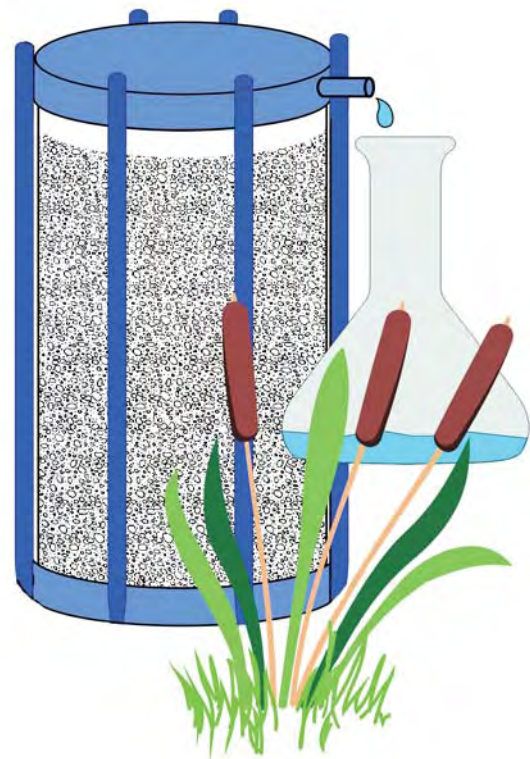# Dispersivity Testing of Zero-Valent Iron Treatment Cells: Monticello, Utah November 2005 Through February 2008

April 2008

**Prepared for
U.S. Department of Energy
Grand Junction, Colorado**

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Dispersivity Testing of Zero-Valent Iron Treatment Cells: Monticello, Utah, November 2005 Through February 2008

April 2008

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Executive Summary

A treatment cell containing a mixture of zero-valent iron (ZVI) and gravel was installed at the Monticello, Utah, project site in June 2005 to supplement a permeable reactive barrier (PRB). Monticello is one of the first remediation sites to use treatment cell technology. Because of the success at Monticello, other sites are considering use of treatment cells to address ground-water contamination.

The treatment cell is 6 feet in diameter and contains a 5-foot thickness of treatment media consisting of ZVI mixed with pea gravel. Contaminated ground water was pumped through the treatment cell from bottom to top at a flux generally between 4 and 5 gallons per minute (gpm). The treatment cell was used to remove uranium (U) from the contaminated ground water. A second treatment cell was installed April 4, 2007, to increase total treatment capacity to more than 10 gpm. The treatment cells have been effective in cleaning the ground water, as evidenced by effluent concentrations of U that are nearly always less than the ground-water standard of 44 micrograms per liter (μg/L). Influent U concentrations are generally between 300 and 400 μg/L. Replacement of reactive material is the most costly part of the operation and maintenance of the treatment cells.

It is likely that dispersion characteristics of the reactive material change over time due to mineral and gas buildup. It is hypothesized that increasing dispersion and preferential flow causes the contaminated ground water to have less contact time with the reactive material, leading to less efficient treatment. To investigate the importance of dispersion and preferential flow, tracer tests were conducted at various times during operation of the treatment cells. The results are now being used to design more efficient treatment cells that will further extend the lifetime of the treatment cells.

The tracer consisted of dissolved sodium bromide with a bromide (Br) concentration of 100 grams per liter. All tests were conducted at a flow rate of 4 gpm and the Br concentration of the injection ranged from about 179 to 229 milligrams per liter. The injection period was 2 hours and samples were collected for 4 hours after injection ceased. Samples of effluent water were collected at approximately 5-minute intervals and analyzed for Br by ion chromatography.

Because all tests were conducted at the same flow rate, the time lapse prior to the first arrival of the tracer in the effluent stream is a useful parameter in understanding the dispersion or preferential flow properties of the reactive material. First arrivals ranged from 0.30 to 1.30 hours and showed an inverse correlation with the length of time that the treatment cell had operated. The dispersivity of the reactive material was modeled using the geochemical code PHREEQC. Dispersivity values take more effort to calculate but provide two important advantages over first arrival data. One advantage is that tracer data from tests conducted at various flow rates can be compared using dispersivities, whereas first arrival data are only useful if the flow rate is constant among individual tests (as it was in all tests conducted for this study). A second advantage is that the dispersivity model takes into account the entire set of data for an individual test, including both the breakthrough and the recovery periods; whereas, first arrivals only use a small portion of the data. Dispersivities ranged from 0.1 to 0.7 m for this study.

The results of this study clearly indicate that the dispersivity of the reactive material increases steadily over the lifetime of a treatment cell. The increase in dispersivity represents one cause,

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possibly a main cause, of the reduction in efficiency for U treatment over long time periods. Despite very successful results of the initial treatment cells, the economics of the system may be improved if the dispersivity can be minimized. Minimizing dispersion could be as simple as choosing gravel with high porosity (spherical and equidimensional) and that contains minimal dust and other fine-grained material. The ZVI could be sieved to a narrower size fraction to reduce the fines. Sieving the ZVI would increase its cost, but because only a relatively small amount of ZVI is used, the cost advantage of extended life may compensate for it. Rigorous attention to the operation of the treatment cells may also improve efficiency. For example, if the flow rate is kept high, less calcium carbonate is deposited in the reactive material.

1.0   Introduction

A treatment cell (TC1) containing a mixture of zero-valent iron (ZVI) and gravel was installed at the U.S. Department of Energy (DOE) Office of Legacy Management Monticello, Utah, project site in June 2005 to supplement a permeable reactive barrier (PRB). Monticello is one of the first remediation sites to use treatment cell technology. Because of the success at Monticello, other sites are considering use of treatment cells to address ground-water contamination. The purpose of the study was to determine if aging of the treatment cells led to increased matrix dispersion that could decrease performance. To investigate the importance of dispersion and preferential flow, tracer tests were conducted at various times during operation of the treatment cells. The results were expected to lead to more efficient design that will extend the lifetime of the treatment cells. The project was funded by the U.S. Environmental Protection Agency Region 8 (EPA) through an Interagency Agreement between EPA and DOE. DOE subcontracted to S.M. Stoller through Task Order STO8-08.

The treatment cell is 6 feet (ft) in diameter and contains a 5-ft thickness of treatment media (Figure 1 and Figure 2). The treatment media consisted of 2 tons of ZVI mixed with 3/8-inch-diameter pea gravel. The bottom third of the media contained about 10 percent (by volume) ZVI, the middle third about 20 percent, and the upper third about 30 percent ZVI. Contaminated ground water was pumped through the treatment cell from bottom to top at a flux generally between 4 and 5 gallons per minute (gpm). The treatment cell was used to remove uranium (U) and other contaminants from the contaminated ground water. Details of the construction and as-built drawings are available in DOE (2005).

