

The influence of biogeochemical conditions and level of model complexity when simulating cometabolic biodegradation in sorbent-water systems

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Abstract

Eighteen models with different levels of complexity for representing sorption, mass transfer, and biodegradation are used to simulate the biodegradation of toluene (primary substrate) and TCE (cometabolic substrate). The simulations are conducted for hypothetical completely mixed systems of various scenarios with regard to sorbent, microbial composition, and solute concentrations. The purpose of the suite of simulations is to investigate the sensitivity of different modeling approaches in simulating the bio-attenuation of co-existing solutes in sorbent-water systems. The sensitivity of results to the modeling approach depends on the biogeochemical conditions of the system. For example, the results are insensitive to the type of sorption model in systems with low sorption strength and slow biodegradation rates, and insensitive to the biodegradation rate model if mass transfer controlled. Differences among model results are generally greater when evaluated in terms of total mass removal rather than aqueous phase concentration reduction. The fate of the cometabolite is more sensitive to the proper consideration of co-solute effects than is the fate of the primary substrate. For a given system, graphical comparison of a characteristic mass transfer rate coefficient (α_{mt}) versus a characteristic biodegradation rate coefficient (α_{bio}) provides an indication of how sensitivity to the different processes may be expected to change with time and can guide the selection of an appropriate level of model complexity.

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1. Introduction

An ongoing difficulty in simulating the fate of contaminants in subsurface environments is that the modeled macro-scale phenomena are primarily governed by complex micro-scale processes that are hard to isolate and characterize in heterogeneous subsurface environments. For this reason, models developed using overly simplistic assumptions will fail under field conditions

that are outside the bound of their calibration [60]. These failures are often attributable to the small-scale and short-term conditions of laboratory experiments that do not adequately reflect longer-term rate phenomena [61], but also result from simplifications in the model formulations that do not sufficiently account for complex solute–soil, solute–microbial, and solute–solute interactions [32,65,69]. Practical constraints often prevent the full incorporation of all processes into a model, and there is an inherent conflict between the desire to constrain the model complexity (and associated uncertainty of model parameter values) with the need to more mechanistically model complex processes [12,13,42].

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One area in which past model simplifications have been inadequate (and where laboratory data have provided new insight) is in regard to sorption and the related issues of mass transfer (e.g., desorption). Recent studies have underscored the need to better delineate and represent complex sorption mechanisms and desorption/diffusion processes. For example, research has shown that using linear isotherms as a convenient approximation for nonlinear sorption can lead to large errors in predicting aqueous concentrations (e.g., [16,61,68]). Other work has shown that the commonly used first-order rate model for simulating desorption and intraparticle mass transfer oversimplifies sorption and desorption dynamics and can lead to large errors after long times of desorption or under scenarios that involve time-variant boundary conditions external to the sorbent particle (e.g., [37,38,51,59,61,83]). Even highly mechanistic pore diffusion models are often inaccurate for natural sorbents and porous media because they can never precisely account for inherent heterogeneities in particle shapes, sizes, sorption capacities, sorbent-phase pore volumes and internal structures (e.g., [10,22,46,57]). Co-existing solutes also can affect both sorption and mass transfer by competing for sorption sites (e.g., [36,52,62,79]).

Given such complexities, increased sophistication has been incorporated into numerical models to describe pollutant fate and remediation. For example, improved sorption isotherm models are available to more mechanistically describe sorption nonlinearity by more distinctly accounting for the simultaneous absorption into natural organic matter and adsorption onto “harder” substances [2,43,44,77,78,80,81], and models have also been developed to consider competitive sorption in multi-solute systems (e.g., [27,54,62]). Some recently developed models for mass transfer explicitly account for diffusion in particles of different sizes, geometries, and internal porosities [10,46], and others consider particle heterogeneities using multiple rate constants (e.g., [24,45,73]), including stochastic approaches with statistical distributions of rate or combinations of rate and sorption capacity (e.g., [22,39,57]).

Biodegradation kinetics are also modeled with various approaches. Although first-order models offer simplifications valuable for model construction and interpretation, biodegradation models are also available for more mechanistically representing concepts of enzyme saturation and biomass growth. These include not only the classical Monod equation [21,49,55], but also modifications to the Monod equation that can account for the formation of toxic degradation products (e.g., [28,30]), co-solute inhibition, and cometabolism (e.g., [6,26]).

The increased sophistication of sorption, diffusion, and biodegradation models has led to a greater ability to predict and simulate solute fate in many well-defined laboratory experiments. For poorly characterized sys-

tems, however, a drawback to increased model sophistication is that more complex models invariably have a greater number of parameters, not all of which can be independently determined using currently available methods [70]. In such cases, the better fit to experimental data may be only a result of an increase in the degrees of freedom and may not truly reflect a more mechanistic representation of the governing processes [33,34,45]. Thus, when a detailed characterization of biogeochemical properties is impractical or infeasible, what is likely a more mechanistic representation is compromised by assuming a simpler model that can be more easily parameterized and implemented. Given that all models can never be fully mechanistic for complex and heterogeneous media, the choice of an “appropriate” model is often unclear. A general rule (sometimes referred to as Occam’s Razor) is that the most appropriate model for a given situation is that which uses as few unspecified parameters as possible to describe the principal outcomes of concern with reasonable accuracy. Use of such a model will minimize the possibility of nonunique parameters and increase the likelihood that the parameters are appropriately descriptive for the system at hand [42]. In this context, exploring the sensitivity of a model’s results to various simplifying assumptions can offer insight into model selection.

This paper explores model sensitivity for co-solute systems as influenced by solute concentration, sorption, mass transfer, and cometabolic biodegradation in order to provide insight on the level of modeling complexity that is needed for different system conditions. Several models with hierarchical levels of complexity in their process representations are used to simulate cometabolic biodegradation in some selected hypothetical, completely mixed domains that represent volume elements of water-saturated porous media. Toluene and TCE are used as model contaminants for the primary (growth) and cometabolic (nongrowth) substrates. Although a comprehensive analysis of all models and environmental scenarios is obviously not possible, the case studies presented do illustrate how different combinations of biogeochemical factors affect model sensitivity in well-mixed systems that include cometabolic biodegradation.

2. Concepts and methods

2.1. Model development

The assumed modeling domain is a finite-volume, completely mixed, soil–water system in which the solute mass changes over time can be related by the following:

$$\frac{\partial M_T(t)}{\partial t} = \frac{\partial M_w(t)}{\partial t} + \frac{\partial M_s(t)}{\partial t} \quad (1)$$

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