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Finite element modeling of phosphorus leaching through floodplain soils dominated by preferential flow pathways

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Abstract. *Phosphorus is a critical nutrient in soils, providing both positive and negative effects to different systems. While optimum crop growth requires a range of P above 0.2 mg/L, preventing surface water enrichment generally requires P to be below 0.03 mg/L. Proper application and control of phosphorus is important to increase farming efficiency and to protect freshwater systems from toxic algal growth. While the movement of phosphorus through many soil types has been well-documented, the presence of highly conductive, gravel outcrops and macropores in soil can have a significant, poorly-documented effect on phosphorus movement. In the Ozark ecoregion, for example, the erosion of carbonate bedrock (primarily limestone) by slightly acidic water has left a large residuum of chert gravel in Ozark soils, with floodplains generally consisting of coarse chert gravel overlain by a mantle (1 to 300 cm) of gravelly loam or silt loam. Highly conductive gravel outcrops and macropores may create preferential flow pathways for water moving through the soil column, along with any solutes in solution. In previous research, floodplain sites in Oklahoma and Arkansas were chosen due to the presence of cherty gravel outcrops that reached near the soil surface. Soil properties were evaluated, and two-dimensional electrical resistivity data were collected and correlated to hydraulic conductivity. Water was then applied to several plots (1, 10, and 100 m^2) with known concentrations of phosphorus, Rhodamine WT, and chloride for up to 52 hours, and flow towards a nearby stream was monitored with observation wells. The objective of this research was to use finite element modeling to develop a long-term model for this phenomenon for future predictions. Results from the previous research were modeled with HYDRUS-3D, a three-dimensional, finite-element model for flow and contaminant transport (both equilibrium and physical/chemical nonequilibrium transport) through soils. HYDRUS-3D was setup to simulate the 1 m^2 infiltration plot at the Barren Fork Creek site, with initial hydraulic conductivity data calculated from the* *plot scale infiltration experiment for the upper silt loam soil and from 2D geophysical data for the underlying gravel. The mobile-immobile (MIM) phase model within HYDRUS was also utilized, and MIM solute transport parameters were found iteratively using chloride tracer data taken from two wells. Results from this research will be used to predict phosphorus transport parameters and solve for long-term phosphorus transport through these soil profiles.*

Keywords. *HYDRUS, infiltration, preferential flow, subsurface nutrient transport, Ozark ecoregion.*

Introduction

Phosphorus is an important nutrient for crop growth and development, but overloading of freshwater systems with phosphorus can induce significant algae growth. Algal blooms and cyanobacteria outbreaks contribute to hypoxic waters and fish kills, as well as reduce the quality of water for consumption and recreational use (Lopez et. al., 2008). Phosphorous (P) transport has been assumed to take place primarily in surface runoff, although a growing collection of research indicates that subsurface P transport can be significant (Osborne and Kovacic, 1993; Cooper et al., 1995; Gburek et al., 2005; Fuchs et al., 2009). Large scale bank storage of P-laden stream water during high flow discharges can result in P-laden groundwater in alluvial aquifers which migrates back to the stream during baseflow conditions (Heeren et al., 2011). These subsurface P transport rates in Ozark floodplains have been shown to be comparable to surface runoff P transport rates (Mittelstet et al., 2011). In many gravelly floodplains, gravel outcrops and macropores are present resulting in high infiltration rates, some of which are reported to be on the order of 10 to 100 cm hr^{-1} (Heeren, 2012). It has been shown that in porous media with heterogeneous flow properties, the majority of the flow can occur in small preferential flow paths (Gotovac et al., 2009; Najm et al., 2010). Djodjic et al. (2004) performed experiments on P leaching through undisturbed soil columns, and stressed the need to consider larger-scale leaching processes due to soil heterogeneity.

The objective of this paper is to demonstrate the effectiveness of high-end computer modeling tools to simulate the effects of highly porous media on solute transport. The role of mobile-immobile interactions for solute transport is also demonstrated. Results from this work will be used to develop long-term simulations to predict P transport through these soil profiles under different management regimes.