Figure 1. Photo of Instrument Vault and Treatment Cell TC1 Prior to Filling with Reactive Material. Water was pumped through the treatment cell from bottom to top.
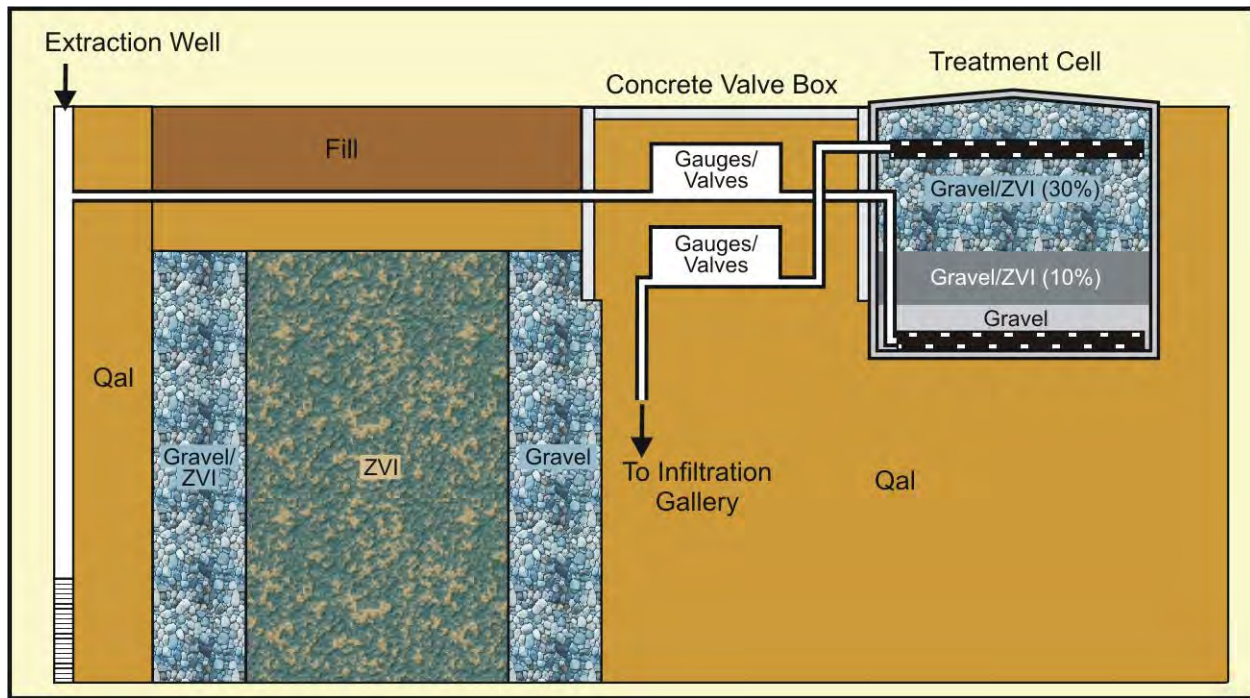
Figure 2. Cross-Section Through Extraction Well, PRB, and Treatment Cell (not to scale)

TC1 (Fill 1) was operated from June 2005 to April 4, 2007, after which the effluent U concentrations increased above ground-water MCLs and TC1 was refilled with fresh reactive material. A second treatment cell (TC2) was installed April 4, 2007, to increase total treatment capacity to more than 10 gpm. TC1 (Fill 2) and TC2 were filled with the same reactive material as TC1 (Fill 1). Although the intent was to have the same reactive material in all treatment cells, subtle (but perhaps important) differences likely occurred. An example of a possible difference is that the pea gravel used in TC1 (Fill 2) and TC2 appeared to be dustier than that used in TC1 (Fill 1).

The treatment cells have been very effective removing contaminants of concern from the ground water, as evidenced by effluent concentrations of U that are generally less than the ground-water standard of 44 micrograms per liter (µg/L) established in Title 40 *Code of Federal Regulators* Part 192 (Figure 3 and Figure 4). As a treatment cell ages, effluent U concentrations gradually increase, and the reactive material eventually has to be replaced. It is likely that dispersion characteristics of the reactive material change over time due to mineral and gas buildup. It is hypothesized that increasing dispersion and preferential flow causes the contaminated ground water to have less contact time with the reactive material, leading to less efficient treatment over time.

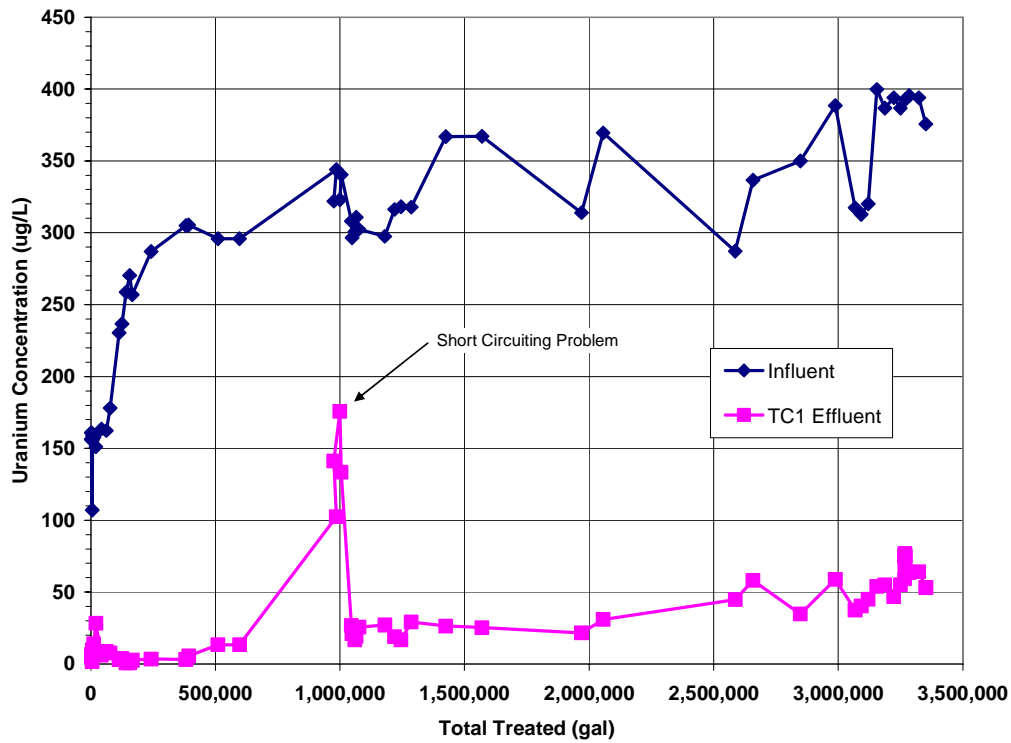*Figure 3. Uranium Concentrations in Treatment Cell TC1 (Fill 1). The increase in U concentration at about 1M gal, was caused by a short circuiting through a well screen within the reactive material; the short circuit was quickly repaired and the high treatment efficiency resumed.*
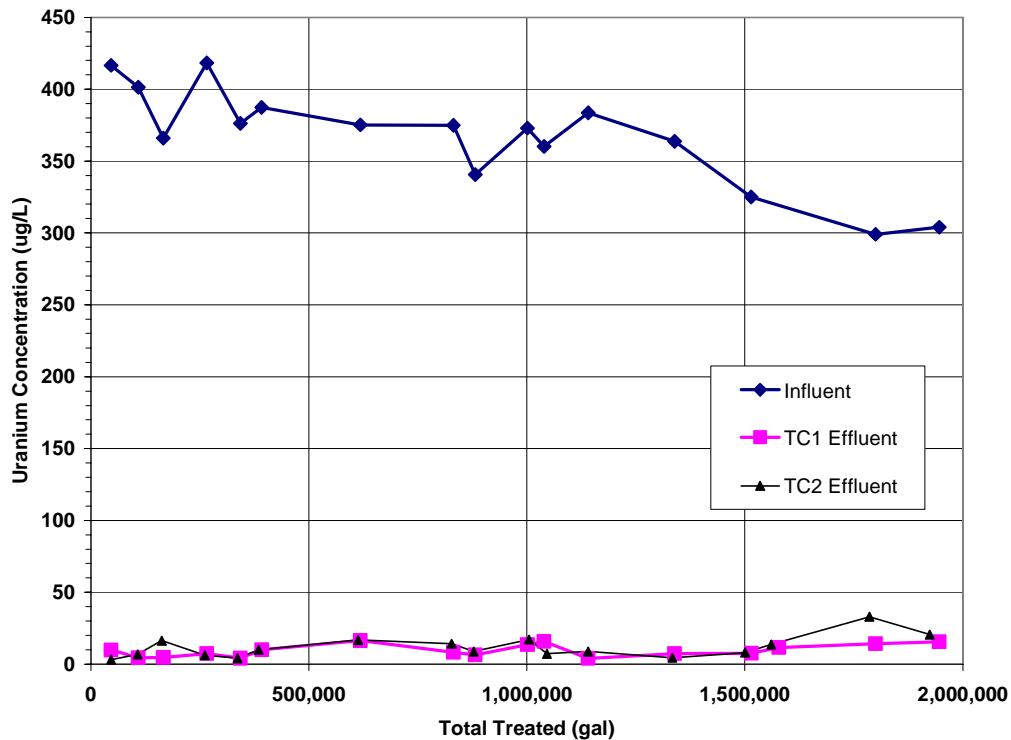

