The Society for engineering
in agricultural, food, and
biological systems

Paper Number: 033103
An ASAE Meeting Presentation

Modeling Sequential Electron Acceptors in Bioremediation

Xiaomin Su

Biological Resources Engineering Department, University of Maryland at College Park.

Yingli Fu

Biological Resources Engineering Department, University of Maryland at College Park.

Jennifer Becker, Ph.D.

Biological Resources Engineering Department, University of Maryland at College Park.

Paul Schreuders, Ph.D.

Biological Resources Engineering Department, University of Maryland at College Park.

Hubert Montas, Ph.D.

Biological Resources Engineering Department, University of Maryland at College Park,
College Park, MD, 20742. montas@umd.edu.

Written for presentation at the
2003 ASAE Annual International Meeting
Sponsored by ASAE
Riviera Hotel and Convention Center
Las Vegas, Nevada, USA
27- 30 July 2003

Abstract**.** This study evaluates the importance of considering sequential electron acceptor processes when modeling hydrocarbon bioremediation downgradient of a leaky subsurface tank. Predictions of transport models ranging from linear reactive to sequential two-electron acceptor model are compared for a typical transport scenario at its steady-state limit. The main result is that the sequence of aerobic and anaerobic metabolisms enhances bioremediation relative to aerobiosis alone. It is concluded that sequential electron acceptor dynamics are important for accurate predictions of bioremediation.

Keywords. Biodegradation, Nonlinear Models, Asymptotic Analysis.

1. Introduction

In the past decade, groundwater pollution by petroleum hydrocarbons caused by leaking underground storage tanks, or leakage from other types of fuel storage facilities, have been reported extensively in the US, Europe and Australia. It is estimated that 10-20% of nearly two million underground storage tanks in the United States are leaking (Atlas and Cerniglia, 1995). Restoration of affected aquifers to regulatory standards is a technically difficult problem, even when the best engineering strategies are applied. The substantial cost and technical challenges involved in the remediation of this contamination have led to increased interest in quantitative investigations of how these compounds may be naturally attenuated by resident subsurface bioagents.

Intrinsic bioremediation, relying on the intrinsic (or naturally developing) biological activity, mainly microbiological degradation of organic compounds, to prevent the migration of contamination away from its source, has gained increased acknowledgment in the last few years for its cost effectiveness and ecological soundness. In the intrinsic bioremediation process, microorganisms degrade the contaminant hydrocarbons by using organic matter as electron donor and oxygen, in aerobic condition, or nitrate, Mn (IV), Fe (III), sulfate or CO_2, in anaerobic condition, as electron acceptors. Theoretically, the differences in energy release from the organic carbon oxidation, by the different electron acceptors, lead to the sequential occurrence of redox processes (Potsma and Jakobsen, 1996) and produce a characteristic spatial or temporal separation of redox zonation in the biodegrading contaminant plume (Ludvigsen et al., 1998). This zonation is thought to affect the rate of bioremediation but quantitative estimates of its effects are lacking.

Mathematical modeling of bioremediation has gained popularity during the past decade for its potential applicability in the design and analysis of effective bioremediation systems. The models often consist of systems of nonlinear partial differential equations because of the complexity of microbial dynamics and transport processes occurring simultaneously during bioremediation. It is not always clear, however, whether such complexity is warranted, whether, for example, a model must be able to represent redox zonation to properly predict plume extent or whether one can get by with the use of a simpler, possibly linear model.

2. Objective

The objective of this contribution is to evaluate the importance of considering sequential electron acceptor processes (redox zonation) when modeling the bioremediation of hydrocarbons emanating from leaky subsurface tanks. This evaluation is performed by comparing the predictions of transport models with varying degrees of sophistication, starting with a linear reactive model and ending with a sequential two-electron acceptor model where the acceptors are oxygen (aerobiosis) and nitrate (anaerobiosis). For simplicity, the study is limited to a single transport scenario (source strength, parameter values, domain geometry, etc…), evaluated at its asymptotic steady-state limit.

3. Materials and Methods

3.1. Transport Scenario and Sequential Electron Acceptor Model

The transport scenario investigated in this study corresponds to the continuous release (leakage) of a relatively soluble hydrocarbon from a buried storage container (cracked). The container is embedded in a water saturated subsurface formation where a uniform, steady and unidirectional horizontal flow field prevails (Figure 1). Advective and dispersive transport processes cause the leaking contaminant to form a plume downgradient of its container. Microbiota located within the plume volume consume the hydrocarbon, using either oxygen or nitrate as electron acceptor. The supply of electron acceptors comes from the aquifer's water transported by the uniform flowfield. At large times after the beginning of the leakage process, the combination of hydrocarbon and electron acceptor supply, and their consumption by microbiota, is expected to produce steady-state (time-independent but spatially variable) distributions of hydrocarbon, oxygen, nitrate and microorganism concentrations denoted respectively by H(x,y,z), O(x,y,z), N(x,y,z) and X(x,y,z) (all in mg/l) (see equation 2.67 of Fisher et al., 1979 for the non-reactive case).

