Technical Basis for Contaminated Pore-Water Extraction from the Vadose Zone – 14052

Michael Truex * and Mart Oostrom *
* Pacific Northwest National Laboratory

ABSTRACT
Pore-water extraction offers the potential to remove a portion of the contaminated water from the vadose zone, which may be beneficial in reducing the flux of vadose zone contaminants to the groundwater. Laboratory and numerical modeling investigations have been conducted demonstrating the ability to induce pore-water extraction from unsaturated sediments. These efforts have led to plans for a field test of the process. Design simulations were used to evaluate operational parameters for pore-water extraction based on the expected range of test site characteristics. Simulations results show that initial water saturation, hydraulic conductivity, and sediment retention parameters have a significant effect on pore-water extraction performance.

INTRODUCTION
Pore-water extraction from the vadose zone is removal of water from unsaturated hydraulic conditions by means of applying suction (vacuum) at a well. Extraction of pore water is in response to the applied pressure gradient, but is limited by the capillary forces in the porous media. Thus, pore-water extraction can only occur when moisture content in the soil is above a threshold that is a function of the soil hydraulic properties (Truex et al. 2013). Multiple laboratory efforts have demonstrated the ability to extract water from some types of unsaturated soil under specific operational conditions of applied gas-phase vacuum (Oostrom et al. 2011; Truex et al. 2013).

Elevated moisture conditions corresponding to the range for which pore-water extraction was successful in the laboratory have been observed in the vadose zone beneath some of the former waste disposal locations at the U.S. Department of Energy (DOE) Hanford Site, especially in higher silt content layers. A proof-of-principle field test of pore-water extraction is being performed by Washington River Protection Solutions for the DOE, Office of River Protection at a test site near the Hanford Site's 241-SX Tank Farm. The test is using the application of negative pressure (vacuum) via soil-gas extraction at a well to induce coincident pore-water extraction. The test design is centered on using tank-farm-deployable, small-diameter, direct-push drilling techniques for well placement.

To support design of this test, numerical simulations were conducted to help define equipment and operational parameters, as described in detail by Truex and Oostrom (2013) and summarized herein. The modeling effort builds from information collected in laboratory studies and from field characterization information collected at the test site. Numerical simulations were used to evaluate pore-water extraction performance as a function of the test site properties and for the type of extraction well configuration that can be constructed using the direct-push installation technique. The output of the simulations included rates of water and soil-gas extraction as a function of operational conditions for use in supporting field equipment design. The simulations also investigated the impact of subsurface heterogeneities in sediment properties and moisture distribution on pore-water extraction performance.

METHODS

Numerical modeling was used as an evaluation tool for scale-up, including simulations to assess the impact of heterogeneities and the extraction well configuration on pore-water extraction performance for targeted field applications at the test site near the Hanford Site's 241-SX Tank Farm. A generalized depiction of the stratigraphic units in the vadose zone at this site is shown in Figure 1. The targeted zone for pore-water extraction, with elevated moisture and contaminant concentration, is the 10-m-thick Cold Creek Unit silt (CCUz) layer. Simulations included three-dimensional configurations with appropriate variations in porous media properties and heterogeneities and with imposed vacuum/pressure conditions for selected scenarios.

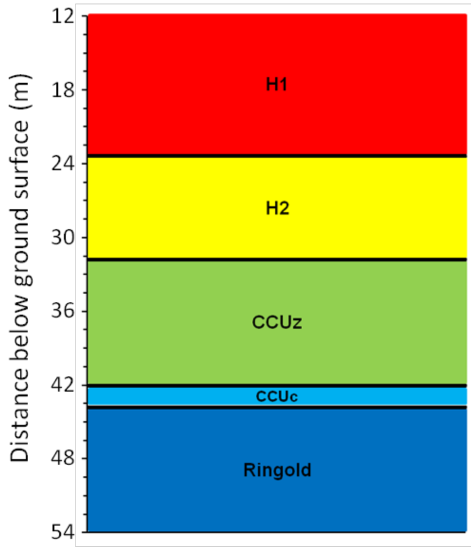

Figure 1. Stratigraphic units in the vadose zone at the test site. H1 and H2 are sand- and gravel-dominated zones. The CCUz is a silt zone with varying amounts of fine sand across the thickness of the zone. The CCUc is a silt zone but with a high degree of calcareous deposits and cementation. The Ringold zone is another sand- and gravel-dominated zone.

