Plume Detachment and Recession Times Following Source Treatment in Bedded Fractured Rock

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Abstract

The influence of source zone remediation on transient plume detachment and recession times in bedded fractured porous media is evaluated using a recently developed three-dimensional semi-analytical model. This solution permits the simulation of source treatment initiated at some time \( t^* \) after the source is introduced to the subsurface, and also considers independent first-order degradation rates in the fracture and the matrix. Other processes of interest include advection, dispersion, sorption in both the fractures and the matrix, forward diffusion into the rock matrix, and back diffusion into fractures. The effects of remediation at the source are represented in the model as a specified concentration versus time function.

Simulations were conducted for a domain impacted with trichloroethene (TCE). Three source zone remediation scenarios were investigated for a monitoring well located 37.5 m downstream from the source: (i) a ‘Type A’, no decay, (ii) a ‘Type B’, instantaneous, complete source removal at \( t^* = 25, 50 \) and 75 years, and (iii) a ‘Type C’, a decaying source concentration, approximated by half-life values of 15 and 30 years, initiated at \( t^* = 25 \) years. Each of these scenarios was evaluated with respect to the time of plume detachment \( t_d \) at a well located downstream of the source, and the time to recession \( t_{rec} \) of the leading edge of the plume, each defined by the 5 ppb concentration contour.

For this example, it was found that \( t_{rec} \) and \( t_d \) were directly proportional to \( t^* \) for the Type B source. When examining Type B and Type C sources with \( t^* = 25 \) years, it was observed that the influence of source zone treatment on \( t_{rec} \) is not significant. Both moderate and aggressive source removal have similar influences on the leading edge of the plume. However, \( t_d \) at the subject monitoring well was strongly influenced by source zone half-life, with the Type B source yielding the most beneficial response. The results of this study demonstrate that back-diffusion from the rock matrix can be the dominant process influencing the length of time that a plume will persist following source treatment.
1.0 Introduction

After many years of passive and active treatment of dense, non-aqueous phase liquid (DNAPL) source zones, the remediation industry has begun to evaluate what effect source zone treatment has on contaminant mass flux and plume evolution (Sale and McWhorter, 2001; Rao and Jawitz, 2003; Saenton et al. (2002); Parker and Park, 2004; Jawitz et al., 2005; Falta et al., 2005). Particularly important dialogue has evolved over the value of partial source mass removal and how aggressively the source should be treated. The exact response of a source to treatment is often difficult to predict because of uncertainty regarding domain heterogeneity, source architecture, and remediation technology efficacy.

DNAPL source zone behaviour in the presence of active and passive treatment is highly complex, and efforts have been undertaken to relate decreases in source zone mass to changes in aqueous phase mass flux. Although the source concentration response to source mass reduction can be highly variable (Parker and Park, 2005), Falta et al. (2005) describes a special case where source concentration is linearly proportional to source mass, and both source mass and source concentration simultaneously exhibit an exponential decaying behaviour. This behaviour has been observed in both field studies (e.g., Newell et al., 2005) and numerical modeling studies (e.g., Parker and Park, 2005).

In this paper, the influence of time-variant source zone treatment on plume evolution is investigated for a fractured rock domain using recently developed semi-analytical solutions. Fractured rock environments are susceptible to penetration by DNAPLs, with DNAPL migration potentially occurring to substantial depths (Kueper and McWhorter, 1991). Three different source treatment functions are considered: (i) a steady-state, constant concentration source designated ‘Type A’, (ii) a ‘Type B’ source simulating the instantaneous complete removal of the source zone at some time \( t^* \), and (iii) a ‘Type C’ exponential decaying source zone concentration initiated at \( t^* \). Two performance metrics are introduced to evaluate source zone treatment efficacy with respect to plume evolution. The time to plume detachment time, \( t_d \), assesses near-source effects, while the time to plume recession, \( t_{rec} \), examines the effect of source treatment on the leading edge of the plume.

2.0 Problem Formulation

2.1 Physical Problem of Interest

The physical problem of interest is conceptualized here as a set of parallel, equally spaced fractures in bedrock (refer to West et al., 2004). It is assumed that the source zone comprises fractures containing residual and pooled DNAPL that is dissolving into flowing groundwater. The direction of groundwater flow is assumed to be parallel to the fractures. A monitoring well is located immediately downstream of the source zone and samples water from the fractures, thereby characterizing the concentration history of the source.
The rock properties adopted in this study are based on those examined by Lipson et al. (2005) and are summarized in Table 1. The solute of interest in this study is trichloroethylene (TCE), a commonly encountered groundwater contaminant.