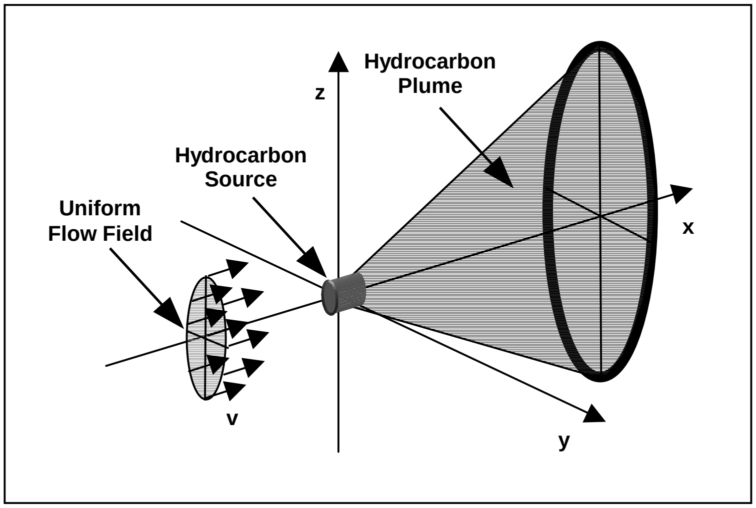

Figure 1: Transport Scenario under Investigation

The underground tank is concentrated at the point (x, y, z) = (0, 0, 0) and assumed to leak hydrocarbon at a constant rate: Q = 25 kg/d, and the background concentrations of hydrocarbon (or equivalent substrate for microbial sustenance), oxygen and nitrate, upgradient of the tank, are assumed to be: $H_0 \equiv H(x \leq 0, y, z) = 0.01$ mg/l, $O_0 \equiv O(x \leq 0, y, z) = 5$ mg/l and $N_0 \equiv N(x \leq 0, y, z) = 20$ mg/l, respectively. The subsurface formation is further taken to have constant porosity: $\theta = 0.4$ (e.g. Bear, 1972).

The growth of microbiota in the subsurface is assumed regulated by the availability of substrate (the hydrocarbon) and electron acceptors (oxygen and nitrate). Oxygen is taken as the primary electron acceptor for metabolism and is preferred to nitrate when its concentration is sufficiently large. As oxygen becomes depleted, the microbes start to use nitrate as electron acceptor and switch to anaerobic metabolism. In this study, a multiplicative Monod model (Borden and Bedient, 1986) is used to represent microbial growth under this sequential electron-acceptor process, and it is coupled with a second-order term that represents microorganism die-off:

$$\frac{\partial X}{\partial t} = \mu_{\max}\left[\frac{H}{K_{sh}+H}\right]\left\{\left[\frac{O}{K_{so}+O}\right]+\left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\right\}X - \lambda X^{2} \tag{1a}$$

where t is time, $\mu_{\max}$ is the maximum growth rate of biota, K_{sh} , K_{so} and K_{sn} are half-saturation constants for metabolism of the substrate H with electron acceptors O and N, respectively, K_{io} is the constant regulating the inhibition of N-mediated metabolism when the concentration of O is large, and λ is the death rate parameter. By considering the limiting forms of (1a) for large and small oxygen concentrations, it is readily verified that it produces the desired gradual switching from aerobic to anaerobic metabolism:

$$O >> K_{io} \qquad \Rightarrow \qquad \frac{\partial X}{\partial t} = \mu_{\max}\left[\frac{H}{K_{sh}+H}\right]\left[\frac{O}{K_{so}+O}\right]X - \lambda X^{2} \qquad \text{aerobic}$$

$$O << K_{io}, K_{so} \qquad \Rightarrow \qquad \frac{\partial X}{\partial t} = \mu_{\max}\left[\frac{H}{K_{sh}+H}\right]\left[\frac{N}{K_{sn}+N}\right]X - \lambda X^{2} \qquad \text{anaerobic}$$

The quadratic death-rate term in (1a) is used to impose a maximum value on the microbial concentration while ensuring that this concentration never becomes negative. The more commonly used zero- and first-order death rates can produce either negative or infinite concentrations that are not biologically plausible. The use of the second-order death-rate gives (1a) the form of a multiplicative-Monod-logistic equation that appears better suited to the present application. The phase space of this model is presented in Figure 2 and illustrates the trajectories of microbial population towards the stable equilibrium curve:

$$X(x,y,z) = \frac{\mu_{\max}}{\lambda}\left[\frac{H}{K_{sh}+H}\right]\left\{\left[\frac{O}{K_{so}+O}\right]+\left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\right\} \tag{1b}$$

The other equilibrium point of (1a) (X = 0 mg/l) is unstable unless the substrate and/or electron acceptor concentrations are null, in which case it fuses with (1b).