Simulations were conducted to evaluate pore-water extraction under conditions relevant to the SX Tank Farm test site. In the simulations, the CCUz layer was assumed to be either 1) homogeneous or 2) heterogeneous with a single 0.3-m (1-ft)-thick high-conductivity sand layer (at various locations with respect to the screen interval) in an otherwise homogeneous zone. The hydraulic properties of the sand porous medium in Carsel and Parrish (1988) were assigned to the high conductivity layer in the CCUz (Table 2). Although it is not likely that a layer with these hydraulic properties will be present in the CCUz at the SX Tank Farm site, lower soil moisture content zones in the CCUz may contain more sand and may have hydraulic properties similar to those for the hypothetical sand layer. A description of the simulation sensitivities is presented in Table 1. The hydraulic sediment properties used in the simulations are listed in Table 2. The Base Case computational domain for this set of simulations is based on the stratigraphy shown in Figure 1. The two-dimensional cylindrical domain (45 degrees) extends from the surface to the water table and consists of five layers (H1, H2, CCUz, CCUc, and Ringold). The reader is referred to Truex et al. (2013) for a justification for this computation domain and descriptions of the hydraulic layers. The well diameter was assumed to be 2.54 cm (1 in.). The domain was discretized in 5-cm × 5-cm grid cells in the *x* and *z* directions except for the first meter adjacent to the boundary nearest the extraction well ($x = 0$), where the cells were 2.5 cm × 2.5 cm. The simulations consisted of two parts. In the first part, a steady-state system with a constant recharge rate was established. In the second part, a gas-phase vacuum of 2 m H_2O (2.8 psi) was imposed over a 0.3-m (1-ft) screen length ranging from 37.5 to 37.8 m below ground surface (bgs) for a simulation period of 3 months. For each simulation, water and gas extraction rates were computed as a function of time.

Table 1. Overview of simulations using the layered system depicted in Figure 1. The hydraulic parameters of the Base Case simulation are listed in Table 2. For the Base Case, the near-well aqueous saturation (*S*) equals 0.8. The hydraulic properties for the simulations with the sand layers are taken from Carsel and Parrish (1988; Table 2). A base-case vacuum of 2 m H_2O (2.8 psi) is imposed over a 0.3-m (1-ft) zone ranging from 37.5 to 37.8 m bgs.

Simulation Name	Modification with Respect to Base Simulation
Base Case	—
High *S*	Average near-well *S* = 0.9
Low *S*	Average near-well *S* = 0.7
3-m Vacuum	Well vacuum: 3 m H_2O
High K_{sat}	Base Case K_{sat} CCUz × 10
Low K_{sat}	Base Case K_{sat} CCUz / 10
High van Genuchten *n*	Base Case CCUz *n* + 1
Low van Genuchten *n*	Base Case CCUz *n* - 1
High van Genuchten α (1/cm)	Base Case CCUz α × 2
High van Genuchten α (1/cm)	Base Case CCUz α / 2
Sand Layer 1	Sand layer between 37.5 and 37.8 m bgs
Sand Layer 2	Sand layer between 37.35 and 37.65 m bgs
Sand Layer 3	Sand layer between 37.27 and 37.57 m bgs
Sand Layer 4	Sand layer between 37.2 and 37.5 m bgs
Sand Layer 5	Sand layer between 37.58 and 37.73 m bgs
Compacted Zone 1	K_{sat} of 5 cm adjacent to well is 0.1 × Base Case K_{sat} CCUz
Compacted Zone 2	K_{sat} of 5 cm adjacent to well is 0.01 × Base Case K_{sat} CCUz

Table 2. Hydraulic properties of the sediments used in the simulations. The values for the H2 unit and CCUz are the averages of the experimental data reported by Truex et al. (2013, Table 9). The values for the other sediments were obtained from Last et al. (2006). The Carsel and Parrish Sand was used in the Sand Layer simulations listed in Table 1.