Figure 4. Uranium Concentrations in Treatment Cells TC1 (Fill 2) and TC2. These cells are still in operation.

An efficient treatment cell provides a long contact time between the contaminated water and the ZVI. Ideal "plug flow," or flow with minimal dispersion, produces the maximum contact time with reactive material. Preferential flow through reactive media accompanied by high dispersivity produces less contact time. Ideal plug flow is indicated by a sharp spike in effluent tracer concentration at a time corresponding to one pore volume. Preferential flow through fractures or high porous media dispersion causes the tracer to arrive earlier than it would for plug flow. Dispersion also causes tails on the concentration spike. More complicated breakthrough curves may result if the tracer flows through various-sized pores. Tracer tests conducted at various time intervals ranging from weeks to months were used to evaluate the changing dispersion in the treatment cells.

2.0 Methods

A series of tracer tests were conducted on the treatment cells. Three tests were conducted on TC1 from March 2006 through March 2007 during its operation with the initial reactive media. From April 2007 through February 2008, four tests were conducted on TC1 after it was refilled and four tests were conducted on TC2.

The tracer consisted of dissolved sodium bromide with a bromide (Br) concentration of 100 g/L. Food coloring was added to help visually observe the injection operation. A Milton Roy (Model LM A141) piston pump inside the valve vault was connected to the influent piping through a check valve to prevent backflow. The stroke and speed of the pump were each set at 60 to 70. These settings produced an injection rate of about 35 to 40 milliliters per minute (mL/min) yielding a Br concentration of about 200 milligrams per liter (mg/L) in the influent water flowing at 4 gpm. All tests were conducted at a flow rate of 4 gpm (plus or minus about 0.05 gpm). The tracer injection rate varied by as much as 10 percent between tests due to imprecision of the injection pump. Thus, the concentration of the injection among individual tests ranged from about 179 to 229 mg/L Br.

A 4-L slug of 100 g/L bromide tracer was injected over a period of 2 hours. Samples were collected for 4 hours after injection ceased. Samples of effluent water were collected at 5-minute intervals (10 minute intervals were used in early tests) for the 6-hour period. Samples were analyzed for Br in the Environmental Sciences Laboratory by ion chromatography (STO 210, procedure AP[Br-2]). Effluent samples were collected in 50-mL plastic vials at the outlet of the treatment cell.

For several of the early tests, concentrations of Br were monitored in the effluent piping in real time using a Cole Palmer solid state (Model C-27504-02) bromide ion selective electrode (ISE) connected to an Orion 520A millivolt meter following ESL procedure AP(Br-1) (STO 210). Data were collected every 20 seconds on a laptop computer using Orion's DataCollect software. The bromide ISE did not always accurately respond to the Br concentration and this method was discontinued. It is likely that the combination of fast-flowing water and accumulation of oxidized iron negatively affected the performance of the ISE.

Dispersion modeling was performed using the geochemical speciation code PHREEQC. The model domain consisted of a one-dimensional column divided into 20 cells, each 0.0762 meter (m) long for a total length of 1.52 m (5 ft). Molecular diffusion was ignored by setting the diffusion coefficient to a low value (10^{-5} m^2/s). Porosity was estimated at 0.5 from preliminary

model curves; however, because porosity was likely to change during operation of the treatment cells, models were run for porosity 0.25, 0.35, and 0.5. Only the 0.5 value provided a reasonable match to the data. At each porosity, models were run for dispersivities of 0.0001, 0.05, 0.1, 0.2, 0.5, and 0.7 m. The model was divided into two stages, injection and recovery. During the injection stage, Br concentration was set at 1 (normalized; unitless) and during recovery at 0. Water flow through the system was maintained at 4 gpm throughout the simulations. A sample input file (porosity 0.25, dispersivity 0.0001 m) is provided as Appendix A.

Effluent Br concentration data from each tracer test were plotted against time and normalized by dividing each value by the input concentration. The input concentration was estimated as the highest value measured during the test. Plots of normalized data were then compared visually by overlaying the modeled plots (Figure 5) on a light table. The model that produced the best fit was used to provide the porosity and dispersivity of the tracer test. While model curves did not exactly match the data, there was reasonable agreement in most cases. The progression of dispersion was matched better using the breakthrough portions of the curves (portion with increasing Br concentration) than using the recovery portion (portion showing decreasing Br concentrations). The small discrepancies in the recovery portions are probably due to small variations in the rate of injection caused by irregularities in the injection pump. For this reason, emphasis was placed on the breakthrough portion of the curves when matching data to models.

3.0   Results

Three sets of tracer tests were conducted: TC1 (Fill 1), TC1 (Fill 2), and TC2 (Table 1). Three tests were conducted on TC1 (Fill 1), and four tests each on TC1 (Fill 2) and TC2. Because all tests were conducted at the same flow rate (4 gpm), the time lapse prior to the first arrival of the tracer in the effluent stream is a useful parameter in understanding the dispersion or preferential flow properties of the reactive material (i.e. decreased arrival times may be indicative of decreased treatment cell performance). The first arrival time was defined as the time before the Br concentration increased to 2 percent of its influent concentration (i.e., a value of 0.02 on the normalized plots). Perfect plug flow would produce a first arrival at about 2 hours based on the 4 gpm flow rate and 500 gallon capacity. First arrivals ranged from 0.30 to 1.30 hours (Table 1).