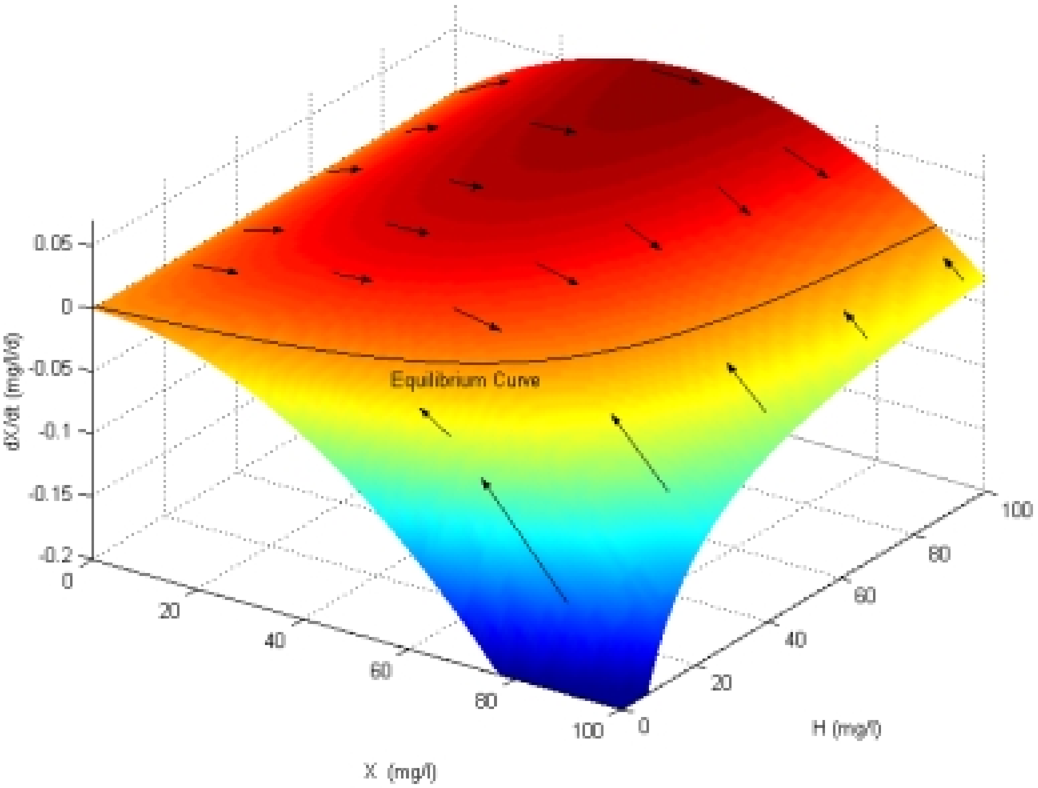

Figure 2. Microbial Dynamics Phase-Space Plot for Model Equation (1a) at High Oxygen Concentration

Equation (1b) (and simplifications defined below in section 3.2) is the steady-state equation used in this study to determine the steady spatial distribution of microbiota within and around the hydrocarbon plume, at large times after the inception of leakage. With parameter values in Table 1, and background concentration given above, it produces a background microbial concentration: $X_0 \equiv X(x \leq 0, y, z) \approx 0.1$ mg/l and a maximum concentration at high H and either high O or N of: $X(x, y, z) = 100$ mg/l. These values correspond approximately to 10^3~10^4 and 10^6~10^7 Colony Forming Units per milliliter (CFU/ml), respectively.

Table 1. Parameter Values for Steady Bioremediation of Hydrocarbon Plume

Parameter	Value	Parameter	Value	Parameter	Value
v (m/d)	0.2	K_{sh} (mg/l)	10.0	Y_h (mg/mg)	0.25
D (m^2/d)	0.03	K_{so} (mg/l)	0.1	Y_o (mg/mg)	0.31
μ_{max} (1/d)	0.0034	K_{sn} (mg/l)	0.5	Y_n (mg/mg)	0.42
λ (l/mg/d)	0.000034	K_{io} (mg/l)	0.2		

Sources: Mayer et al., 2001; MacQuarrie and Sudicky, 2001.

The leaking hydrocarbon, oxygen and nitrate are transported through the aquifer by the advective-dispersive process generated by the flow field, and they are simultaneously consumed by the microorganisms. Their spatio-temporal dynamics are assumed to be correctly represented by the commonly used advective-dispersive-reactive system of partial differential transport equations with reactive terms derived from (1a):

$$\begin{aligned}
\frac{\partial H}{\partial t} &= -\frac{\mu_{\max}}{Y_h}\left[\frac{H}{K_{sh}+H}\right]\left\{\left[\frac{O}{K_{so}+O}\right]+\left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\right\}X - v\frac{\partial H}{\partial x} + D\Delta H \\
\frac{\partial O}{\partial t} &= -\frac{\mu_{\max}}{Y_o}\left[\frac{H}{K_{sh}+H}\right]\left[\frac{O}{K_{so}+O}\right]X - v\frac{\partial O}{\partial x} + D\Delta O \qquad (2a) \\
\frac{\partial N}{\partial t} &= -\frac{\mu_{\max}}{Y_n}\left[\frac{H}{K_{sh}+H}\right]\left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]X - v\frac{\partial N}{\partial x} + D\Delta N
\end{aligned}$$

where v is the velocity of groundwater, D is the dispersion coefficient of the transport process, Δ is the three-dimensional Laplacian operator, and Y_h , Y_o and Y_n are metabolic yield coefficients for H, O and N, respectively (see Table 1).