Sediment Mixture	van Genuchten α (1/cm)	van Genuchten *n*	Residual Saturation (m^3_{liquid}/ $m^3_{pore\ space}$)	Hydraulic Conductivity, K_{sat} (cm/s)	Porosity (–)
H1	1.00×10^{-2}	2.177	0.118	3.67×10^{-5}	0.356
H2	7.87×10^{-3}	2.372	0.121	8.19×10^{-4}	0.393
CCUz	6.30×10^{-3}	2.172	0.086	1.29×10^{-3}	0.389
CCUc	1.80×10^{-2}	1.727	0.214	5.04×10^{-4}	0.306
Ringold	1.32×10^{-2}	1.753	0.334	1.06×10^{-4}	0.297
Carsel and Parrish Sand	1.45×10^{-1}	2.680	0.105	8.25×10^{-3}	0.430

RESULTS

The water and gas extraction rates after 90 days of water extraction, as well as the time when water is first being produced, are reported in Table 3 for all of the simulations listed in Table 1. The water-extraction rates range from 0 L/day for the Sand Layer 1 simulation to approximately 165 L/day for the High K_{sat} simulation. All simulations showed gas extraction; values ranged from 0.28 L/min (0.01 ft^3/min) for the Compacted Zone 1 simulation, to about 2200 L/min (78 ft^3/min) for the Sand Layer 1 simulation. Tables and figure show gas extraction in ft^3/min to correspond to typical equipment specification units. Most of the simulations demonstrate water extraction shortly (<0.1 day) after the vacuum was imposed in the well.

Table 3. Water and gas extraction rates after 90 days of vacuum extraction and arrival time of water at the extraction well for the simulations listed in Table 1.

Simulation Name	Water Extraction Rate (L/day)	Gas Extraction Rate (ft^3/min)	First Water Extraction (days)
Base	14.75	0.38	<0.1
High *S*	39.38	0.31	<0.1
Low *S*	1.33	0.44	6.8
3-m Vacuum	50.50	0.67	<0.1
High K_{sat}	165.01	3.67	<0.1
Low K_{sat}	1.03	0.39	<0.1
High van Genuchten *n*	32.99	0.29	<0.1
Low van Genuchten *n*	3.77	0.39	<0.1
High van Genuchten α (1/cm)	2.71	0.72	<0.1
Low van Genuchten α (1/cm)	41.72	0.15	<0.1
Sand Layer 1	0	78.14	>90
Sand Layer 2	3.34	64.73	7.2
Sand Layer 3	4.96	48.02	1.4
Sand Layer 4	11.86	0.87	<0.1
Sand Layer 5	2.51	39.12	19.4
Compacted Zone 1	2.82	0.09	<0.1
Compacted Zone 2	0.32	0.01	<0.1

As an example of the temporal and spatial responses to imposed vacuum, results for the Base Case simulations are shown in Figures 2 through 5. The gas extraction plots in Figures 2 and 3 indicate that gas extraction is fairly stable over time, with only a minor reduction during the first few days when water saturations increase in the near-well zone. Water extraction rates slowly increase to almost 15 L/day after 90 days of imposing the 2-m H_2O (2.8 psi) vacuum. For this case, it takes about 0.01 day before the near-well water saturation at the lowest part of the screen is high enough so that water can move into the borehole. Water saturations and velocities at the end of the simulation are shown in Figure 4 for a 1.5-m × 1.5-m (5-ft × 5-ft) area adjacent to the borehole. In this area, the water saturation ranged from 0.76 to 0.82, with higher values directly adjacent to the extraction screen. The water velocity vectors clearly demonstrate that below the well screen, no water is moving downward, meaning that for the conditions covered by this simulation, no potentially contaminated water is able to migrate below the zone of influence of the pore-water extraction zone. The gas pressure plot for this case (Figure 5) shows that the gas pressure increases from 2 m H_2O (2.8 psi) at the well to atmospheric conditions over a zone of approximately 3 m (10 ft).

