based analytical solution ROI ranges are different from the STOMP-based contaminant plume calculations. Unlike the analytical solution, which is applicable to steady state moisture flow, STOMP can account for transient moisture flow as well as mass transport (i.e., advection, diffusion, and dispersion) processes. Unlike the analytical solution, STOMP can model the macroscopic, field-scale variable state-dependent (i.e., moisture-dependent) anisotropy. Consideration of these processes leads to a considerably larger ROI estimate, including a bigger range, compared to the approximate analytical solution.

Nonetheless, the analytical as well as the numerical results show a consistent behavior. As time progresses and near steady state conditions prevail, the calculated ROI depends essentially on the available moisture holding capacity (i.e., $\theta wet - \theta dry$); a higher value yields a lower ROI estimate and vice versa. A smaller water holding capacity, however, is expected for the highly gravelly media Stage B field site, and the ROI estimate (8.5 m), for example, at 16 hours for the S1 simulation case is more reasonable. It should also be noted that the ROI estimates are based on a threshold concentration of 20%; a lower threshold will yield a larger ROI estimate. Moreover, the EHM approximation was used to represent the highly heterogeneous gravelly media at the field site. An alternate modeling approach would be to develop multiple Monte Carlo (MC) realizations to represent the discrete heterogeneities for the spatially variable gravelly media. For a network of injection wells, the calculated ROI values based on EHM modeling for Cases S1 through S8 are expected to encompass the spatial variability of ROIs for the MC based heterogeneous field site. Compared with EHM modeling, however, an MC based discrete heterogeneous field is expected to result in a larger smearing of the simulated polyphosphate concentration front and, consequently, higher ROI estimates.

STOMP modeling does not account for density effects and any chemical reactions that would occur from polyphosphate injection. The effect of media heterogeneity is expected to overwhelm any variations due to density effects. The final injection concentration is estimated to be about 10,000 to 12,000 mg/L total dissolved solids (TDS). In comparison, the seawater concentration is about 35,000 mg/L TDS. Thus, the density effects are not expected to be significant. The work scope for this ECF does not address apatite formation as part of the polyphosphate injection; the scope is to estimate the ROI and its variability due to media heterogeneities.