The steady-state version of the system (2a) is obtained by setting time-derivatives to zero, neglecting longitudinal dispersion (direction x), introducing the radial coordinate $r = \sqrt{y^2 + z^2}$, and substituting (1b) for X to obtain, explicitly:

$$\begin{aligned}
\frac{\partial H}{\partial x} &= -\frac{\mu_{\max}^2}{v\lambda Y_h}\left[\frac{H}{K_{sh}+H}\right]^2\left\{\left[\frac{O}{K_{so}+O}\right]\right. \\
&\qquad \left. + \left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\right\}^2 + \frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial H}{\partial r}\right) \\
\frac{\partial O}{\partial x} &= -\frac{\mu_{\max}^2}{v\lambda Y_o}\left[\frac{H}{K_{sh}+H}\right]^2\left\{\left[\frac{O}{K_{so}+O}\right]^2\right. \\
&\qquad \left. + \left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\left[\frac{O}{K_{so}+O}\right]\right\} + \frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial O}{\partial r}\right) \qquad (2b) \\
\frac{\partial N}{\partial x} &= -\frac{\mu_{\max}^2}{v\lambda Y_n}\left[\frac{H}{K_{sh}+H}\right]^2\left\{\left[\frac{N}{K_{sn}+N}\right]^2\left[\frac{K_{io}}{K_{io}+O}\right]^2\right. \\
&\qquad \left. + \left[\frac{N}{K_{sn}+N}\right]\left[\frac{K_{io}}{K_{io}+O}\right]\left[\frac{O}{K_{so}+O}\right]\right\} + \frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial N}{\partial r}\right)
\end{aligned}$$

This system of coupled nonlinear partial differential equation (and simplifications corresponding to those of (1b) in section 3.2 below) is used to evaluate the steady spatial distribution of hydrocarbon (the plume), oxygen and nitrate downgradient of the leaky storage tank, at large times. It is notable that it has the form of a system of diffusive-reactive transport equations where the role of time is played by the spatial ordinate x. This suggests that analytical and/or numerical analysis and solution strategies commonly used for diffusive-reactive systems may also be used to analyze or solve (2b).

The solution domain corresponding to the transport scenario of Figure 1 and the model system (2b) is (in view of symmetries about r = 0) the quadrant:

$$\begin{aligned} 0 &\le x \le \infty \\ 0 &\le r \le \infty \end{aligned} \tag{3}$$

Background concentrations (in mg/l) and the hydrocarbon source at x = 0 are represented by the boundary conditions:

$$\begin{aligned} H(0,r) &= 0.1 + \frac{Q}{v\theta}\delta(r) \\ O(0,r) &= 10 \\ N(0,r) &= 100 \end{aligned} \tag{4a}$$

Boundary conditions at the radial limits of the domain (for an arbitrary transported entity, U, representing either H, O or N) are:

$$\left.\frac{\partial U}{\partial r}\right|_{r=0} = 0 \quad \text{and} \quad \left.\frac{\partial^n U}{\partial r^n}\right|_{r=\infty} = 0, \quad \text{with} \quad n \ge 0 \tag{4b}$$

3.2. Analysis Methods and Simplified Models

The system (2b) and simplified forms of this system that neglect electron-acceptor switching dynamics are solved either analytically (when possible) or numerically over the domain (3) with boundary conditions (4a,b). Numerical solutions (when needed) are obtained using Galerkin Finite Elements with linear basis functions to discretize the radial component of the equations (Huyakorn and Pinder, 1983). A Crank-Nicolson discretization is used to treat the spatial derivative in the longitudinal (x) direction. The resulting system of nonlinear algebraic matrix equations is solved by Picard fixed point iteration for each spatial step in direction x.

The spatial characteristics of steady hydrocarbon plumes obtained using (2b) and its simplifications are compared to each other based on two measures distributed along the x-axis: a) hydrocarbon content and; b) plume transverse area. Hydrocarbon content, expressed in gram per longitudinal meter is calculated as:

$$m_0(x) = 2\pi\theta \int_0^\infty \left[H(x,r) - H(x,\infty)\right] r\, dr \tag{5}$$

where r is in meters. This measure, and especially its slope, is indicative of the effectiveness with which biota is able to degrade the hydrocarbon in the plume. Plume transverse area, expressed in square meters, is calculated as:

$$m_2(x) = \frac{2\pi\theta}{m_0(x)} \int_0^{\infty} \left[H(x,r) - H(x,\infty) \right] r^3 dr \qquad (6)$$

which is readily identified as the variance of the transverse spatial distribution of hydrocarbon within the plume.

Results obtained with the full sequential electron-acceptor bioremediation model (2b) will be compared to those of three simplified models to identify the importance of biotic spatial variability, biotic response to oxygen levels and metabolic switching from aerobiosis to anaerobiosis on the spatial characteristics of the steady hydrocarbon plume. The three simplified models are presented in the following subsections.

3.2.1. Linear Reactive Hydrocarbon Transport with Constant Microbe Level (“H”)

A frequently used simplification of (1)-(2) considers that hydrocarbon concentration is small, oxygen concentration is large (non-limiting) and microbiota concentration is constant (say X_c). The resulting biodegradation model is linear and completely neglects the role of electron acceptor limitations on biodegradation. It has the form:

$$\frac{\partial H}{\partial x} = -kH + \frac{D}{vr}\frac{\partial}{\partial r}\left(r \frac{\partial H}{\partial r} \right) \qquad \text{where:} \quad k = \frac{\mu_{\max} X_c}{v Y_h K_{sh}} \qquad (7a)$$

The analytical solution of this simple linear model is well known and can be obtained from equation 2.67 of Fisher et al. (1979) or Polianin (2002). It consists of an exponentially decaying Gaussian with variance that increases linearly with position. The solution and plume characteristics obtained via (5)-(6) are:

$$H(x,r) = \left[H_0 + \frac{Q}{4\pi D x \theta} e^{-\frac{vr^2}{4Dx}} \right] e^{-kx}$$

$$m_0(x) = \frac{Q}{v} e^{-kx}$$

$$m_2(x) = 4\frac{Dx}{v}$$

The linear reactive term causes hydrocarbon concentration to decay exponentially as one moves away from the leaky tank in the downgradient direction and transverse dispersion causes it to also decay away from the problem’s centerline (r = 0). Plume mass similarly decays exponentially with downgradient distance while plume transverse area increases linearly with distance. These characteristics are compared to other models in section 4.