Table 1 –Parameters for Fractured Porous Media(1)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol &amp; Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial source concentration</td>
<td>$C_0$ (mg/L)</td>
<td>789</td>
</tr>
<tr>
<td>Source zone width</td>
<td>$2B$ (m)</td>
<td>20</td>
</tr>
<tr>
<td>Hydraulic gradient</td>
<td>$\nabla h$</td>
<td>0.005</td>
</tr>
<tr>
<td>Fracture aperture</td>
<td>$2b$ (µm)</td>
<td>140</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>$2T$ (m)</td>
<td>1.42</td>
</tr>
<tr>
<td>Fracture aqueous phase decay half-life</td>
<td>$T(\lambda)_{1/2}$ (yrs)</td>
<td>15</td>
</tr>
<tr>
<td>Fracture retardation factor</td>
<td>$R$</td>
<td>1.0</td>
</tr>
<tr>
<td>Fracture longitudinal dispersivity</td>
<td>$\alpha_L$ (m)</td>
<td>1.0</td>
</tr>
<tr>
<td>Fracture transverse dispersivity</td>
<td>$\alpha_T$ (m)</td>
<td>0.1</td>
</tr>
<tr>
<td>Matrix aqueous phase decay half-life</td>
<td>$T(\lambda)_{1/2}$ (yrs)</td>
<td>15</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>$\theta'$</td>
<td>0.077</td>
</tr>
<tr>
<td>Matrix fraction organic carbon</td>
<td>$f_{oc}$</td>
<td>0.0036</td>
</tr>
<tr>
<td>Matrix dry bulk density</td>
<td>$\rho_b$ (g/cm$^3$)</td>
<td>2.49</td>
</tr>
<tr>
<td>Matrix tortuosity</td>
<td>$\tau$</td>
<td>0.2</td>
</tr>
<tr>
<td>Free-water diffusion coefficient$^2$</td>
<td>$D^*$ (m$^2$/s)</td>
<td>$1.0 \times 10^{-9}$</td>
</tr>
<tr>
<td>Octanol-Carbon Partition Coefficient$^3$</td>
<td>$K_{oc}$ (ml/g)</td>
<td>126</td>
</tr>
</tbody>
</table>

1 – Parameters from Lipson et al., (2005)
2 – Pankow and Cherry, 1996
3 – Pankow and Cherry, 1996

2.2 Source Concentration Function

The conceptual framework for the Type A, B, and C source zone functions are illustrated in Figure 1, and described in detail below. Each of these source Types are utilized in semi-analytical solutions for reactive solute transport in the fractured porous media (West and Kueper (2007, in preparation).

2.2.1 Type A Source

A ‘Type A’ source provides a constant concentration versus time signature in monitoring well A, located immediately downstream of the DNAPL source zone. The concentration in monitoring well A is assumed to be reflective of groundwater concentrations throughout the source zone, and is maintained at $C_0$ for all time. An aqueous phase plume evolves in the downstream direction and achieves a steady-state length ($L_p = L_{max}$) at time ($t = t_S$). The ‘plume’ is defined here as all concentrations exceeding 5 ppb, a typical regulatory limit for several chlorinated VOCs of interest. The value of 5 ppb was selected for convenience only; the concepts illustrated here apply to any concentration used to define the leading edge of the plume. After time $t_S$, the plume no longer expands in the downstream direction. Monitoring well B is located along the plume centerline and exhibits a breakthrough curve reaching a maximum concentration $C_m < C_0$ at time $t_m < t_S$. Groundwater concentrations downstream of monitoring well B will reach their steady-state values at times greater than $t_m$. Once all concentrations along
the plume centerline above 5 ppb are no longer increasing, the plume has reached steady-state. It is clear that the constant concentration nature of the Type A source precludes plume detachment from occurring at any point in time. In addition, the plume will not exhibit recession.