In addition to first arrivals, changes in the dispersivity of the reactive material were calculated using PHREEQC. In all models, the porosity was assumed to be 0.5, because it provided the best fit to the tracer data. Dispersivity values take more effort to calculate but provide two important advantages over first arrival data. One advantage is that tracer data from tests conducted at various flow rates can be compared using dispersivities, whereas first arrival data are only useful if the flow rate is constant among individual tests (as it was in all tests conducted for this study). A second advantage is that the dispersivity model takes into account the entire set of data for an individual test, including both the breakthrough and the recovery periods; whereas, first arrivals only use a small portion of the data. Dispersivities ranged from 0.1 to 0.7 m for this study (Table 1).
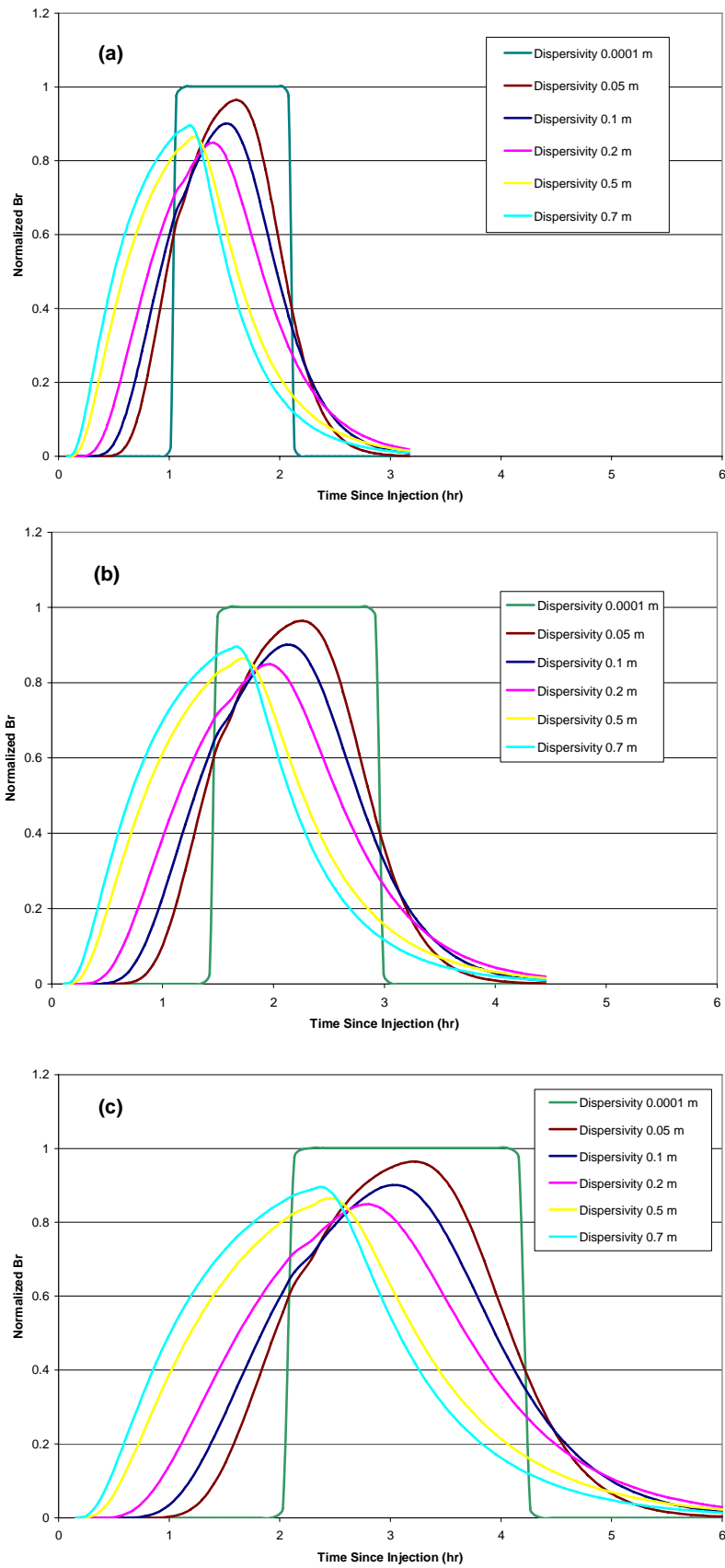
Figure 5. Modeled Bromide Tracer Tests for Varied Dispersivity and Porosity. Normalized to an input concentration of 1. Porosity (a) 0.25, (b) 0.35, and (c) 0.50.

Table 1. Details of Bromide Tracer Tests

Cell	Test Date	Time Since Fill (days)	Cum. Volume Treated (Mgal)	[a]First Arrival (h)	[b]Dispersivity (m)	Effluent U Conc. (µg/L)
TC1(Fill1)	Mar 23, 2006	275	1.22	0.55	0.3	19
TC1(Fill1)	Aug 30, 2006	435	2.22	0.40	0.6	35
TC1(Fill1)	Mar 9, 2007	626	3.27	0.30	0.7	72
TC1(Fill2)	Apr 18, 2007	14	0.10	1.10	0.1	4
TC1(Fill2)	July 25, 2007	112	0.88	0.95	0.2	6
TC1(Fill2)	Nov 27, 2007	237	1.58	0.50	0.5	12
TC1(Fill2)	Feb 15, 2008	317	1.94	0.45	0.45	16
TC2	Apr 19, 2007	15	0.10	1.30	0.1	7
TC2	July 26, 2007	113	0.88	1.10	0.2	9
TC2	Nov 28, 2007	238	1.56	0.40	0.7	14
TC2	Feb 16, 2008	318	1.92	0.45	0.45	21

[a]First arrival (normalized): first value exceeding 0.02 (i.e. 2% of influent concentration).
[b]Dispersivity estimated from PHREEQC modeling.