Methods

Barren Fork Creek Field Site

The Barren Fork Creek floodplain site was located in the Ozark region of northeastern Oklahoma, which is characterized by karst topography, including caves, springs, sink holes, and losing streams. The erosion of carbonate bedrock (primarily limestone) by slightly acidic water has left a large residuum of chert gravel in Ozark soils, with floodplains generally consisting of coarse chert gravel overlain by a mantle of gravelly loam or silt loam (Figure 1). Topsoil depth in the floodplains ranged from 1 to 300 cm in the Oklahoma Ozarks, and generally increased with increasing stream order. Common soil series include Elsah (frequently flooded, 0-3% slopes) in floodplains; Healing (occasionally flooded, 0-1% slopes) and Razort (occasionally flooded, 0-3% slopes) in floodplains and low stream terraces; Britwater (0-8 % slopes) on high stream terraces; and Clarksville (1-50%) on bluffs.

At the Barren Fork Creek site, located five miles east of Tahlequah, Oklahoma (latitude: 35.90°, longitude: -94.85°) and just downstream of the Eldon U.S. Geological Survey (USGS) gage station (07197000), soils were Razort gravelly loam. The silt loam layer was from 30 to 200 cm thick, and the chert gravel layer, ranging from 3 to 5 m, extended down to limestone bedrock. The gravel subsoil, classified as coarse gravel based on the Wentworth (1922) scale, consists of approximately 80% (by mass) of particle diameters greater than 2.0 mm, with an average particle size (d_{50}) of 13 mm (Fuchs et al., 2009). Estimates of hydraulic conductivity for the gravel subsoil range between 140 and 230 m d^{-1} based on falling-head trench tests (Fuchs et al., 2009). The gravel layer itself is a complex alluvial deposit (Figure 1) that includes both clean gravel lenses associated with rapid flow and transport (Fox et al., 2011) as well as layers of fine gravel that can cause lateral flow in the silt loam and subsequent seepage erosion (Correll et al., 2013). The anisotropic horizontal layering results in a propensity for lateral flow.

Figure 1. Streambank at the Barren Fork Creek field site including the bank profile (left) and a seepage undercut (right). Note the sloughed material in the bottom of each picture from recent bank failures. These complex alluvial deposits include both clean gravel lenses associated with rapid flow and transport (left) as well as fine gravel lenses that can cause lateral flow and seepage erosion.

Soil Profile Characterization

Previous geophysical research was used to characterize the soil profile at the Barren Fork Creek floodplain site (Heeren et al., 2010, 2011; Mittelstet et al. 2011; Miller, 2012). Resistivity mapping involves measuring the electrical properties of near-surface earth materials, which vary with grain size, mineral type, solute content of pore water, and pore-space saturation. Miller (2012) collected electrical resistivity data using a SuperSting R8/IP Earth Resistivity Meter (Advanced GeoSciences Inc., Austin, TX) with a 56-electrode array. Two-dimensional electrical resistivity (ERI) transects were acquired at multiple locations with a 1 m electrode spacing, with an associated depth of investigation of 11 m, and utilized a proprietary routine devised by Halihan et al. (2005) for the resistivity sampling and subsequent inversion. The ERI data from 87 to 94 m along the Barren Fork main roll-along (Figure 2) were used as the ERI base for the modeling. Detailed electrical resistivity data for the Barren Fork Creek site are reported in the appendix of Miller (2012).

Miller et. al. developed a positive linear relationship ($R^2 = 0.57$) to correlate ERI data to hydraulic conductivity using a vadose zone borehole permeameter designed for coarse gravel (Miller et al., 2011). Using the conversion factor of 0.11 m d^{-1} Ω-m^{-1}, hydraulic conductivity was estimated from resistivity data.