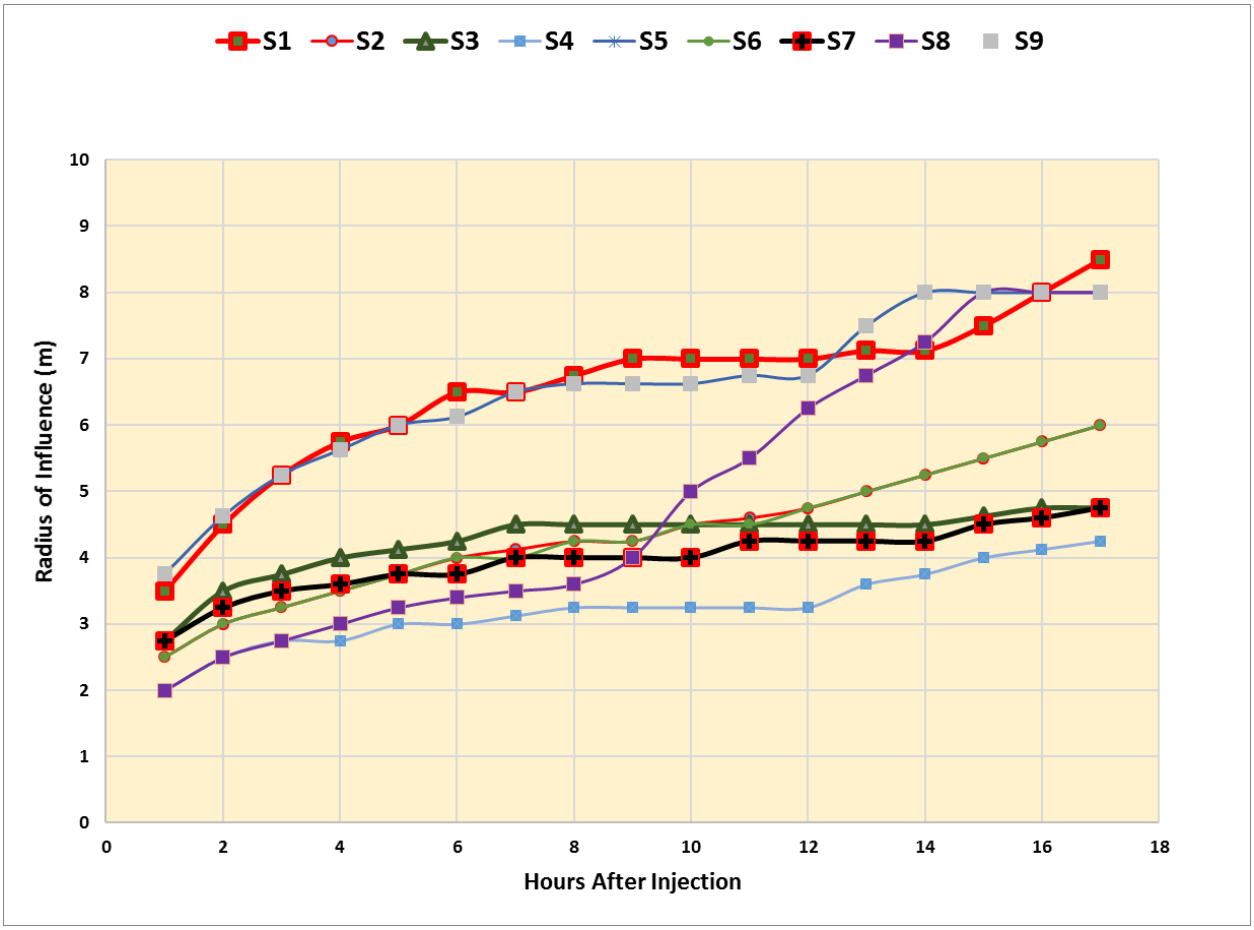

Figure 24. Change of ROI with Injection Period for All Simulation Cases

Table 4. Calculated ROI for Simulation Cases S1 through S9

Simulation Case	ROI at 8 hours (m)	ROI at 16 hours (m)
S1	7	8.5
S2	4.25	6
S3	4.50	4.75
S4	3.25	4.25
S5	6.625	8
S6	4.25	6
S7	4	4.75
S8	4	8
S9	6.625	8

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Appendix A

Analytical Solution for Estimating Radius of Influence during Injection

Note: The material in this appendix is based on Warrick, 2003, *Soil Water Dynamics*.

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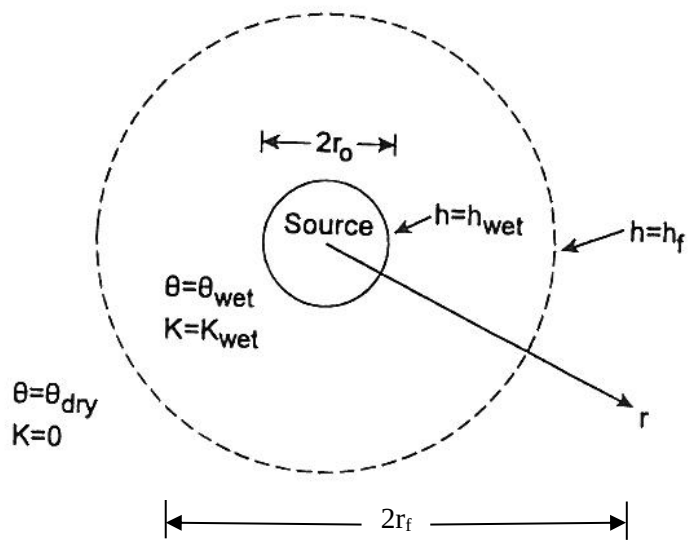
A1 Spherical Source at Constant Potential (Three Dimensions)

Considering the time-dependent absorption in radial direction and from a spherical source, as shown in Figure A-1, the volumetric flow rate, q (m^3/s) across radius $r = r_0$ is $q = q(t)$, t = time. Following a sharp wetting front approximation during injection, unsaturated hydraulic conductivity $K = K_{wet}$ and moisture content $\theta = \theta_0$ behind the front, that is, are assumed for the region $r_0 < r < r_f$ (Figure A-1). This simplified analysis is referred to as a Green and Ampt analysis. Ahead of the front, unsaturated hydraulic conductivity $K = 0$ and the moisture content $\theta = \theta_{\text{dry}}$ (Figure A-1). The pressure head is h_{wet} at radius $r = r_0$ and h_f at radius $r = r_f$. As described in Warrick, 2003, *Soil Water Dynamics*, these are comparable to the Philip, 1969, "Hydrostatics and Hydrodynamics in Swelling Soils," delta function hydraulic properties, at least if the pressure head at the source is $h_0 \leq 0$.