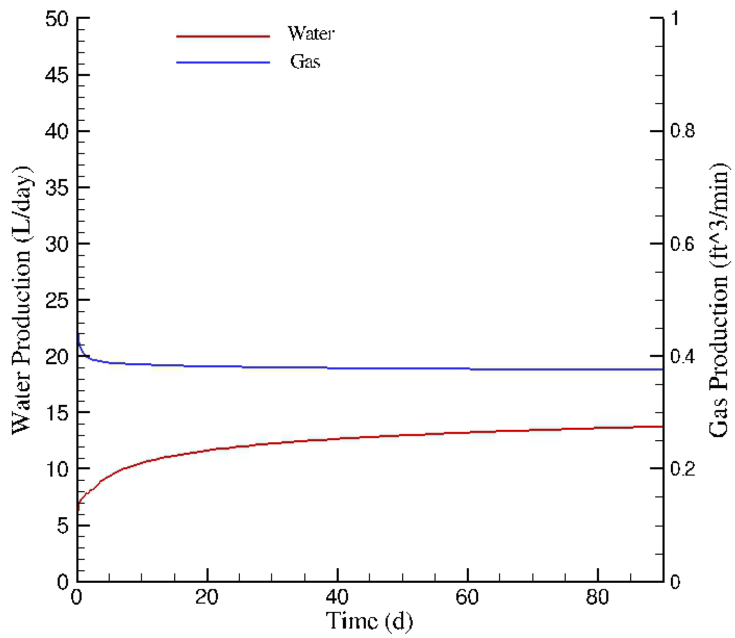

Figure 2. Water and gas extraction rates as a function of time for the Base Case simulation.

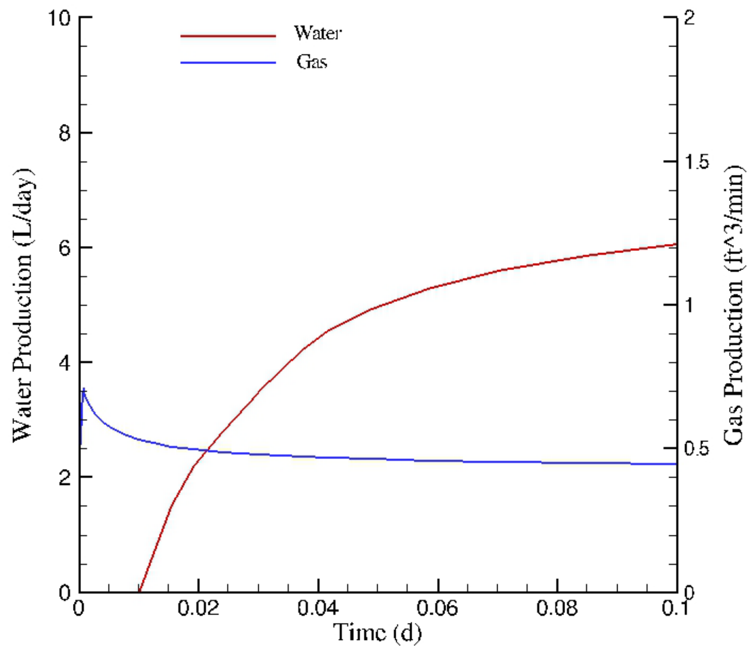

Figure 3. Water and gas extraction rates as a function of time for the Base Case simulation during the initial stages of the vacuum application.