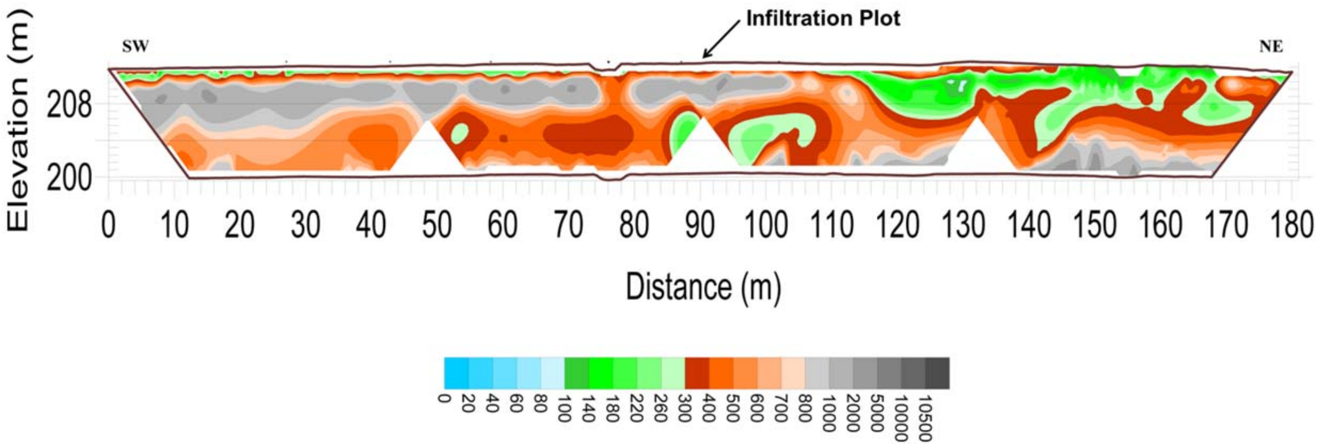

Figure 2. Electrical resistivity (Ω-m) data from the Barren Fork Creek floodplain site. Gray areas indicate high resistivity course gravels, interpreted to be buried gravel bars. Adapted from Heeren et al. (2010).

Plot Scale Infiltration Experiments

In this research, a berm method (Heeren et al., 2013) was used to confine infiltration plots and maintain a constant head of water. An infiltration experiment for a 1 m by 1 m plot at the Barren Fork Creek site was performed for 22 hr (Heeren, 2012). Chloride (Cl^-) was used as a conservative (nonsorbing) tracer. The RhWT was regarded as a slightly sorbing solute since the soils were expected to have organic matter contents of less than 2%, resulting in a minor amount of Rhodamine WT sorption. Phosphorus (highly sorbing) concentrations were used to represent poultry litter application rates. Observation wells were installed with a Geoprobe Systems drilling machine (6200 TMP, Kejr, Inc., Salina, KS), and low flow sampling with a peristaltic pump was used to collect water samples from the top of the water table. Two wells were selected to create a representative sample for the purposes of modeling (Figure 3).

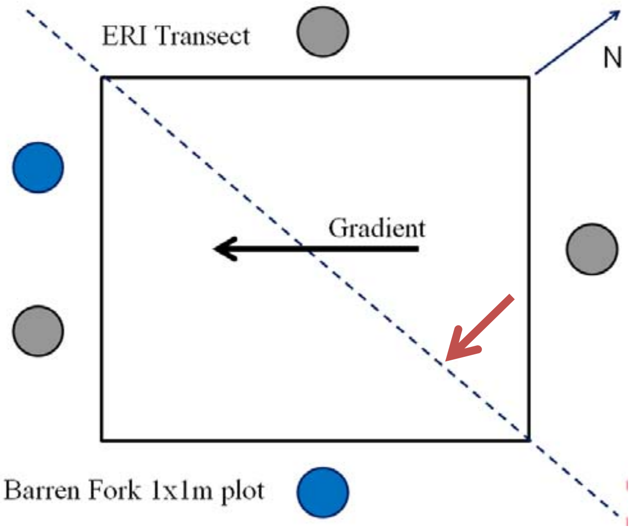

Figure 3. Overhead view of the shallow gravel 1 m by 1 m test plot. Circles indicate observation wells, with wells in blue indicating those selected for modeling calibration. The red arrow indicates the position of a high conductivity gravel bed.

Vadose Zone Flow and Transport Modeling

Chloride fate and transport was modeled using the HYDRUS 3-D software. HYDRUS 3-D is a software package that utilizes numerical methods to solve the Richards equation for water flow and solute transport equations to solve movement of heat and contaminants in subsurface systems (Šejna, 2011). HYDRUS 3-D is capable of solving water and solute movement in variably saturated media, and is adaptable to varying levels of heterogeneity. HYDRUS-3D can simulate both small- and large-scale water and contaminant transport through unsaturated and saturated soils (Akay and Fox, 2007; Akay et al., 2008).