2.2.2 Type B Source

A ‘Type B’ source provides a constant concentration $C_o$ until time $t^*$, beyond which concentrations throughout the source are maintained at $C = 0$. Conceptually, this
condition would be achieved if the entire source zone is physically removed at time $t^*$. The middle plot in Figure 1 shows that the plume will continue to expand in the downstream direction for times beyond $t^*$, up until time $t_{rec}$ when plume recession begins. Monitoring well B, located along the plume centerline a certain distance downstream of the source zone, will exhibit increasing concentrations beyond the time of source removal if that region of the plume had not reached steady-state conditions at the time of source removal. This increase in concentration will continue until time $t_m$ (time of maximum concentration), after which concentration will decrease and eventually reach 5 ppb, at which time ($t_d$) the plume will have detached itself from that location.

### 2.2.3 Type C Source

A ‘Type C’ source provides a constant concentration $C_o$ until time $t^*$, beyond which the source exhibits an exponential decay in concentration with time. The exponential decay in concentration is assumed to result from either the implementation of an in-situ mass removal technology within the source zone, or from natural processes (e.g., DNAPL depletion) (Falta et al., 2005; McGuire et al., 2006). The rate of concentration decay is characterized by a half-life, with more aggressive and complete technology implementation giving rise to a smaller half life than less aggressive and complete technology implementation. As with the Type B source discussed above, the plume will continue to expand in length for times beyond $t^*$ if the plume has not already reached its steady-state length by time $t^*$. At some time $t_{rec}$ the plume begins to recede in length. Monitoring well B is located along the plume centerline a certain distance downstream of the source zone and exhibits an increase in concentration for some length of time beyond $t^*$. Once concentrations have declined to below 5 ppb, the plume will have detached itself from this location.

### 3.0 Boundary Value Problem and Semi-Analytical Solutions

A detailed depiction and mathematical description of the boundary value problem can be found in West et al. (2004). The semi-analytical solution for transport in a fracture is derived from (1), but requires an additional equation for reactive transport in the contiguous matrix. The governing equation for two-dimensional reactive solute transport in a homogeneous, isotropic fracture plane, assuming uniform-steady flow, with a source/sink is given by:

$$0 \leq x \leq \infty$$
$$0 \leq y \leq H$$
$$0 \leq z \leq b$$

$$\frac{\partial c}{\partial t} + \frac{v \partial c}{R \partial x} - \frac{D_x \partial^2 c}{R \partial x^2} - \frac{D_y \partial^2 c}{R \partial y^2} + \lambda c - \frac{2q}{R(2b)} = 0$$

where $c = c(x,y,t)$ is the concentration of the solute $[M/L^3]$, $x$ is the longitudinal spatial coordinate $[L]$, $y$ is the horizontal transverse spatial coordinate $[L]$, $t$ is time $[T]$, $v$ is the average linear steady-state groundwater velocity in the fracture and assumed to be unidirectional in $x$ $[L/T]$, $D_x$ is the coefficient of longitudinal dispersion $[L^2/T]$, $D_y$ is coefficient of horizontal transverse dispersion $[L^2/T]$, $H$ is the finite width of the
transverse domain [L], $q$ is the source/sink term representing diffusion of solute across the matrix wall, $2b$ is the fracture aperture [L], and $R$ is the retardation coefficient for the fracture walls, and $\lambda$ is the aqueous phase decay constant [1/T] in the fracture. The governing equation for one-dimensional diffusive transport in the matrix is described by:

$$\frac{\partial c'}{\partial t} - \frac{D'}{R'} \frac{\partial^2 c'}{\partial z^2} + \lambda' c' = 0$$

$$b \leq z \leq T$$
$$0 \leq y \leq H$$
$$0 \leq x \leq \infty$$

(2)

where $c' = c'(x,y,z,t)$ is the concentration in the porous rock matrix [M/L^3], $\lambda'$ is the aqueous phase decay constant [1/T] in the matrix, $T$ is the half-width between centerlines of equally spaced, parallel fractures [L], $R'$ is the matrix retardation factor, and $z$ is the spatial coordinate perpendicular to the fracture plane [L].

As described in West et al. (2004), (1) and (2) are coupled by $q$, which is approximated using Fick’s first law:

$$q = -\theta D' \frac{\partial c'}{\partial z} \bigg|_{z=b}$$

(3)

where $c'$ is concentration in the matrix [M/L^3], $\theta$ is the matrix porosity, and $D'$ is the effective matrix diffusion coefficient [L^2/T], which the product of $\tau$ (for the matrix) and $D^o$. For the sake of brevity, details regarding other input parameters are not presented here and can be found in West et al. (2004). Furthermore, beyond Figure 1, the mathematical description of initial and boundary conditions are omitted and the interested reader is referred to West et al. (2004) and West and Kueper (2007, in preparation).

