A MODEL OF *IN SITU* BIOREMEDIATION THAT INCLUDES THE EFFECT OF RATE-LIMITED SORPTION AND BIOAVAILABILITY

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ABSTRACT

In situ bioremediation is a groundwater and soil remediation technology that makes use of indigenous or introduced microorganisms to degrade contaminants in the subsurface. One factor affecting the feasibility of *in situ* bioremediation is the availability of the contaminant to the microorganisms. It is typically assumed that the contaminant is only available for biodegradation in the aqueous phase. However, many organic contaminants of interest are sorbed to soil in the subsurface, and the sorbed contaminant is presumably unavailable for bioremediation. If bioremediation is attempted, the rate of desorption of contaminant from the sorbed phase is a factor in determining the availability of the contaminant to the degrading microorganisms and hence, the efficacy of the remediation. In this work, a transport model is presented that accounts for both biodegradation and desorption kinetics. The model is run using realistic parameter values obtained from a recent field evaluation of *in situ* aerobic cometabolic bioremediation at Edwards AFB, to demonstrate the potential impact of rate-limited sorption on bioremediation efficacy. The model allows remediation managers to better understand the impact of the *in situ* bioremediation technology on the fate and transport of contaminants, ultimately helping these managers design and implement solutions to contamination problems.

Key words: modeling, bioavailability, sorption, cometabolism, bioremediation

BACKGROUND

In situ bioremediation is a technology that is currently being studied (and increasingly implemented) in the hope that it may be useful in remediating the nation's hazardous waste sites. One factor affecting the feasibility of *in situ* bioremediation is the availability of the contaminant to the indigenous or introduced microorganisms that degrade it. It is typically assumed that the contaminant is only available for biodegradation in the aqueous phase (Fry and Istok, 1994). However, many organic contaminants of interest are sorbed to soil in the subsurface. The sorbed fraction is presumably unavailable for bioremediation. If bioremediation is attempted, the rate of desorption of contaminant from the sorbed phase is a factor in determining the availability of the contaminant to the degrading microorganisms and hence, the efficacy of the remediation. Most models of contaminant transport in the groundwater neglect the rate of desorption, even though desorption rate may be crucial in determining bioavailability, and hence efficacy of remediation (Fry and Istok, 1994).

A recent demonstration of *in situ* bioremediation to treat trichloroethylene (TCE)-contaminated groundwater was conducted at Edwards AFB (McCarty et al., 1998). The remediation at the Edwards AFB site was based upon aerobic cometabolism of TCE whereby indigenous bacteria are induced to fortuitously oxidize TCE when they are provided a primary substrate (a source of energy) under aerobic conditions. The two-well treatment system shown in Figure 1 depicts the system that was used in the Edwards AFB field evaluation. Figure 1 shows toluene (the primary substrate) and oxygen injected into the treatment wells and mixed into the contaminated groundwa-

ter flowing through the wells. Each treatment well is screened at two depths, with one well operated in an upflow mode, the other in a downflow mode. Since water being injected into the aquifer from the treatment wells contains contaminant (TCE), primary substrate (toluene), and oxygen, *in situ* bioactive zones are created around the injection screen of each treatment well. In the bioactive zone, the indigenous microorganisms aerobically metabolize the primary substrate and cometabolize the contaminant. The treatment is *in situ* and contaminated water is never brought to the surface. Figure 2 presents an example remediation scenario, similar to the implementation at the Edwards AFB evaluation site, where *in situ* bioremediation is employed to contain the transport of TCE-contaminated groundwater. The figure depicts a treatment system-installed downgradient of a source of contamination.

MODEL

The partial differential equations describing aerobic cometabolic biodegradation in one dimension are presented in Semprini and McCarty (1991, 1992). The model presented by Semprini and McCarty (1991, 1992) accounts for sorption/desorption kinetics by using a first-order rate expression. In the current work, these one-dimensional equations are incorporated into a three-dimensional model and numerically solved using an efficient self-adaptive, partial-implicit approach. The three-dimensional model permits simulation of bioremediation in the complex groundwater flow field induced by the two dual-screened treatment wells depicted in Figure 1. The model used in this work incorporates the following processes: (1) multi-dimensional flow, (2) advection and dispersion, (3) equilibrium or rate-limited sorption, and (4) biodegradation. Equilibrium sorption may be described using linear, Freundlich, or Langmuir isotherms. Rate-limited sorption may be described using either first-order kinetics or Fickian diffusion through various simple geometries. Biodegradation is described using either Monod kinetics or cometabolic transformation kinetics. Fate and transport of contaminant, primary substrate, oxygen, and microorganisms are described by a set of nonlinear partial differential equations. The equations are numerically solved using a customized self-adaptive, partial-implicit approach. This numerical approach examines each term in the governing equations at every cell and time step. If the term is rapidly changing in space or time, an implicit solution method is used. An explicit method is used when the term is stable. The approach permits use of much larger time steps than would otherwise be allowed.