HYDRUS was set up to model the shallow gravel 1 m by 1 m infiltration plot (June 30, 2011) at the Barren Fork

Creek site (Heeren, 2012). A two-dimensional model was developed using the concentration data from the infiltration experiment and hydraulic conductivity data derived from Miller (2012) for the gravelly subsoil. Values for gravel hydraulic conductivity ranged between 1900 cm hr $^{-1}$ and 66000 cm hr^{-1}. The effective saturated hydraulic conductivity (K_{eff}), calculated to be 9.6 cm hr^{-1} based on the plot scale infiltration experiments, was used for the upper silt loam soil layer. A finite element (FE) mesh was developed and was fitted with a media material distribution (Figure 4). The material distribution for each region has an average hydraulic conductivity value that gives a good representation of the region and allows for the model to operate more smoothly during computations. The FE mesh density is also tailored to allow for optimum computation time and sensitivity of the model. The system was discretized into 775 27 cm x 17 cm rectangular units; each unit is composed of two triangular units.

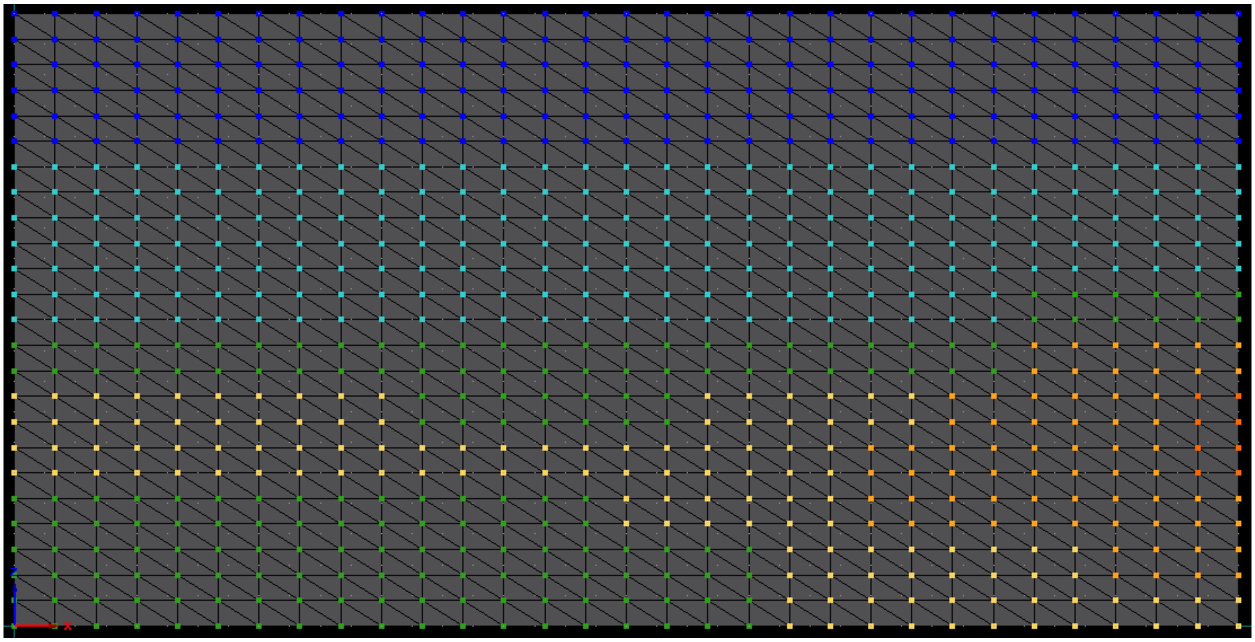

Figure 4. Vertical FE Mesh overlain with media material distribution. Dark blue indicates a silt loam soil. Other colors indicate gravels of increasing conductivity, with light blue being less conductive and red being highly conductive. Orientation of the profile is from SW (left) to NE (right). The y-axis is 5 m, from bedrock at the bottom to the soil surface at the top. The infiltration gallery is located at the top center. The initial water table is 1 m from the bottom.