Tracer data for treatment cell TC1 (Fill 1) are shown in Figure 6. Tracer tests were not conducted for the early portion of the operation of TC1 (Fill 1); the first test was conducted after 275 days of operation. The injection pump operated at less than 75 percent of the desired value during the March 2007 test, resulting in a lower maximum Br concentration (Figure 6a). First arrivals for this set of tests ranged up to 0.55 hour and decreased to 0.30 hours as the reactive material aged (Table 1). The normalized plots show a progressive drift of the curves toward earlier arrival times, reflecting increasing dispersion (Figure 6b). Calculated dispersivities range from 0.3 to 0.7 m and the dispersivity values increased monotonically as the treatment cell aged. The effluent U concentration also increased monotonically as the treatment cell aged, suggesting a positive correlation with media dispersivity (Table 1). A decision was made to replace the media in TC1 (Fill 1) after effluent U concentrations increased to levels above the 44 µg/L treatment goal.
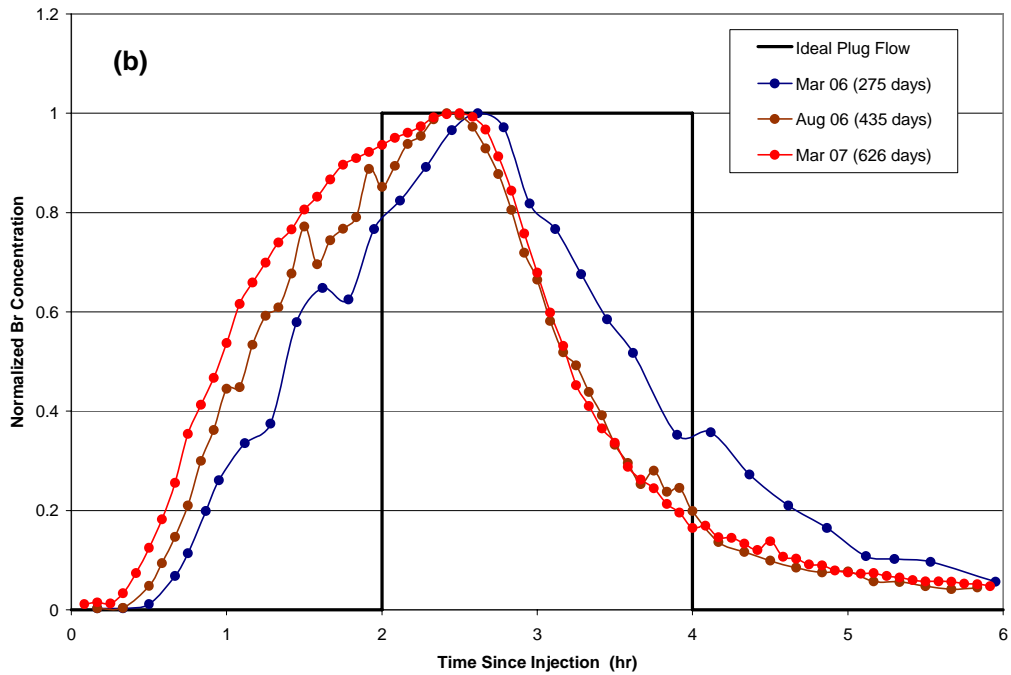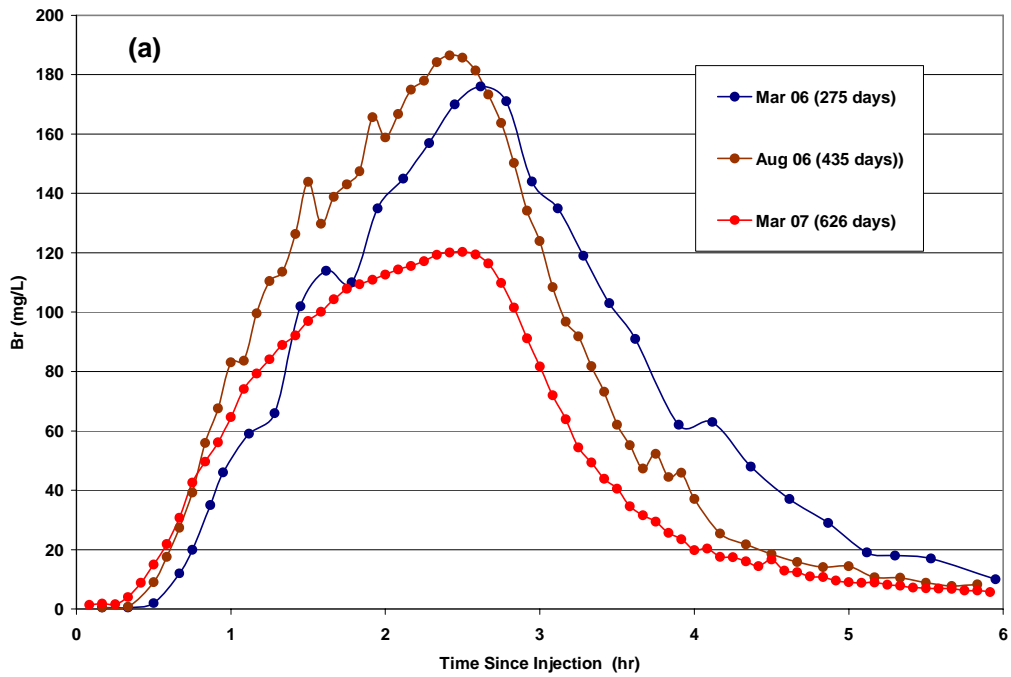
Figure 6. Data from Treatment Cell TC1 (Fill 1) (a) raw data, (b) normalized. Numbers in parentheses are the number of days the treatment cell operated prior to the tracer tests.

Tracer data for treatment cell TC1 (Fill 2) are depicted in Figure 7. First arrivals for this set of tests ranged up to 1.10 hours and decreased to 0.45 as the reactive material aged (Table 1). The normalized plots show a progressive drift of the curves toward earlier arrival times, reflecting increasing dispersion (Figure 7b). Calculated dispersivities range from 0.1 to 0.5 m, and the dispersivity values increased monotonically as the treatment cell aged. An exception is the data for November 2007, which had a slightly higher calculated dispersivity than the February 2008 data. Because of a malfunction with the injection pump, the November 2007 test data are suspect. Without the November 2007 curve, there is a systematic progression of the breakthrough curves toward earlier times, indicating increasing dispersion of the reactive material. Effluent U concentrations increased from 6 to 16 µg/L during the study period and showed a positive correlation with dispersivity (Table 1).

Tracer data for treatment cell TC2 are shown in Figure 8. First arrivals for this set of tests ranged up to 1.30 hours and decreased to 0.40 hours as the reactive material aged (Table 1). The normalized plots show a progressive drift of the curves toward earlier times, reflecting increasing dispersion (Figure 8b). An exception is the data for November 2007, which plotted far to the left of the other data. Because of a malfunction with the injection pump, the November 2007 test data are suspect and are disregarded in the ensuing discussion. Calculated dispersivities range from 0.1 to 0.45 m (omitting November 2007), and the dispersivity values increased monotonically as the treatment cell aged. There is a systematic progression of the breakthrough curves toward earlier times, indicating increasing dispersion of the reactive material. Effluent U concentrations increased from 7 to 21 µg/L during the study period and showed a positive correlation with dispersivity (Table 1). Treatment cells TC1 (Fill 2) and TC2 are still in operation (as of April 2008), and are still treating U to concentrations less than the 44 µg/L goal.