The semi-analytical solutions that incorporate the Type A, B, and C source functions are presented in West & Kueper (2007, in preparation).

### 4.0 Simulations

The Table 1 parameters were utilized to generate all plots and all simulations are summarized in Tables 2 and 3. Two sets of simulations were conducted for the Type B treatment. The first set of simulations examined the three $t^*$ values to obtain plume length ($L_p$) versus time plots. Similarly, the second set of simulations examined the three $t^*$ values to obtain breakthrough curves at a monitoring well located 37.5 m downstream from the source zone. The Type C simulations utilize a similar strategy as the Type B simulations and are summarized in Table 3. Type A simulations were generated, where appropriate, to compare and contrast the influence of Type B and C treatment.
Table 2 – Summary of ‘Type B’ Simulations

<table>
<thead>
<tr>
<th>Scenario</th>
<th>(t^*) (yrs)</th>
<th>(t_{rec}) vs (t^*)</th>
<th>(L_p) vs time &amp; (t_{rec}) vs (t^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) Base Case</td>
<td>25, 50, 75</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Plots: \(C\) vs time & \(L_p\) vs \(t^*\)

<table>
<thead>
<tr>
<th>Scenario</th>
<th>MW location (m)</th>
<th>(t^*) (yrs)</th>
<th>(T(\gamma)^{1/2}) (yrs)</th>
<th>(t_d) vs (t^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) Base Case</td>
<td>37.5</td>
<td>25</td>
<td>(\infty), 30, 15, 0</td>
<td></td>
</tr>
</tbody>
</table>

Plots: \(C\) vs time & \(t_d\) vs \(t^*\)

Notes:
- Type A is equivalent to \(T(\gamma)^{1/2} = \infty\)
- Type B is equivalent to \(T(\gamma)^{1/2} = 0\) yrs

Table 3 – Summary of ‘Type C’ Simulations

<table>
<thead>
<tr>
<th>Scenario</th>
<th>(t^*) (yrs)</th>
<th>(T(\gamma)^{1/2}) (yrs)</th>
<th>(L_p) vs time &amp; (t_{rec}) vs (t^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) Base Case</td>
<td>25</td>
<td>(\infty), 30, 15, 0</td>
<td></td>
</tr>
</tbody>
</table>

Plots: \(C\) vs time & \(t_d\) vs \(t^*\)

<table>
<thead>
<tr>
<th>Variable</th>
<th>MW location (m)</th>
<th>(t^*) (yrs)</th>
<th>(T(\gamma)^{1/2}) (yrs)</th>
<th>(t_d) vs (t^*)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) Base Case</td>
<td>37.5</td>
<td>25</td>
<td>(\infty), 30, 15, 0</td>
<td></td>
</tr>
</tbody>
</table>

5.0 Results & Discussion

5.1 Type B Simulations

5.1.1 Time to recession

The time for the influence of source zone remediation to manifest itself as a beneficial plume response is often a forefront concern. Figure 2 plots the position of the 5 ppb leading edge contour with time for the simulations listed in Table 2.

From Figure 2 the maximum length of the plume (\(L_{max}\)) occurs at approximately 100 years for a \(t^*\) of 25 years and increases to approximately 150 years for \(t^*\) equal to 75 yrs, with the corresponding \(L_{max}\) ranging between 380 and 400 m. The time at which \(L_{max}\) occurs is the time to recession. The plume requires an additional 100 years to diminish below 5 ppb throughout the domain. The Type B simulation is plotted in plan view in Figure 3 to further illustrate the characteristics of the plume for \(t^* = 25\) years.

From Figure 3, the time to recession of the leading edge occurs at approximately 105 years. Thereafter, the leading edge gradually recedes until compliance is achieved. It can also be observed that the leading edge of the plume recedes faster than the back edge of the plume moves forward (detaches). This stems from the fact that back diffusion from the rock matrix near the source contributes more mass to the fractures than back diffusion at the leading edge of the plume because of the larger amount of mass sequestered in the matrix near-source.
5.1.2 Time to detachment

Figure 4 considers the concentration history at a monitoring well located 37.5 m downstream of the source for $t^* = 25$ years. Figure 4 coincides with Figure 3. It can be observed that the time to plume detachment ($C \leq 0.005$ mg/L) is directly proportional to $t^*$ at this well with $t_d$ equal to approximately 180, 210, and 240 years for $t^*$ values equal to 25, 50, and 75 years, respectively.