The model also features a mobile-immobile component (Šimůnek and van Genuchten, 2008). Mobile-immobile (MIM) models adapt the porous media to allow for some pores to be closed off to water and/or solute transport (Figure 5). This distinction can yield different results in a system, such as higher pore velocities or reduced solute concentrations in observation wells. For this model, immobile pores were designated as being closed to water flow, but open to solute transport through diffusion. After initial parameters were input, the model was calibrated. The θ_{im} (cm^3 mobile pore space cm^{-3} total soil volume), the immobile porosity, and ω (hr^{-1}), the solute transport rate between mobile and immobile pores, were optimized by iteratively by changing values and examining the resultant concentration breakthrough curves.

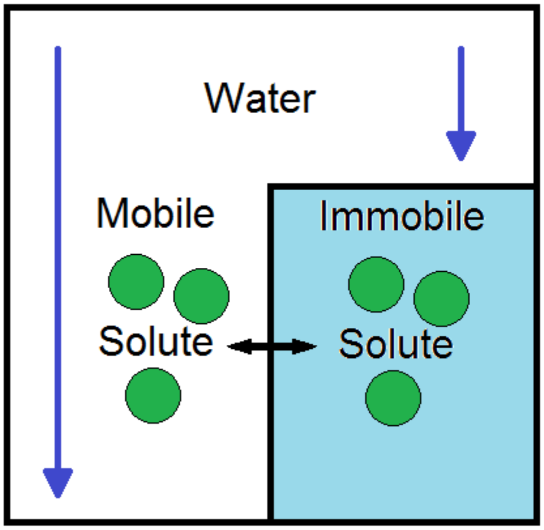

Figure 5. The mobile-immobile model. This cartoon illustrates a case where water flow is restricted to only a fraction of the pore space, but is open to diffusive solute transfer between the mobile and immobile phases.

Results and Discussion

Calibration was performed for three scenarios. The first scenario used the concentration breakthrough curve at the bottom of the observation wells. The modeled concentration breakthrough curves were compared to observed data (Figure 6a). The model predicted the concentration with an $R^2 = 0.68$ and an RMSE = 0.519.Research from others at this site (Correll et al., 2013) suggests the possibility of a confining gravel layer which may have caused lateral flow in the silt loam layer to the wells, then vertical flow down the borehole annulus to the water table where samples were collected. Therefore, a second scenario tested the plume response where the silt loam layer meets the gravel layers (Figure 6b). Calibrated values were adjusted to show the plume response under these conditions. The model predicted the concentration with an $R^2 = 0.61$ and an RMSE = 0.73. A control scenario tested the plume response given no MIM interaction (Figure 6c). The model predicted the concentration with an $R^2 = 0.47$ and an RMSE = 0.974. Table 1 lists the calibrated parameters for each scenario.

Table 1. Calibrated parameters for three test scenarios.

	Silt Loam θ_{im} (cm^3 cm^{-3})	Silt Loam ω (hr $^{-1}$)	Gravel θ_{im} (cm^3 cm^{-3})	Gravel ω (hr $^{-1}$)	R^2	RMSE
MIM (no confining gravel layer)	0.3	0.07	0.2	0.05	0.68	0.519
MIM (confining gravel layer)	0.2	0.1	0.2	0.1	0.61	0.731
No MIM	0	0	0	0	0.47	0.974

The calibrated HYDRUS model reasonably matched conditions found experimentally by Heeren (2012) when simulating conditions at the water table with MIM phases (Figure 6a). Concentration response was reduced in the early stages of the trial, but closely matched the observed data as the trial progressed. The confining gravel layer trial had a lower accuracy of prediction than the first trial. While the model closely predicted the steep concentration increase seen in the observed data, it overestimated the concentration in the later stages of the trial (Figure 6b). The accuracy of the model was reduced even further when the MIM phases were removed. In this trial, the model failed to predict both the initial concentration increase and the later concentration trends (Figure 6c). Oscillations in the data are due to numerical dispersion. Numerical dispersion is instability in the model created by mesh characteristics or equation results near boundaries.