The first arrival and dispersivity data for each tracer test (with the exception of the suspect November 2007 tests) are plotted with the volume of water treated on Figure 9. The first arrival data show a negative correlation with volume treated. It appears that TC1 (Fill 1) has a more gradual slope than the other two, suggesting that dispersivity in TC1 (Fill 2) and TC2 are developing faster than it did in TC1 (Fill 1). This effect may be attributed to the dirtier gravel used in the latter two tests; however, because of the limited number of tests, the results of the three reactors may not be statistically different. The dispersivity values increase monotonically with volume treated and suggest a similar conclusion as derived from the first arrival data (Figure 9b).
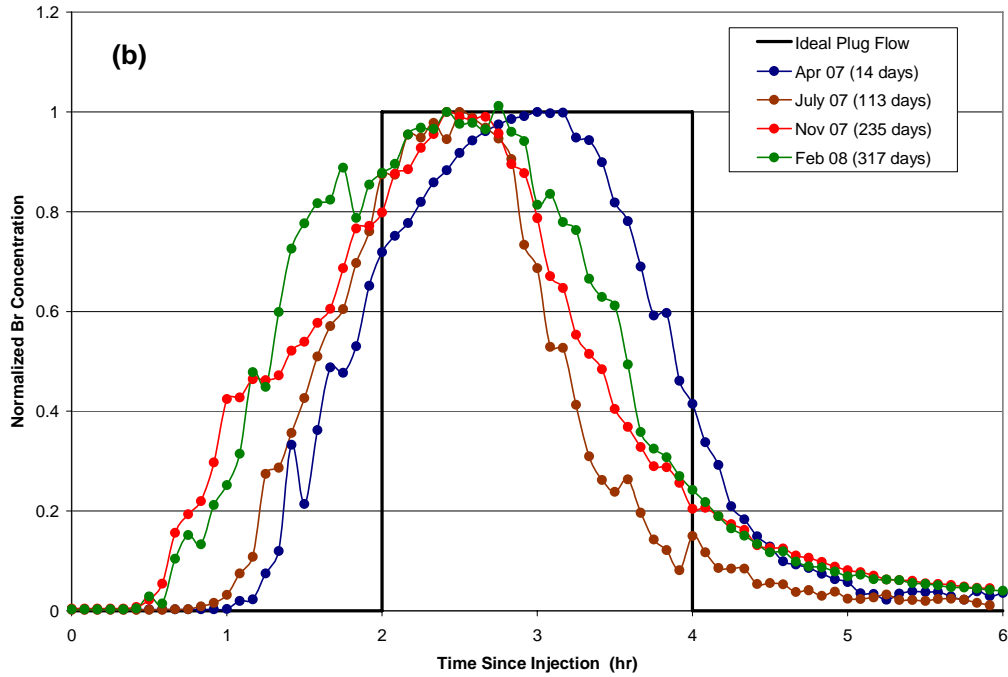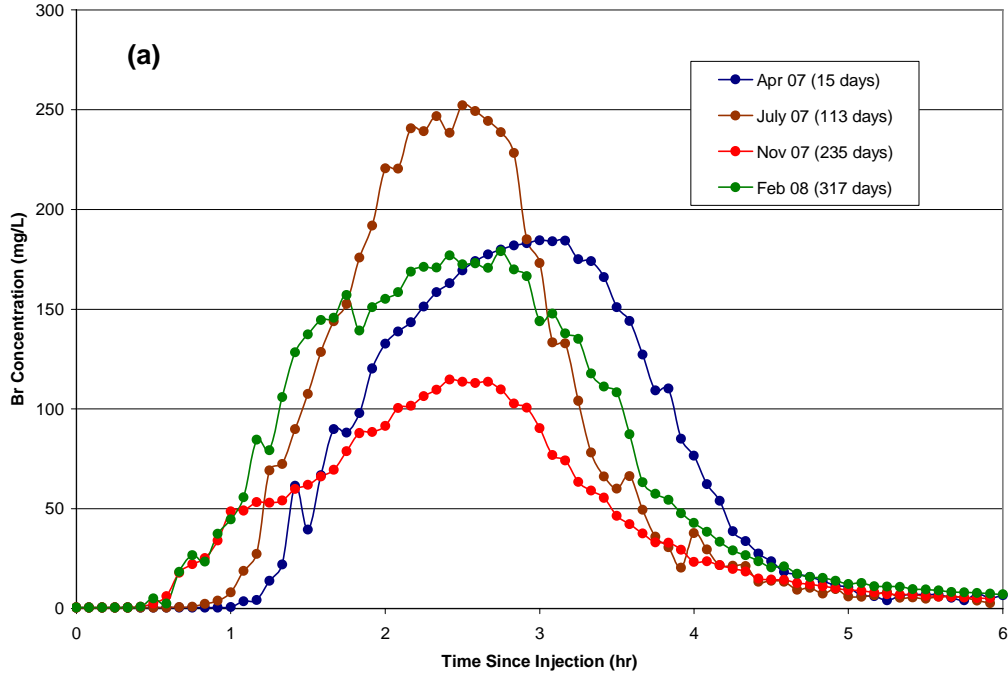
Figure 7. Data from Treatment Cell TC1 (Fill 2) (a) raw data, (b) normalized. Numbers in parentheses are the number of days the treatment cell operated prior to the tracer tests.
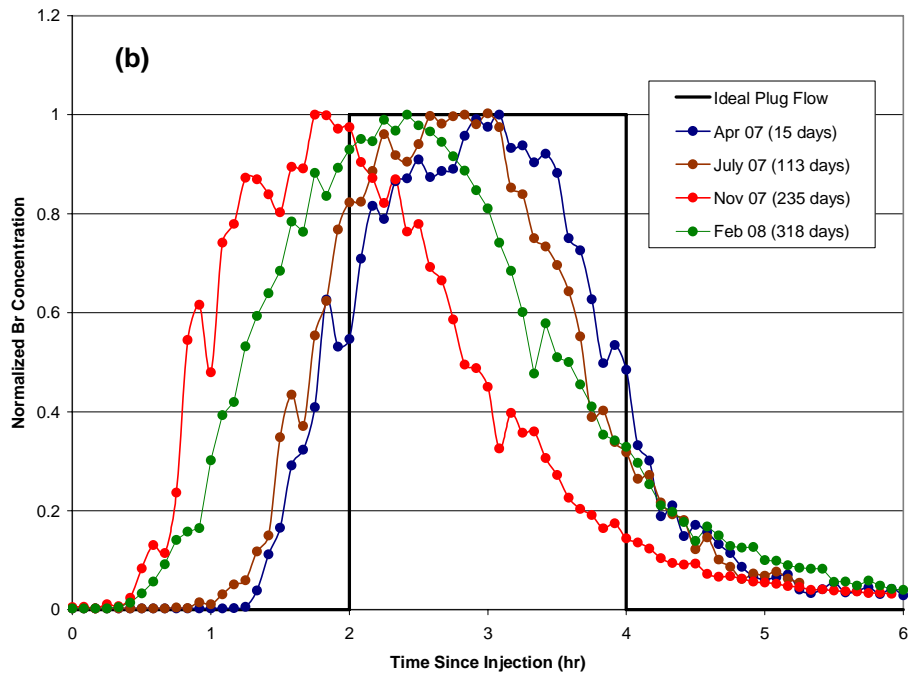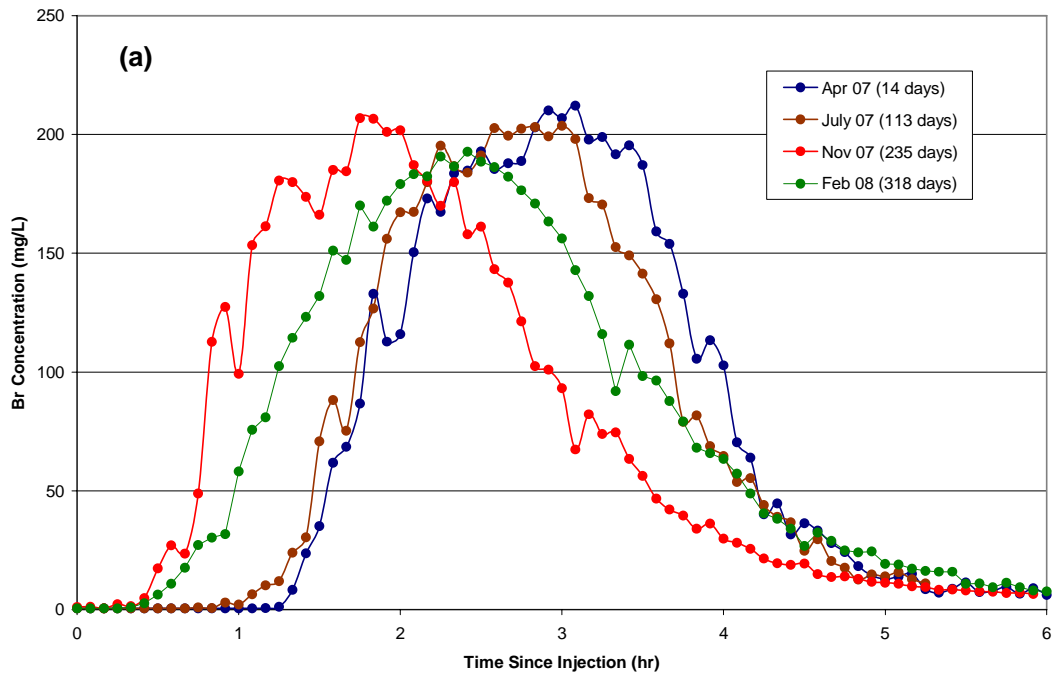
Figure 8. Data from Treatment Cell TC2 (a) Raw Data, (b) Normalized. Numbers in parentheses are the times the treatment cell operated prior to the tracer tests.
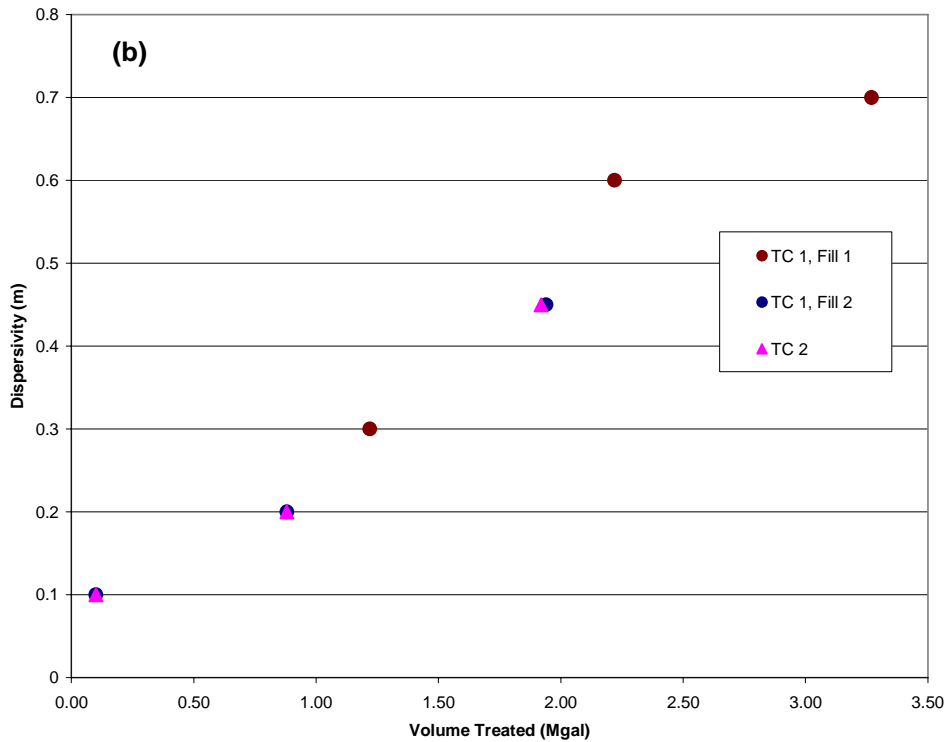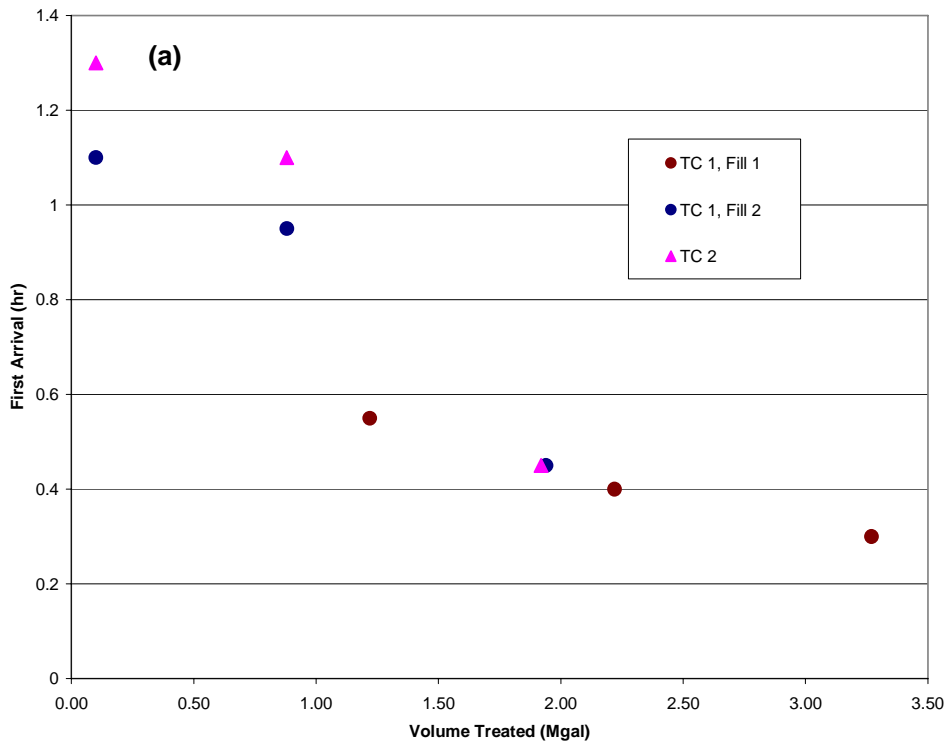
Figure 9. Summary Plots Showing Progression of Change in Reactive Material Properties as Treatment Progresses: (a) First Arrivals, (b) Dispersivities. Data from the November 2007 tests were omitted.