3.2.2. Hydrocarbon Transport with Variable Biota Concentration ("HX")

A milder simplification of (1)-(2) assumes that hydrocarbon concentration is not necessarily small and may affect microbial concentrations but maintains the high electron-acceptor concentration assumption of the previous model. In this case, the steady distribution of biota becomes (from (1b)):

$$X(x,r)=\frac{\mu_{\max}}{\lambda}\left[\frac{H}{K_{sh}+H}\right]$$

and the corresponding form of the system (2b) is:

$$\frac{\partial H}{\partial x}=-\frac{\mu_{\max}^2}{v\lambda Y_h}\left[\frac{H}{K_{sh}+H}\right]^2+\frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial H}{\partial r}\right) \tag{7b}$$

This model is expected to represent the effects, on biodegradation, of the biotic response to hydrocarbon concentration variability better than (7a). However, in similarity to (7a), it neglects any limitative effect that electron acceptor concentration and switching may have on the process. The model is nonlinear due to its squared-Monod reactive term that behaves as a zero-order decay reaction at high hydrocarbon levels and as a second-order decay reaction at low H levels. Spatial characteristics of the solution to this equation may be investigated using analytical techniques (Murray, 2003) but, here, it will simply be solved numerically prior to computing plume characteristics via (5) and (6).

3.2.3. Hydrocarbon and Oxygen Transport with Variable Biota Concentration ("HXO")

The third simplified version of (1)-(2) considers both hydrocarbon and oxygen transport, as well as spatial variability of biotic concentrations, but neglects the potential use of nitrate as electron acceptor for anaerobic metabolism. Accordingly, (1b) is simplified to the multiplicative Monod form:

$$X(x,y,z)=\frac{\mu_{\max}}{\lambda}\left[\frac{H}{K_{sh}+H}\right]\left[\frac{O}{K_{so}+O}\right]$$

and (2b) reduces to the pair of equations:

$$\begin{aligned}\frac{\partial H}{\partial x} &= -\frac{\mu_{\max}^2}{v\lambda Y_h}\left[\frac{H}{K_{sh}+H}\right]^2\left[\frac{O}{K_{so}+O}\right]^2+\frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial H}{\partial r}\right)\\ \frac{\partial O}{\partial x} &= -\frac{\mu_{\max}^2}{v\lambda Y_o}\left[\frac{H}{K_{sh}+H}\right]^2\left[\frac{O}{K_{so}+O}\right]^2+\frac{D}{vr}\frac{\partial}{\partial r}\left(r\frac{\partial O}{\partial r}\right)\end{aligned} \qquad (7c)$$

This model system is nonlinear and will be solved numerically. Its main deviations from the sequential model (2b) are expected to occur in zones where increased bioactivity has led to significant oxygen depletion, triggering anaerobiosis. Comparison of the plume characteristics predicted by (7c) and (2b) will help in identifying the importance of considering the latter process when modeling natural bioremediation in the present transport scenario.

4. Results and Discussion

Steady hydrocarbon plumes predicted by models (7a), (7b), (7c) and (2a) are presented in Figure 3 where the models have been labeled “H”, “HX”, “HXO” and “HXON”, respectively, according to the entities whose spatial distribution they consider. For model “H” (i.e. (7a)), the decay constant (k) was computed with X_c = 10 mg/l which produces a plume of comparable extent to those of other models.