The results of the model suggest several important conclusions. First, the model experiences higher levels of accuracy when comparing predicted curves to observed data at the water table. While this does not disprove the presence of a confining gravel layer suggested by others (Correll et al., 2013), it does give credence to the idea that contaminants will be removed quickly from the system by way of highly conductive gravel layers. This matches predictions and findings from Heeren (2012) and Fox et al. (2011). Second, the model certainly emphasizes the importance of MIM phases. Mobile-immobile phases explain several phenomena in the observed data. The presence of pores closed to water flow increases the average pore velocity in the system, which in turn allows for water and dissolved solutes to travel through the system faster. Also, the exchange of solutes between the mobile and immobile phases explains how the concentration can remain low when compared to the input concentration into the system. The better fit of the MIM simulations to the field data is consistent with Gao et al. (2009), who found the MIM approach to better characterize laboratory soil column data than the convective dispersion equation alone. The implications of the MIM model are that phosphorus-laden water will move through the soil profile more quickly than expected, but a significant portion of that phosphorus will be left behind in immobile pore spaces. Finite-element modeling is capable of modeling complex subsurface systems. While less sophisticated models would be unable to handle the extreme variability in media properties that are common to the Ozark ecoregion, finite element modeling breaks the modeling process into small enough regions that these conditions can be modeled.