4.0   Conclusions and Recommendations

The ex-situ treatment cells at the Monticello site are efficiently and cost-effectively treating U. Preliminary estimates of treatment costs indicate that the treatment cells are much more cost-effective than the permeable reactive barrier (EPA 2006). Because of the success of the treatment cells, this study was undertaken to gain a better understanding of the dispersion, which could lead to improvements in the design of the reactive material.

The results of this study clearly indicate that the dispersivity of the reactive material increases steadily over the lifetime of a treatment cell. The increase in dispersivity represents one cause, possibly a main cause, of the reduction in efficiency for U treatment over long time periods. The results of the initial treatment cells indicate a successful treatment process; however, the efficiency of the system may be improved if the dispersivity can be minimized.

It is beyond the scope of this study to thoroughly evaluate the ways that the treatment cells could be improved, but a few preliminary thoughts are provided based on the premise that limiting development of dispersion will increase treatment cell efficiency. Improvements to reactive material could be as simple as choosing gravel with high porosity (spherical and equidimensional) and that contains minimal dust and other fine-grained material. The ZVI could be sieved to a narrower size fraction to reduce the fines. Sieving the ZVI would increase its cost, but because only a relatively small amount of ZVI is used, the advantage of extended life may compensate for the increased cost. Rigorous attention to the operation of the treatment cells may also improve efficiency. For example, if the flow rate is kept high, less calcium carbonate (a principal cause of plugging and dispersivety) will be deposited in the reactive material.

In addition to the relatively simple approaches of selecting gravel and ZVI, more aggressive approaches could be tested, such as the injection of chemical compounds into the influent stream. For example, chelating compounds may help keep iron in solution and reduce the amount of iron oxide that forms in the treatment cells. Although increased dissolved iron may be undesirable, the iron would likely precipitate in the aquifer as iron hydroxide, particularly if a biodegradable chelating compound was used. Commercial iron chelating compounds are available for this purpose that are currently being used to lessen iron oxide scaling in air-sparging systems. Chemical reductants, such as dithionite, could also be investigated as a means to lessen oxidation in the ZVI. These chemical additions would require laboratory testing prior to field testing. The environmental effects would need to be carefully considered, and biodegradable compounds should be favored.