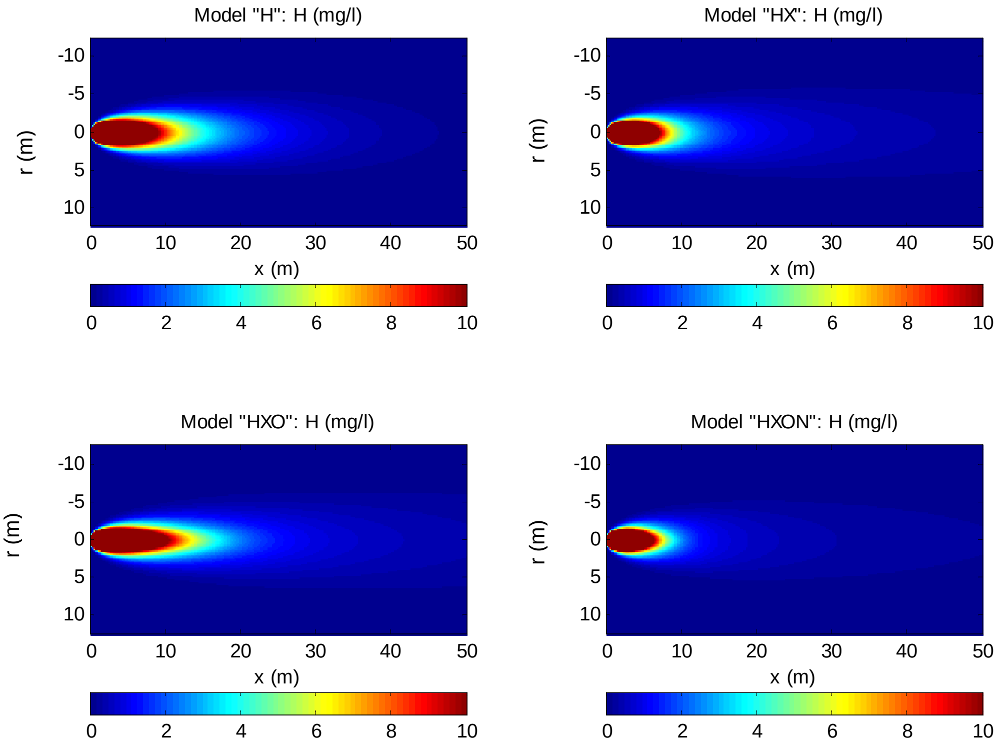

Figure 3. Steady Hydrocarbon Plumes Predicted by the Models

All plumes have oblong shapes with equi-concentration contours that are essentially ellipsoidal (the plots are truncated at a maximum concentration of 10 mg/l for display purposes). The longitudinal extents of the plumes are seen to vary by model. The oxygen-limited model "HXO" produces the longest plume with 10 mg/l contour extending more than 10 meters downgradient of the source. The full sequential electron acceptor model produces the most compact plume with a 10 mg/l contour that extends only half as far longitudinally as the "HXO" plume. The second smallest plume is produced by the "HX" model and the linear "H" model produces a plume comparable (but shorter) to that of the "HXO" model. The transverse extents of the plumes generally appear to be consistent across models.

The masses and transverse areas of the hydrocarbon plumes, computed with (5) and (6), are presented in Figure 4. Plume masses decay with increasing distance from the leaking source which reflects the influence of the biodegradative process. Decay rates are similar for the "H" and "HXON" models up to a downgradient distance of 20 m and they are slower than for the other two models. The redox zonation model "HXON" predicts significantly faster decay with a hydrocarbon mass that is less than half that of the "HXO" model from 5 m from the source onwards. Predictions of the non-oxygen limited Monod "HX" model are intermediate between the "HXO" and "HXON" model as observed also in the plumes of Figure 3.

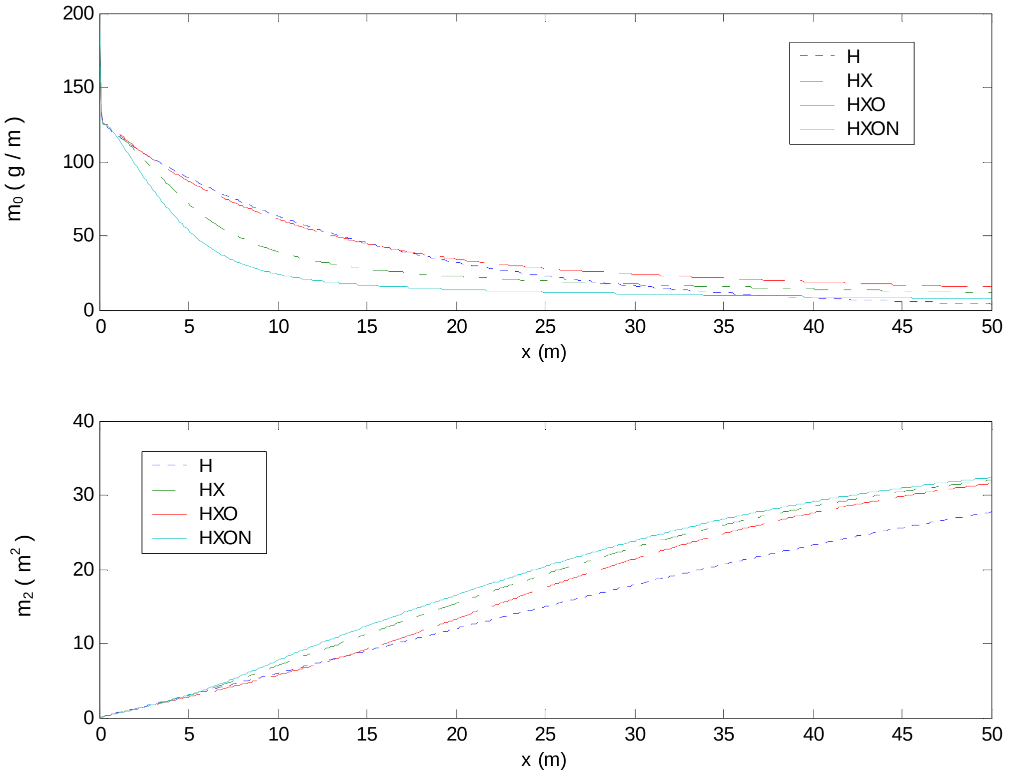

Figure 4. Longitudinal Mass Distribution and Cross-Sectional Area of the Predicted Steady Hydrocarbon Plumes

The cross-sectional areas of all steady plumes increase with distance from the source, as expected. Plumes predicted by models considering biotic spatial variability (“HX”, “HXO”, “HXON”) generally produce slightly wider plumes than when this variability is neglected (model “H”). Here again, predictions of models “HX” and “HXON” are observed to be closer to one another than to other models while “H” and “HXO” agree up to 15 m downgradient of the source.