For the above simplification, the flux J_r by Darcy's law for the region $r_0 < r < r_f$ (Figure A-1) is:

$$J_r = -K_{wet}\frac{\partial h}{\partial r} \qquad \text{(Equation A-1)}$$



Reference: Warrick, 2003, *Soil Water Dynamics*.

Figure A-1. Absorption from Spherical or Cylindrical Source for a Green and Ampt Soil

Also, the flux J_r satisfies:

$$J_r = \frac{q}{4\pi r^2} \qquad \text{(Equation A-2)}$$

Where the flow rate (q) is a function of time (t), a combination of (A-1), (A-2), and boundary conditions gives:

$$h = \frac{q}{4\pi K_{wet}}\left(\frac{1}{r} - \frac{1}{r_0}\right) + h_{wet} \qquad \text{(Equation A-3)}$$

and:

$$q(t) = 4\pi\, K_{wet}\left(h_{wet} - h_f\right)\left(\frac{1}{r} - \frac{1}{r_0}\right)^{-1} \qquad \text{(Equation A-4)}$$

or:

$$q(t) = 4\pi\, K_{wet} \Delta h r_0 \left(1 - \frac{r_0}{r_f}\right)^{-1} \qquad \text{(Equation A-5)}$$

with the change in head:

$$\Delta h = \left(h_{wet} - h_f\right) \qquad \text{(Equation A-6)}$$

A continuity relationship is found by equating water stored to the volume injected $Q(t)$:

$$Q(t) = \frac{4\pi}{3}\left(r_f^3 - r_0^3\right)\Delta\theta \qquad \text{(Equation A-7)}$$

with:

$$\Delta\theta = \left(\theta_{wet} - \theta_{dry}\right) \qquad \text{(Equation A-8)}$$

The flow rate, q (m^3/s), is related to the volume of water stored, Q (m^3), by:

$$\frac{dQ}{dt} = q \qquad \text{(Equation A-9)}$$

The radius of influence, i.e., the wetting front coordinate r_f (Figure A-1), is from Equation A-7:

$$r_f = r_0 \left(1 + \frac{3Q}{4\pi\Delta\theta r_0^3}\right)^{1/3} \qquad \text{(Equation A-10)}$$

or:

$$r_f = r_0 (1 + aQ)^{1/3} \qquad \text{(Equation A-11)}$$

where:

$$a = \frac{3}{4\pi\Delta\theta r_0^3} \qquad \text{(Equation A-12)}$$

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Appendix B

Process-Level Model Based on STOMP Flow and Transport Simulator

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B1 Process-Level Model Based on STOMP Flow and Transport Simulator

This appendix describes detailed process-level numerical models based on the Subsurface Transport Over Multiple Phases (STOMP) code, which was used to simulate three-dimensional flow and transport through the Stage B enhanced attenuation area integrated saturated-unsaturated media. To calculate water flow, the STOMP based numerical model includes the assumption that the vadose zone and unconfined aquifer system can be represented and approximated by an equivalent porous continuum. Each heterogeneous geologic unit is represented in the model by an equivalent homogeneous media having either a constant or a moisture-dependent macroscopic anisotropy. With each heterogeneous unit assigned its upscaled or effective hydraulic properties, the simulated flow fields predict the bulk or mean flow behavior at the field scale. Upscaling, in effect, accounts for the differences in scale between small, core-scale measurements and large, field-scale modeling.

The STOMP based numerical model solves a conservation of mass equation using a finite difference approximation to the matric potential form of the Richards' equation (Jury and Horton, 2004, *Soil Physics*) that calculates fluid flow entering, exiting, and accumulating within the finite numerical volumes as follows:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[K(h)\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[K(h)\frac{\partial h}{\partial y}\right] + \frac{\partial}{\partial z}\left[K(h)(\frac{\partial h}{\partial z} + 1)\right] \pm S \qquad \text{(Equation B-1)}$$

where:

h	=	matric potential h = h(x,y,z,t), t=time
C(h) = dθ/dh	=	specific moisture capacity, C for a given h, and is equal to dθ/dh, i.e., the inverse slope of the matric potential-moisture content, θ, relation (cm)
K(h)	=	the hydraulic conductivity (cm/s), which may be anisotropic and is dependent on matric potential
S	=	the amount of water added (source) or subtracted (sink) per unit volume through time (1/s).