MODELING RESULTS

The model is run using realistic parameter values obtained from the Edwards AFB evaluation of *in situ* aerobic cometabolic bioremediation (McCarty et al., 1998). Using the model, variations in TCE, toluene (the primary substrate), oxygen, and microbial concentrations in time and space can be simulated. Figure 3 shows the simulated breakthrough of TCE at a monitoring well downgradient of the treatment system, depicting the impact on TCE-breakthrough of assuming

equilibrium and rate-limited sorption. In the equilibrium case, a linear sorption isotherm is assumed. In the rate-limited case, a first-order expression is used to model nonequilibrium between the aqueous and sorbed phases. Note that although rate-limited sorption has a transient impact on remediation effectiveness (earlier breakthrough and late-time tailing), at steady state, both assumptions result in equal TCE concentrations at the downgradient well. The simulations demonstrate that if this bioremediation system is being used to implement a contaminant containment strategy, whether one assumes equilibrium or rate-limited sorption is not critical in the long-term. The model also allows testing of other assumptions and parameter values. The model is a tool that will allow remediation managers to better understand the impact of *in situ* bioremediation technology on the fate and transport of contaminants, ultimately helping these managers design and implement better technology solutions to contamination problems.

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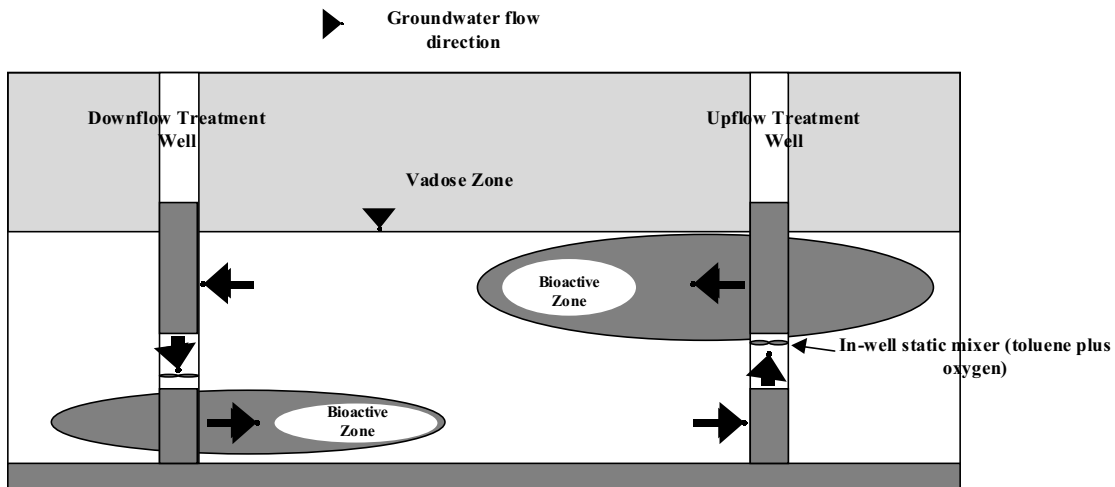**Figure 1.** *In situ* bioremediation-treatment-well system to treat TCE-contaminated groundwater.

Figure 2. Treatment system layout showing streamlines entering and leaving upper screens of treatment wells.
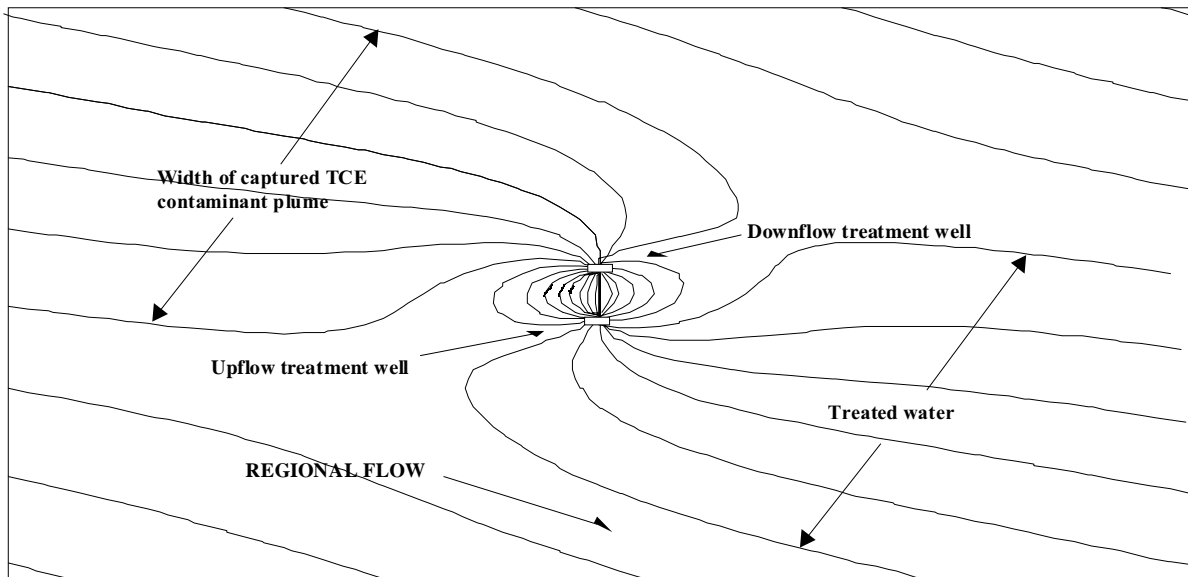
Figure 3. Comparison of TCE concentrations at a monitoring well downgradient of treatment system (TCE concentration upgradient of system = 1 mg/L) assuming equilibrium and rate-limited sorption.

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