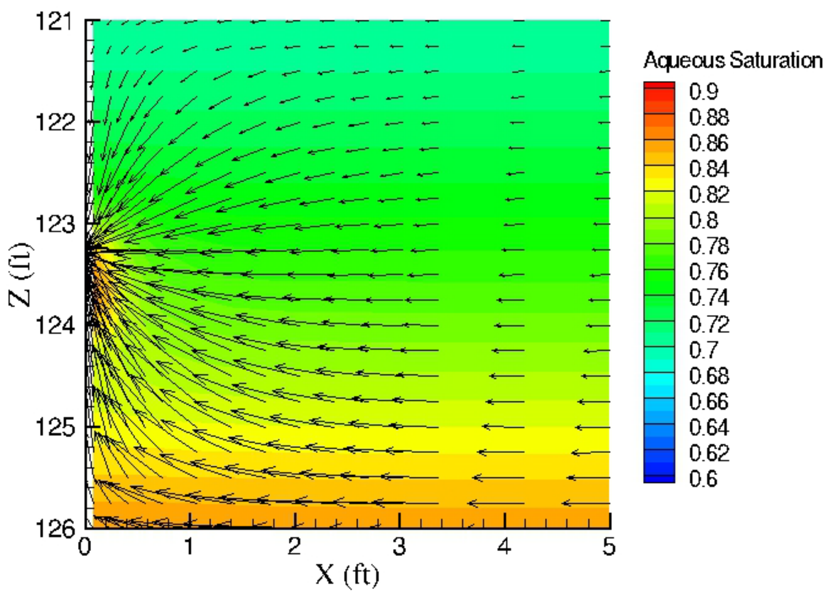

Figure 4. Near-well water saturations and velocities for the Base Case simulation during steady-state conditions.

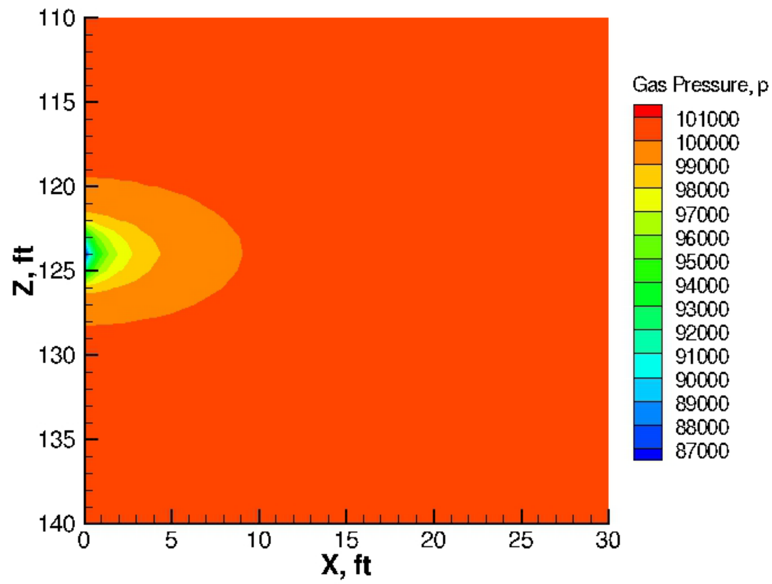

Figure 5. Gas pressures (Pa) for the Base Case simulation during steady-state conditions.

The High *S* simulation (Table 1), representing a higher initial saturation (0.9) than the Base Case, increases the water extraction by a factor of 3. The gas extraction rate, however, is only slightly lower than for the Base Case. Reducing the initial saturation to 0.7 (Low *S* simulation; Table 1) results in a tenfold decrease in water extraction with only a minor increase in the gas extraction rate. The results for the Base Case and the High *S* and Low *S* simulations show a high sensitivity of the water extraction rate to initial water saturation because the rate increases from about 1 L/day to around 40 L/day for a change in water saturation of only 0.2. Based on recent borehole data obtained at the site, such variations in water saturation are not uncommon in the targeted CCUz zone. The simulation data also suggest that below water saturations of 0.7, extraction rates will be very low. For each sediment type at a specified imposed vacuum, there is a water saturation at which the pore-water extraction rate becomes zero (Truex et al. 2013). In addition, simulation results show that a reduction of the initial saturation delays the arrival time of the first water in the extraction well (Table 1); almost 7 days are required for water to be produced for the Low *S* simulation compared to < 0.1 day for the Base Case and High S simulations.

The effects of hydraulic conductivity changes on extraction are nearly linear, with almost tenfold increases and decreases in rate, respectively, compared to the Base Case.

Arrival times of the first water in the extraction wells for both cases are relatively fast (<0.1 day). A two-order-ofmagnitude range in hydraulic conductivity is not uncommon for the site sediments. Thus, in addition to the initial water saturation, hydraulic conductivity is another sensitive parameter in relation to pore-water extraction.