The different plume extent predictions of the 4 models underline the importance of biodynamic assumptions in bioremediation modeling. The neglect of anerobiosis in the oxygen-limited model “HXO” causes it to underpredict total biodegradation and hence produce a longer hydrocarbon plume than the other models. On the other hand, inclusion of this metabolic mechanism, in the sequential electron-acceptor model “HXON”, produces the shortest predicted plume. In this case, the hydrocarbon in zones where oxygen is depleted still undergoes biodegradation but with biota using nitrate as the electron acceptor. The spatial distribution of oxygen and nitrate predicted by these models are presented in Figure 5. The long anaerobic core predicted by model “HXO” is caused by hydrocarbon availability and the assumption that microorganisms use only oxygen as electron acceptor. Low oxygen levels in this core cause low biodegradation rates and hence a longer hydrocarbon plume. The “HXON” model predicts a shorter core as microbes switch to anaerobic metabolism where O levels are low and metabolize the hydrocarbon with nitrate as electron acceptor. Decreased N levels, within the anaerobic core, illustrate the redox zonation predicted by this model.

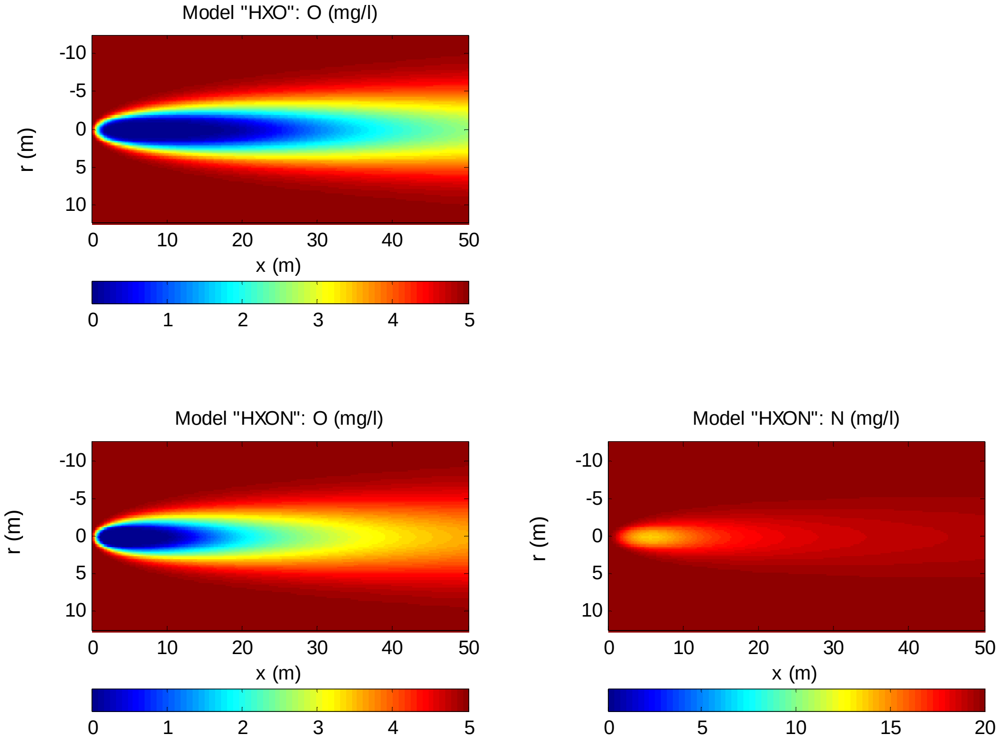

Figure 5. Steady-State Distributions of Oxygen and Nitrate

Further insight into the differences between models can be gained by observing the predicted steady distributions of biota concentration (Figure 6). In the oxygen-limited “HXO” model, microorganism growth and activity are controlled by the availability of both hydrocarbon, from the leaky tank, and oxygen, from the background water flow. The availability of the latter is controlled by transverse dispersion which, in the present case, does not act fast enough, relative to consumption by biota, to replenish the anaerobic core (Cirpka et al., 1999). Consequently, significant biotic growth and activity are limited to the head and periphery of the hydrocarbon plume. Availability of background nitrate, and its use during anaerobiosis, as considered by the “HXON” model, lead on the other hand to a more uniform distribution of biotic activity, with no “hole” at the hydrocarbon plume’s core. This distribution resembles that of the non-electron-acceptor-limited model “HX” and explains the relative similarity of hydrocarbon plumes predicted under “HX” and “HXON” assumptions.

