



A software tool for simulating contaminant transport and remedial effectiveness in sediment environments

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ABSTRACT

Sediments have often acted as sinks for contaminants that possess strong affinity for solids near historical pollution sources. Mathematical models describing the evolution of contaminant concentrations in sediment environments provide a scientific basis for decision support and remediation design. Herein, novel software (CapSim) is introduced including processes relevant to natural attenuation and *in-situ* treatment and containment (capping). The tool has been used as a basis for remedial design at a number of sites throughout the United States. CapSim is built on the concept of an arbitrary number of layers that each exhibit traditional porous media transport processes including sorption (linear and non-linear, transient or local equilibrium), advection, diffusion, dispersion, multicomponent linked reactions and, critically, processes specific to the sediment-water interface including bioturbation of both solids and porewater, deposition, consolidation, and interaction with the overlying surface water. A summary of recent applications and selected simulations of key features are presented.

1. Introduction

Historical failures to control pollution sources have generated a legacy of contaminated sites near industrial areas throughout the world. Sediments frequently act as sinks for such contamination, particularly when the constituents exhibit affinity for solids. There are few economically viable options for management of contaminated sediments. *In-situ* management, which includes monitored natural recovery (MNR), *in-situ* treatment with sorptive or reactive materials, and *in-situ* containment via placement of a capping layer, represent some of the most cost-effective approaches. MNR is a remedy that uses known naturally occurring processes to contain, eliminate or reduce the bioavailability and toxicity of contaminants in sediment. Generally, MNR involves contaminant source control, evaluation of potential attenuation mechanisms and long-term monitoring to confirm the performance. *In-situ* treatment normally involves the incorporation of a sorbent such as biochar or activated carbon directly into the sediment layer to reduce bioavailability but other sorbents or reagents encouraging contaminant transformation have been proposed. *In-situ* capping refers to the placement of a subaqueous covering of clean material over contaminated sediment that provides new substrate and buries the contaminants below the biologically active zone. The cover material may include a homogeneous medium such as sands or sediments but may also include

amendments to aid containment or degradation of the contaminants. Each of these remedies seeks to reduce the availability or mobility of the contaminants over the long-term and full performance can rarely be assessed with short term monitoring. A modeling tool capable of simulating the availability, mobility and transformation of the contaminant is needed to predict whether the long-term performance criteria may be achieved. Such a tool can also be used to predict short-term performance that can be directly compared to post-remedy monitoring.

Recent studies have demonstrated the efficacy of sand caps to mitigate environmental risks associated with sediments provided the depth exceeds that of bioturbation by benthic organisms and the amount of groundwater upwelling is not substantial (Lampert, 2010; Lampert et al., 2011, 2013; Reible et al., 2006; Thomas et al., 2014). With substantial upwelling, amended caps or *in-situ* treatment with sorptive materials such as organoclay (Sharma et al., 2009; Reible et al., 2007, 2008), biochar or activated carbon (Lin et al., 2014), and apatites (Peld et al., 2004) have been employed to improve the efficacy of the remedy. Activated carbon can be effective for hydrophobic organic compounds such as PAHs and PCBs and certain metals such as mercury. Sometimes the carbon may be placed within a capping material such as sand or within a geotextile to aid retention of the relatively light material. Clay layers have been proposed to decrease pore water advection

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and the associated contaminant transport (Reible et al., 2006), although this can lead to accumulation of upwelling water and microbially produced gas (Yuan et al., 1995). Benthic communities that contain bacteria with specific reductase enzymatic functions have been proposed if the environmental conditions are feasible for community growth (Himmelheber et al., 2008; Hyun et al., 2006; Johnson et al., 2010). Zero-valent iron as a capping material has also been proposed for treating nitroaromatics, chromium, lead, DDT, and related compounds (Agrawal and Tratnyek, 1996; Sayles et al., 1997; Wang et al., 2011; Reible et al., 2014). Yan and Reible (2015) demonstrated the potential of electrode-enhanced capping using electrodes in combination with natural degradation of phenanthrene, as well as an increase in polycyclic aromatic hydrocarbon (PAH) degrading genes in the benthic community surrounding the electrodes. Wang et al. (2014) developed a bio-reactive cap membrane comprised of polysulfone, granular activated carbon, and immobilized microorganisms (PS/GAC+) to remove nitrobenzene from sediment. The results indicated that more than 70% of the nitrobenzene present in the sediment was removed using the PS/GAC + membrane cap. Meric et al. (2014) experimented with reactive core mats (RCMs) and found that the geotextile filtering layers provided advantageous filtering for low advective fluxes to capture COCs, while the reactive core in-between the geotextile layers provides good sorption of COCs during high advective fluxes. Red soil rich in iron, aluminum, and oxygen was used by Xia et al. (2016) to control the release of nitrogen and phosphorous from sediment to the water body, and effectively increased the water standard by decreasing the chances of algal blooms. The metallic oxides enhanced the adsorption of the nutrients.