It is recommended that tracer tests be continued during the search for improvements to the treatment cells. Results from this study indicated that first arrival data were nearly as informative as the dispersivity values in determining performance. First arrival data can be obtained at about one-third the cost because (1) the tests are shorter, reducing field time, (2) less analytical work is required, and (3) there is no need for modeling.

5.0   References

STO 210, continuously updated. *Environmental Sciences Laboratory Procedures Manual*, U.S. Department of Energy Office of Legacy Management, Grand Junction, Colorado.

DOE (U.S. Department of Energy), 2005. *Construction Summary and As-Built Report for Ground Water Treatment System Monticello, Utah, Permeable Reactive Barrier Site*, ESL-RPT-2005-05, U.S. Department of Energy Office of Legacy Management, Grand Junction, Colorado, Available at http://www.lm.doe.gov/land/esl_reports.htm.

EPA (U.S. Environmental Protection Agency), 2006. "Hydraulic Conductivity Loss at the Monticello PRB Leads to Trial Use of Ex-Situ Treatment Cell," *Technology News and Trends*, March 2006, U.S. Environmental Protection Agency, Washington, D.C.

Appendix A

Input File for PHREEQC Dispersion Models

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```
TITLE Model of dispersion in treatment cell to match Br tracer data.
#
#
#Use the graph output (grid tab) for transferring to Excel
#Use PHREEQC.DAT database
#Injection solution 0 Br=1 mg/L Normalized
#Injection Phase = 2.132 hours
#For porosity 0.50, 1 PV = 500 gallons, and residence time = 2.08 hr
#For porosity 0.35, 1 PV = 350 gallons, and residence time = 1.46 hr
#For porosity 0.25, 1 PV = 250 gallons, and residence time = 1.04 hr
#Dispersivity is varied
# ####Indicates variables that are changed for different simulations
SOLUTION 0 #Composition of injectate (after mixing with flow stream)
  units mg/l
  pH  7.0
  pe  13.0
  Br  1.0 # Influent Br with injection
  Na  0.29
SOLUTION 1-20 # Composition of water in cell prior to injection (initial
condition)
#Assume pure water (no Br) with high ORP and neutral pH. Only Br conc
matters.
  units mg/l
  pH  7.0
  pe  13.0
PRINT
     -reset            true
TRANSPORT
#Advection
  -cells 20 #number of cells in model
#Shifts controls how long the injection period is: for 20 shifts, the
injection period
# is: 2.08*20.5/20 (see USER_GRAPH below) = 2.132 hrs (injection phase)
     -shifts 20  #number of shifts, movement of fluid to next cell; time
steps
#     -time_step 144    #length of time step in sec; shifts*time_step=Total
time
#     -time_step 14.4   #length of time step in sec; shifts*time_step=Total
time
  -flow_d forward #Forward flow
  -boundary_conditions constant flux #BC for first and last cell
#Assume 10^-5 for diffusion coefficient. Won't affect results much as long as
it is low value.
  -diffusion_coefficient 1.0e-5     #diffusion coefs for each cell (m2/s)
#Length of cell based on total length of reactive material / number of cells
#For 5 ft (1.52 m) thick; length is 1.52/20=0.076 m
  -lengths 0.0762 #length of each cell in meters
#Dispersivity is varied to obtain best fits (values have been 0.35 to 0.6 m)
  -dispersivities 0.0001
 ####dispersivities in meters
     -correct_disp     #correction for column tests; see PHREEQE manual
#  -stagnant 1 6e-6 0.0 0.1   #Number of immobile cells associated with
mobile cells
  -punch   20
  -punch_frequency 1
  -print   20
  -print_frequency 20
save solution 1-20
```

```
USER_GRAPH
      -headings time(hr) Na Br
      -chart_title "Monticello Treatment Cell"
      -axis_titles "Time (hr)" "Effluent Concentration (mg/L)"
      -axis_scale x_axis 0 5 1
      -axis_scale y_axis 0 250 10
      -initial_solutions false
#      -plot_concentration_vs x
      -plot_concentration_vs t
      -start
#      10 GRAPH_X (STEP_NO + 0.5) / 20
# Multiplier 2.08 is travel time through the treatment cell in hours
# 500 gal/4 gpm = 2.08 (porosity = 0.5)
#### For porosity of 0.25, use 1.04 for travel time
#### 2.08 for porosity=0.5
#### 1.46 for porosity 0.35
      10 GRAPH_X 1.04*(STEP_NO + 0.5)/20

#      10 GRAPH_X DIST
#The following instruction convert Na and Br to mg/L for graph only
#Use the graph output (grid tab) for transfering to Excel
      20 GRAPH_Y TOT("Na")*23000, TOT("Br")*80000
      -end
PRINT
      -user_graph true
SELECTED_OUTPUT
  -file   Monticello_Br.sel
  -totals   Na Br
      -molalities Br-
END
#Recovery phase
SOLUTION 0
  units mg/l
  pH  7.0
  pe  13.0
PRINT
      -reset            true
TRANSPORT
#Advection
  -cells 20 #number of cells in model
#Shifts controls the time period for the recovery phase goes.
#Need to have it long enough to cover the recovery period.
      -shifts 40  #number of shifts, movement of fluid to next cell; time
steps
#      -time_step 144    #length of time step in sec; shifts*time_step=Total
time
#      -time_step 14.4    #length of time step in sec; shifts*time_step=Total
time
  -flow_d forward #Forward flow
  -boundary_conditions constant flux #BC for first and last cell
#Diffusion coef, lengths, and dispersivity should match injection phase
  -diffusion_coefficient 1.0e-5     #diffusion coefs for each cell (m2/s)
  -lengths 0.0762 #length of each cell in meters
  -dispersivities 0.0001 #####dispersivities in meters
      -correct_disp     #correction for column tests
#  -stagnant 1 6e-6 0.0 0.1   #Number of immobile cells associated with
mobile cells
  -punch    20
  -punch_frequency 1
```

```
      -print    20
      -print_frequency 20
USER_GRAPH
#       -headings time(hr) Na Br
#       -chart_title "Monticello Treatment Cell"
#       -axis_titles "Time (hr)" "Effluent Concentration (mg/L)"
#The following controls the graph axes - override those for injection phase
        -axis_scale x_axis 0 7.00 1
        -axis_scale y_axis 0 1.2 0.1
        -initial_solutions false
#       -plot_concentration_vs x
        -plot_concentration_vs t
        -start
#       10 GRAPH_X (STEP_NO + 0.5) / 20
#First value in following graph is time from injection phase.
#e.g. From Injection Phase 2.08*20.5/20 = 2.132 hr
# For porosity 0.35 1.46*20.5/20 = 1.4965 hr
# For porosity 0.25 1.04*20.5/20 = 1.066 hr
#####Second value is time for each step during recovery phase (in hr) e.g.
2.08
        10 GRAPH_X 1.066+(1.04*(STEP_NO + 0.5)/20) #For 20 shifts in sim 1
#       10 GRAPH_X 1.612+(2.08*(STEP_NO + 0.5)/20) # For 15 shifts in sim 1
#       10 GRAPH_X 1.30+(2.08*(STEP_NO + 0.5)/20) # For 12 shifts in sim 1

#       10 GRAPH_X DIST
        20 GRAPH_Y TOT("Na")*23000, TOT("Br")*80000
        -end
PRINT
        -user_graph true
end
```

End of current text