Moisture content is a function of soil matric potential, and the soil matric potential-moisture retention relationship is described for the Stage B hydrostratigraphic unit using the following empirical relationship (van Genuchten, 1980, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils;" EPA/600/2-91/065, *The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils*):

$$\theta(h) = \theta_r + (\theta_s - \theta_r)\{1 + [\alpha h]^n\}^{-m} \qquad \text{(Equation B-2)}$$

where θ(h) is the moisture content, here expressed explicitly as a function of the soil matric potential, and the other terms are defined as follows:

θ_r	=	residual moisture content (dimensionless)
θ_s	=	saturated moisture content (dimensionless)
α	=	a fitting parameter (cm^{-1})

n = a fitting parameter (dimensionless)

m = 1 - 1/n

Combining the van Genuchten model with the model from Mualem, 1976, "A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media," for unsaturated conductivity produces the following relationship for hydraulic conductivity and soil matric potential:

$$K(h) = \frac{K_s\{1-(\alpha h)^{mn}[1+(\alpha h)^n]^{-m}\}^2}{[1+(\alpha h)^n]^{ml}} \qquad \text{(Equation B-3)}$$

where K(h) is the hydraulic conductivity (cm/s), which is, as expressed, dependent on the soil matric potential; K_s is the saturated hydraulic conductivity (cm/s); and l is a pore-connectivity parameter (dimensionless) that Mualem (1976) estimates to be about 0.5 for many soils and is assumed to equal 0.5 in this analysis.

Solute transport within the STOMP code is described by the conventional advective-dispersive transport solution to the conservation of mass equation described by Jury and Horton (2004) and applied to finite difference volumes:

$$\frac{\partial}{\partial t} M_c = \frac{\partial}{\partial \mathrm{x}}\left(D_e \frac{\partial C_l}{\partial \mathrm{x}}\right) + \frac{\partial}{\partial \mathrm{y}}\left(D_e \frac{\partial C_l}{\partial \mathrm{y}}\right) + \frac{\partial}{\partial \mathrm{z}}\left(D_e \frac{\partial C_l}{\partial \mathrm{z}}\right) - \frac{\partial}{\partial \mathrm{x}}(J_x\, C_l) - \frac{\partial}{\partial \mathrm{y}}(J_y\, C_l) - \frac{\partial}{\partial z}(J_z\, C_l) - M_c \frac{ln(2)}{t^{1/2}} \qquad \text{(Equation B-4)}$$

where:

$\frac{\partial}{\partial t} M_c$ = the change in contaminant mass or activity present in the finite volume (g or Ci) through time and the mass or activity is calculated according to the equation:

$$(\rho_b\, C_a + \theta\, C_l)$$

ρ_b = soil bulk density (g/cm^3)

C_a = adsorbed solute concentration (g or Ci per g soil)

θ = moisture content (dimensionless), and dependent on the soil matric potential

C_l = dissolved solute concentration (g or Ci per cm^3 water)

J_x, J_y, J_z = water or moisture flux (cm/s) along the x, y, and z directions, respectively

D_e = effective dispersion/diffusion coefficient (cm^2/s)

$t^{1/2}$ = radioactive half-life(s); entire term represents the mass of solute lost to radioactive decay

In Equation B-4, positive is used to indicate solute entering the finite volume, and negative is used to indicate what is exiting or lost to decay. The adsorbed and dissolved solute concentrations are related through an equilibrium linear sorption coefficient (K_d mL water per g soil) formulation: $C_a = K_d\, C_l$. No temperature effects are considered for the vadose zone model (i.e., the model used is isothermal).

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Appendix C

Software Installation and Checkout Form

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CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM

Software Owner Instructions:

Complete Fields 1-13, then run test cases in Field 14. Compare test case results listed in Field 15 to corresponding Test Report outputs. If results are the same, sign and date Field 19. If not, resolve differences and repeat above steps.

Software Subject Matter Expert Instructions:

Assign test personnel. Approve the installation of the code by signing and dating Field 21, then maintain form as part of the software support documentation.