The appropriate design approach for sites where sediment contamination requires remedial action depends on successful modeling of the long-term behavior of contaminants. Site specific conditions and desired remediation goals based upon water body uses, water standards, and habitat restoration (Reible et al., 2014) govern the capping design and must be established. When employing a cap or *in-situ* treatment, it is vital to choose the appropriate materials to meet remediation goals and to do so in an economical manner. Remediation goals may be a concentration at the sediment-water interface, a flux through the surface layers and into the overlying water or a porewater concentration which seeks to directly control the most available and most mobile fraction of contaminants. Materials that might be employed vary greatly in contaminant fate and transport properties. Mathematical models of the fate and transport of contaminants provide critical insight into the expected long-term behavior of various alternatives that guide remedial action and design.

Contaminant transport models often treat sediment processes relatively simply with exchange coefficients to and between one or more layers of sediment, e.g. to provide a boundary condition for water column models, or assume linear behavior to allow analytical solutions that can be readily computed (Lampert, 2010; Reible et al., 2014; Lampert and Reible, 2009). However, activated carbon amendments and/or black carbon in sediments exhibit non-linear and sometimes kinetically limited sorption (Yang et al., 2012; Hong and Luthy, 2008; Murphy et al., 2006; Werner et al., 2006). To address these and other limitations and more realistically describe surficial sediment processes, the CapSim model was developed. Key features of CapSim include the ability to simulate multiple layers of materials including mixtures of inert material and sorbents, advection/diffusion/dispersion processes, bioturbation, or mixing associated with benthic macroorganisms, resulting in transport of both solid particles and pore water, groundwater upwelling and tidal (or other oscillating) flows, sediment consolidation and deposition (i.e., moving domain), transient or equilibrium linear or nonlinear sorption, exchange at the sediment-water interface, and dynamics of multiple species with linked reactions in sediments. The model can be used to simulate the contaminant transport and release from an unremediated sediment, simulate natural recovery of sediments or predict the effectiveness of *in-situ* treatment or capping.

Table 1

Conventional and unconventional and sediment specific processes simulated by CapSim software.

Conventional Process	Unconventional/Sediment Processes
Advection	Bioturbation including particle mixing
Diffusion	Consolidation
First-order decay	Benthic exchange with overlying water
Equilibrium sorption/desorption	Deposition
	Multispecies reaction
	Kinetic sorption and desorption (linear/nonlinear)

2. Model features and software design

CapSim accounts for multiple layers of varying properties and allows the user to input specific properties of the material or use typical values from a database of characteristics for different materials. The thickness of layers can be varied to describe arbitrary variations in conditions in sediment or to determine the most economical solution for a given set of design criteria. The model incorporates traditional porous media transport processes including advection, diffusion, dispersion, reaction and sorption, but also includes the capability to simulate processes specific to the near-surface sediment including deposition, consolidation, bioturbation, and exchange with the overlying water as summarized in Table 1.

2.1. Governing equations and key processes

The sediment with any potential cap or *in-situ* treatment is conceptualized as a one-dimensional stratified system composed of multiple layers with various physical and chemical properties. The top and the bottom of the system are in contact with the overlying water body and the underlying sediment, respectively. All layers are simulated as saturated porous media with the solid particles as immobile except in the bioturbation zone near the surface, where particles can be moved by the activities of benthic organisms (Matisoff, 1995) and when sediment continuously deposits to the surface. Dissolved organic carbon (DOC), which can preferentially absorb hydrophobic organic contaminants, is treated as a third phase besides the water and the sediment solids. This phase can contribute to the total porewater burden of these contaminants. The contaminants are distributed to all three phases and transported within the layer and across the interface between layers. The mass conservation equation for the one-dimensional multi-layered multi-species porous media system is given in Equation (1).

$$\sum_m \left(\varepsilon_m \frac{\partial \phi_m C_n (1 + \rho_{DOC,i} K_{DOC,n})}{\partial t} + \rho_{b,m} \frac{\partial \phi_m q_{m,n}}{\partial t} \right) = - \frac{\partial F_n}{\partial z} + \left(\sum_m \varepsilon_m \phi_m \right) \sum_l a_{l,n} r_{xn_{l,i}} \quad (1)$$

The mass loading of the *n*th contaminant in mobile phase consists of the free-molecular concentration C_n and its DOC associated concentration, which is calculated by the DOC concentration in the *i*th layer $\rho_{DOC,i}$ and the porewater-DOC partitioning coefficient, $K_{DOC,n}$ (Burkhard, 2000). The generation or consumption of the *n*th contaminant by reactions in porewater is summarized as $\sum_l a_{l,n} r_{xn_{l,i}}$, where $r_{xn_{l,i}}$ is the reaction rate of the *l*th reaction in the *i*th layer and $a_{l,n}$ is the stoichiometric coefficient of the *n*th chemical in the *l*th reaction. The porewater concentrations are continuous through layers while the DOC concentration and the reaction terms are assumed to be limited in the defined layer. ε_m and $\rho_{b,m}$ are the porosity and bulk density of the *m*th material. The porosities and the bulk densities of solid mixtures in the system are assumed to be the linear sums of the individual solid components properties weighted by their volumetric fractions ϕ_m . If the property of the mixture is known to be different, the mixture can be

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