Since the monitoring well is relatively near the source (for this example), the concentration response to the Type B treatment is abrupt. The concentration signature will be less pronounced for wells further downstream, as the biodegradation, and forward- and back-diffusion processes will dampen the response.

5.2 TYPE C Simulations

5.2.1 Time to recession

The influence of Type A, B, and C source zone functions on the length of the plume ($L_p$) versus time is presented in Figure 5. For Type A, steady-state is achieved after 200 years; this curve is the benchmark for subsequent evaluation. When considering Type B and C source zone functions, differences in $L_p$ versus time can be observed for each source decay rate with a $t^*$ of 25 years. When examining all curves, it can be observed that some treatment or concentration decay ($T(\gamma)_{1/2} = 30$ or 15 years) of the source reduces the time to recession ($t_{rec}$) approximately the same degree that complete source removal does, and decreasing $T(\gamma)_{1/2}$ from 30 to 15 years reduces the time to compliance ($C \leq 0.005$ mg/L) by approximately two-fold.
Interestingly, the difference between $T(\gamma)_{1/2} = 15$ years and the instantaneous Type B treatment is marginal with respect to the recession time ($t_{rec}$); the difference is approximately 20 years. The differences become more significant when examining the time to compliance.

Figure 3 – Plan view plot of Type B source zone for $t^* = 25$ years.
5.2.2 Time to detachment

Figure 6 presents breakthrough curves for the plume at a monitoring well located 37.5 m downstream of the source zone for Type A, B and C source treatment functions. Clearly, the value of $T(\gamma)_{1/2}$ also has a significant influence on the time to detachment for the monitoring well with a time to detachment of 180, 280 and 510 years for $T(\gamma)_{1/2}$ equal to 0 years (Type B), 15, and 30 years, respectively.
As with Figure 5, moderate source zone decay rates (15 and 30 years) are highly beneficial when compared to the Type A case. Figure 6 demonstrates that there is a continuum of Type C decay rates between the limits of behavior exhibited by the Type A and Type B cases.

6.0 Conclusions

New semi-analytical solutions were utilized to study the influence of source remediation on plume recession and detachment times in discretely fractured rock. Three source treatment functions were considered: (i) a Type A concentration versus time function representing the case of no source treatment, (ii) a Type B concentration versus time function representing instantaneous source removal, and (iii) a Type C concentration versus time function representing treatment yielding a source concentration that can be described by first order decay initiated at a specified point in time after the source is introduced. The influence of source treatment on the plume was evaluated in the presence of biodegradation.

Two performance metrics were introduced to evaluate the effect of source zone remediation on the evolution of a TCE plume. The near-field (near-source) plume behaviour was ascertained by examining the time to plume detachment, $t_d$, at a specific monitoring well. The influence of source treatment on the far-field (leading edge of the plume) was evaluated using the time to plume recession, $t_{rec}$.

The Type A source zone function produces a steady-state (naturally attenuated) plume as a result of dispersion and biodegradation processes. For Type B source zone treatment, it was observed that $t_{rec}$ is directly proportional to $t^*$; the sooner treatment is
initiated, the sooner the leading edge of the plume begins to recede. Similarly, \( t_d \) was proportional to \( t^* \) for this example.

When considering Type C strategies it was found that the \( t_{rec} \) response to source zone decay half-life, \( T(\gamma)^{1/2} \), was largely negligible. There was some benefit to the time to compliance, however. These results suggest that if the goal of remediation is to slow (or stop) the leading edge of the plume, aggressive Type B source zone treatment is unwarranted, and more moderate \( T(\gamma)^{1/2} \) values (e.g., 15 and 30 years) will suffice. The time to detachment was strongly influenced by \( T(\gamma)^{1/2} \) as well. The Type B source yielded the shortest \( t_d \) value (180 years), while the more moderate Type C source zone functions yielded increases in \( t_d \). Based on these observations regarding \( t_{rec} \) and \( t_d \), stakeholders should carefully weigh the costs of aggressive remediation against the benefits.

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References


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