GENERAL INFORMATION:

1. Software Name: STOMP (Subsurface Transport Over Multiple Phases) Software Version No.: Bld 4

EXECUTABLE INFORMATION:

2. Executable Name (include path):

```
All executable files installed in directory                    /bin
--------------------------------  ---------------------------
MD5 File Signature                Executable File Name
--------------------------------  ---------------------------
6536b8e12d8c5b83dca76f2c947b6153  stomp-wae-bcg-chprc04i.x
e0cdf04bc1a2f6c55c5a1b499939f663  stomp-wae-bcg-chprc04l.x
6e72340bb39f6056e232fe5ff241c4d4  stomp-wae-bd-chprc04i.x
3f837a0fb8d9f47dbcada686f542d7fc  stomp-wae-bd-chprc04l.x
7e5b4cc36a8991b3d5a8ea2ed155ce47  stomp-wae-cgsq-chprc04i.x
00a898c0c3ec06817485781ad1c9ec46  stomp-wae-cgsq-chprc04l.x
f18ff5ab5667065d8ab12657344fb6a0  stomp-wae-cgst-chprc04i.x
061af86cf21ad8435b046d0efabe971b  stomp-wae-cgst-chprc04l.x
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84b129786aba9c4be884e15e45a67389  stomp-w-r-bd-chprc04i.x
e990f1566c8099a8d54508de3da9cd88  stomp-w-r-bd-chprc04l.x
18a589a2b55aab2db290efea19b39351  stomp-w-r-cgsq-chprc04i.x
6569959476772a137df35ce874821889  stomp-w-r-cgsq-chprc04l.x
```

3. Executable Size (bytes): MD5 signatures above uniquely identify each executable file

COMPILATION INFORMATION:

4. Hardware System (i.e., property number or ID):

Tellus Subsurface Modeling Platform

5. Operating System (include version number):

Linux tellusmgmt.rl.gov 2.6.18-308.4.1.el5 #1 SMP Tue Apr 17 17:08:00 EDT 2012 x86_64 x86_64 x86_64 GNU/Linux

INSTALLATION AND CHECKOUT INFORMATION:

6. Hardware System (i.e., property number or ID):

GREEN Linux Cluster (INTERA owned)

7. Operating System (include version number):

Ubuntu Linux 14.04.1;
Linux green 4.4.0-38-generic #57~14.04.1-Ubuntu SMP Tue Sep 6 17:20:43 UTC 2016 x86_64 x86_64 x86_64 GNU/Linux

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: STOMP (Subsurface Transport Over Multiple Phases) Software Version No.: Bld 4

8. Open Problem Report? (●) No ( ) Yes PR/CR No.

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]/itc

10. Procedure(s):

CHPRC-00211 Rev 1, STOMP Software Test Plan

11. Libraries:

N/A (static linking)

12. Input Files:

Input files for ITC-STOMP-1, ITC-STOMP-2, and ITC-STOMP-2
(Baseline for comparison are results files from ATC-STOMP-1, ATC-STOMP-2, and ATC-STOMP-3 prepared on Tellus during acceptance testing)

13. Output Files:

plot.* files produced by STOMP in testing

14. Test Cases:

ITC-STOMP-1, ITC-STOMP-2, and ITC-STOMP-3

15. Test Case Results:

Pass for all executable files listed above.

16. Test Performed By: WE Nichols

17. Test Results: (●) Satisfactory, Accepted for Use ( ) Unsatisfactory

18. Disposition (include HISI update):

Installation already recorded in HISI; this is a retest following upgrade of the Linux operating system on GREEN (operational testing) to confirm correct operation after upgrade. Installation is approved for all GREEN users who have completed required STOMP software QA reading assignments.

William E. Nichols Digitally signed by William E. Nichols DN: cn=William E. Nichols, o=CHPRC, ou=Risk & Modeling Integration, email=william_e_nichols@r.gov, c=US Date: 2016.11.02 09:19:27 -07'00'

Prepared By:

19. _____ Software Owner (Signature)	WE Nichols Print	_____ Date

20. Test Personnel:

_____ Sign	WE Nichols Print	_____ Date
_____ Sign	_____ Print	_____ Date
_____ Sign	_____ Print	_____ Date

Approved By:

21. _____ Software SME (Signature)	N/R (per CHPRC-00211 Rev 1) Print	_____ Date

A-6005-149 (REV 0)