Increasing the vacuum to 3 m H_2O (4.3 psi) leads to a simulated water extraction rate of more than 50 L/day and a doubling of the gas extraction rate. Although this might seem attractive at first glance, laboratory studies (Oostrom et al. 2011) have shown that maintaining good hydraulic contact between the well screen and sediments might be difficult for relatively high extraction vacuum values.

The influence of pore-geometry effects on extraction rates are shown to also be important. An increased uniformity (High van Genuchten *n* simulation; Table 1) yields considerably more water because the relative water permeability increases. The opposite effect causes a reduction in water extraction when the sediment pore-geometry is assumed to be less homogeneous. The range in tested pore-geometry values represents what can be expected for a CCUz sediment (Last et al. 2006). The van Genuchten α is an indication of the largest pore sizes for the sediment and $1/\alpha$ may be considered to be equivalent to the air-entry pressure. A reduction of the α increases the entry pressure and yields a more uniform water saturation around the average of 0.8, compared to the Base Case. As a result, the observed water extraction rate increases. The opposite is true for the higher α value. Based on the simulated results, both van Genuchten parameters (*n* and α) are considered to be sensitive parameters for water extraction. Both parameters have a much smaller influence on the gas extraction rates; their values are far less than 28.3 L/min (1 ft^3/min) for all considered cases.

The simulations Sand Layer 1 through Sand Layer 4 investigate the effect of the location of a horizontal 0.3-m-high (1-ft) permeability sand layer with respect to the extraction well screen. Although it is not likely that a layer with these specific hydraulic properties will be present in the CCUz at the SX Tank Farm site, lower soil moisture content zones intersecting the well’s screened interval may cause a similar impact on pore-water and gas extraction rates as observed in simulations with the hypothetical sand layer. However, the results of these simulations should be considered to yield conservative (low) pore-water extraction rates and conservative (high) gas extraction rates compared to expected actual conditions at the SX Tank Farm field test site. If the sand layer is directly adjacent to the screen, no water is produced during the simulation time. The gas extraction rate, on the other hand, approaches 2200 L/min (78 ft^3/min). When the location of this high-permeability zone is moved up compared to the screen location, the water extraction rate increases as a function of the contact area between the screen and the CCUz (Table 3). When the sand layer is fully above the screen (Sand Layer 4), the water extraction rate starts to approach the rate obtained for the Base Case. The trend in the gas extraction rates is opposite to what happens to the water rates. The data in Table 3 show that gas extraction rates are considerably higher than for the Base Case as long as some part of the screen is in direct contact with the high-permeability sand layer. Of interest also is the case in which the sand layer is 0.15-m (0.5-ft) thick located at the center of the extraction well screen ("Sand Layer 5" simulation, Table 1). For this case, the water extraction is close to what was obtained for the Sand Layer 2 simulation where the sand layer is 0.3-m (1-ft) thick but also contacts the screen over a 0.15 m (0.5 ft) length. However, the gas extraction rate is almost double for the Sand Layer 2 0.3-m (1-ft)-thick sand-layer simulation. The results for these five simulations show that the location and thickness of high-permeability zones might have a large effect on extraction rates. As long as such a layer is not in direct contact with the extraction screen, the effects on both water and gas extraction are relatively minimal. However, when the screen is completed directly adjacent to a high-permeability zone, the water extraction rates are expected to decrease rapidly with concurrent large increases in gas extraction rates.

The final two simulations listed in Table 1 considered the effects of compaction near the screen. Due to the nature of direct-push well installation, some compaction is expected, resulting in a zone around the well with a lower effective hydraulic conductivity. In the two compaction simulation scenarios, it was assumed that the hydraulic conductivity was reduced over a 5-cm zone adjacent to the screen. Both simulations show a considerable impact for this modification; water extraction rates were reduced by a factor of about 5 for the Compacted Zone 1 simulation (Table 1) and a factor of approximately 50 for the more compacted near-well zone in the Compacted Zone 2 simulation. Although water extraction was strongly reduced by compaction in both simulations, the rates did not reduce to negligible values. For both of these compacted zone simulations, gas extraction is much lower than for the Base Case.