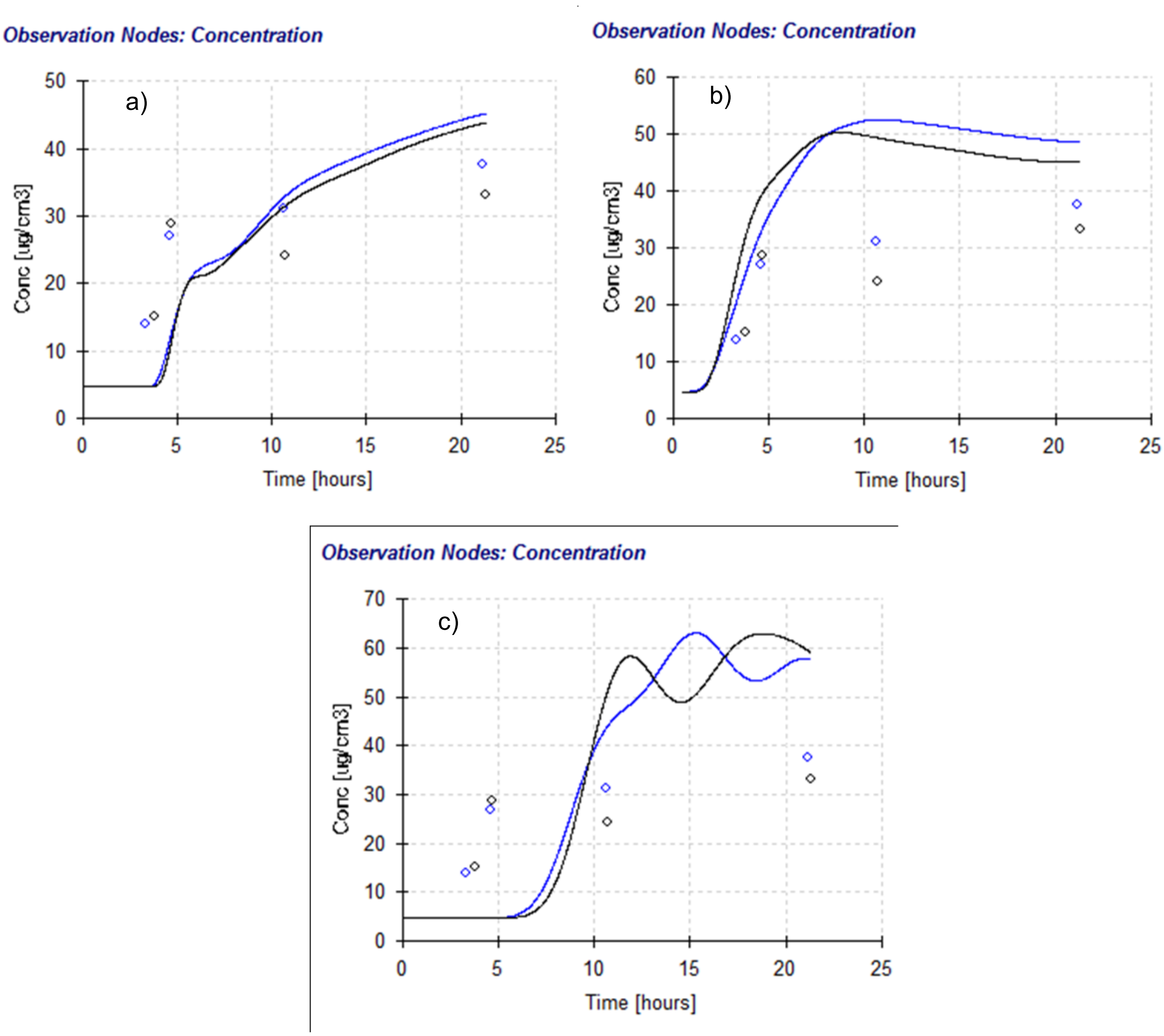

Figure 6. Concentration response curves for wells at the water table with MIM phases (a), seepage down the well column from the confining gravel layer with MIM phases (b), and for wells at the water table with no MIM phases (c). Solid lines indicate concentration breakthrough curves predicted by the model; dots indicate observed data.

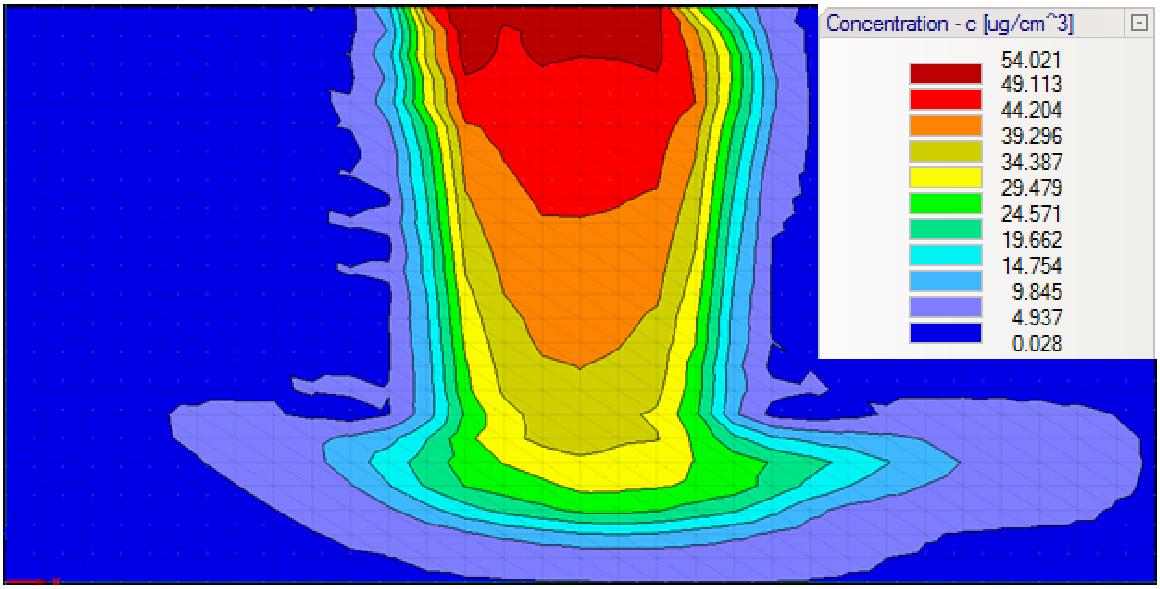

Figure 7. Chloride plume calculated by HYDRUS 3D. Note the fingering on the side of the plume due to numerical dispersion.

Future Work

Additional work needs to be performed to adapt the findings of this paper to long-term simulations of phosphorus transport. The next step is to calibrate the model for phosphorus sorption and transport parameters using the θ_{im} and ω parameters found in this work. Once phosphorus transport parameters have been established, long-term simulation can be conducted to determine fate and transport of phosphorus and other potential contaminants from the Barren Fork site.

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