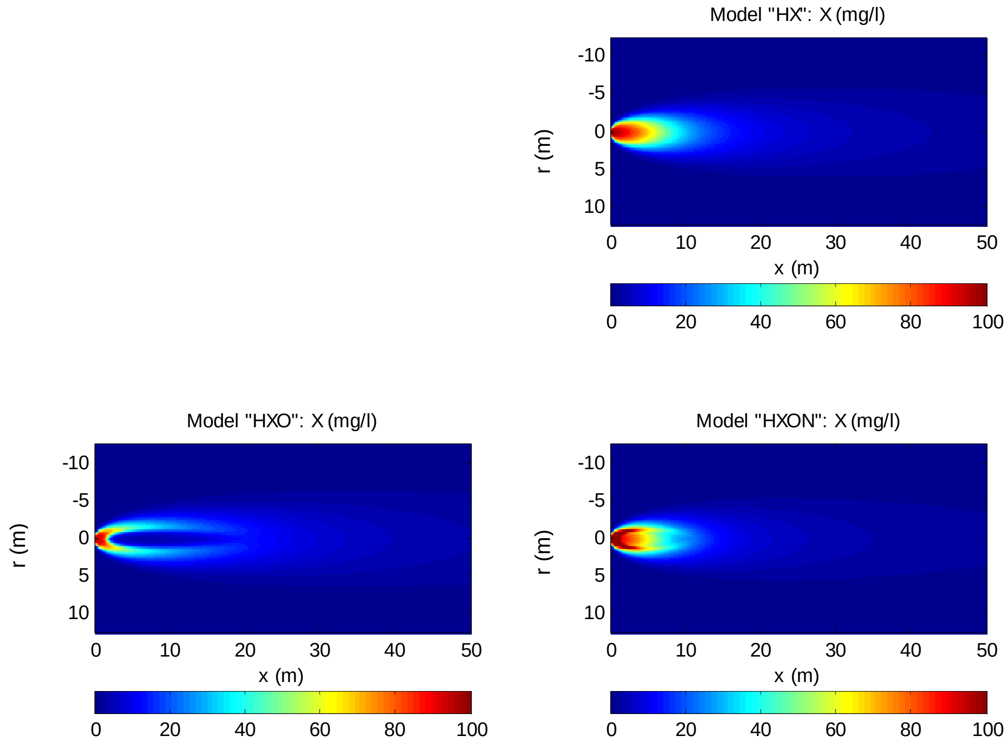

Figure 6. Steady-State Distributions of Microorganisms Predicted by the Models

5. Summary and Conclusions

This contribution evaluated the importance of considering sequential electron acceptor processes when modeling hydrocarbon bioremediation downgradient of a leaky subsurface tank. This was performed by comparing predictions of transport models ranging from linear reactive (“H”) to sequential two-electron acceptor model (“HXON”) and was limited to a single transport scenario at its steady-state limit. The main result is that the sequence of aerobic and anaerobic metabolisms enhances bioremediation relative to aerobiosis alone and is not well represented by a single electron-acceptor aerobic model (“HXO”). The single equation nonlinear model (“HX”) produces a better approximation of the two-electron acceptor model but underestimates bioremediation. The simplest linear model (“H”) underestimates biodegradation and is difficult to apply because of the need to estimate the constant biota concentration (X_c). The conclusion is that sequential electron acceptor dynamics are important for bioremediation predictions and, for the present case, model “HX” approximates them better than “X” or “HXO”.

Acknowledgements

This material is based upon work supported by the National Science Foundation under Grant No. 0134424. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

References

Atlas, R.M. and C.E. Cerniglia, 1995. Bioremediation of petroleum pollutants: diversity and environmental aspects of hydrocarbon biodegradation. Biosci. 45(5):332-338.

Bear, J., 1972. Dynamics of Fluids in Porous Media. Dover, Mineola, NJ.

Borden, R.C. and P.B. Bedient, 1986. Transport of dissolved hydrocarbons influences by oxygen limited biodegradation, 1. Theoretical development. Water Resour. Res., 22:1973-1982.

Cirpka, O.A., E.O. Frind and R. Helmig, 1999. Numerical simulation of biodegradation controlled by transverse mixing. J. Contam Hydrol., 40(1999):159-182.

Fischer, H.B., E.J. List, R.C.Y. Koh, J. Imberger and N.H. Brooks, 1979. Mixing in Inland and Coastal Waters. Academic Press Inc., New York, NY.

Huyakorn, P.S. and G.F. Pinder, 1983. Computational Methods in Subsurface Flow. Academic Press, New York, NY.

Ludvigsen, L., H.J. Albrechtsen, G. Heron, P.L. Bjerg and T.H. Christensen, 1998. Anaerobic microbial redox processes in a landfill leachate contaminated aquifer. J. Contam. Hydrol., 33(1998):273-291.

MacQuarrie, K.T.B. and E.A. Sudicky, 2001. Multicomponent simulation of wastewater-derived nitrogen and carbon in shallow unconfined aquifers: I. Model formulation and performance. J. Contam. Hydrol., 47(2001):53-84.

Mayer, K.U., S.G. Benner, E.O. Frind, S.F. Thornton and D.N. Lerner, 2001. Reactive transport modeling of processes controlling the distribution and natural attenuation of phenolic compounds in a deep sandstone aquifer. J. Contam. Hydrol., 53(2001):341-368.

Murray, J.D., 2003. Mathematical Biology, II: Spatial Models and Biomedical Applications. Springer, New York, NY.

Polianin, A.D., 2002. Handbook of Linear Partial Differential Equations for Engineers and Scientists. Chapman & Hall, New York, NY.

Potsma, D. and R. Jakobsen, 1996. Redox zonation: equilibrium constraints on the Fe(III)/SO4- reduction interface. Geoch. Cosmo. Act., 60(17):3169-3175.