CONCLUSIONS

A limited sensitivity analysis of hydraulic properties identified hydraulic conductivity and the van Genuchten parameters *n* and □ as having the most impact on pore-water extraction performance. Changes in hydraulic conductivity have a nearly linear correlation with water extraction rates. An increase in the pore geometry factor *n* or a decrease in the air entry pressure factor □ both resulted in considerably higher extraction rates, with limited effects on the gas extraction rates. All the investigated parameter value variations were within the ranges of potential values for the field test site, indicating that a wide range of possible water extraction rates may occur in the field test. Initial water saturation and presence of high permeability layers can also have a significant impact on pore-water extraction performance.

Of importance for equipment design and test operations, the gas extraction rates of most simulations yielded values of less than 28.3 L/min (1 ft^3/min). Values considerably higher than 28.3 L/min (1 ft^3/min) were obtained for simulation cases in which (part of) the well screen was located directly adjacent to a high-permeability zone. These high gas extraction rates correlate with low water extraction rates and delayed water arrival times at the extraction well. At the field test site, the combination of these observations (high gas extraction rate, low water extraction rate, delayed water arrival) is a strong indication that a high-permeability zone with low moisture content is negatively affecting the pore-water extraction performance.

Near-well compaction occurring during well installation will reduce both water and gas extraction rates but will not reduce these rates to zero. Field indicators of such conditions are relatively low water extraction rates in combination with low gas extraction rates. Based on testing within boreholes recently installed at the field test site, well development through surging and purging with relatively small volumes of water appears to have the ability to reduce near-well compaction effects and to improve pore-water extraction performance.

This modeling study provides estimates of pore-water extraction for a variety of potential conditions in the field. The study builds on the previous efforts to verify and quantify the pore-water extraction process (Oostrom et al. 2011; Truex et al. 2013). The modeling study results can be used to help guide equipment selection, operational strategies, and interpretation of the field test results. The following specific recommendations for the field test configuration are based on these modeling results.

- Vacuum monitoring locations will be most effective within 3 m (10 ft) of the extraction well.
- Test equipment should accommodate pore-water extraction rates of up to tens of L/day, with associated gas extraction rates of between 2.8 and 56.6 L/min (0.1 and 2 ft^3/min) for the expected subsurface conditions at the field test site.
- To improve the pore-water extraction rate, extraction well screens should target high-moisture zones and avoid intersecting zones with low moisture content. With the observed variation in moisture content at the field test site, a well screen interval of 0.3 m (1 ft) is expected to enable effective targeting of a high moisture content zone.
- Well development efforts are recommended to loosen the compacted zone of sediment adjacent to the well bore at the screened interval and improve the permeability of this zone using the techniques previously tested in a site borehole.

REFERENCES

1. Carsel RF and RS Parrish. 1988 "Developing Joint Probability Distributions of Soil Water Retention Characteristics." *Water Resources Research* 24(5):755–769.

2. Last GV, EJ Freeman, KJ Cantrell, MJ Fayer, GW Gee, WE Nichols, BN Bjornstad, and DG Horton. 2006. *Vadose Zone Hydrogeology Data Package for Hanford Assessments*. PNNL-14702, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

3. Oostrom M, VL Freedman, TW Wietsma, and MJ Truex. 2011. *Pore-Water Extraction Intermediate-Scale Laboratory Experiments and Numerical Simulations*. PNNL-20507, Pacific Northwest National Laboratory, Richland, Washington.

4. Truex, M.J., M. Oostrom, T.W. Wietsma, G.V. Last, and D. Lanigan. 2013. Pore-Water Extraction Scale-Up Study for the SX Tank Farm. PNNL-21882, Pacific Northwest National Laboratory, Richland, WA.

5. Truex, M.J. and M. Oostrom. 2013. Field Test Design Simulations of Pore-Water Extraction for the SX Tank Farm. PNNL-22662, Pacific Northwest National Laboratory, Richland, WA.

6. White MD and M Oostrom. 2006. *STOMP: Subsurface Transport Over Multiple Phases, Version 4.0, User's Guide*. PNNL-15782, Pacific Northwest National Laboratory, Richland, Washington.

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