REMEDIATION TECHNOLOGIES
Technical Reference

MODELING FOR THE DESIGN OF ACTIVE LAYERS FOR CONTAMINATED SEDIMENT CAPS

An interactive Excel spreadsheet (TR-843b) was developed by Dr. Danny Reible, University of Texas at Austin, to model active capping of contaminated sediment. The following guide provides information on the use of the model for contaminated sediment cap design.

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Modeling for the Design of Active Layers for Contaminated Sediment Caps

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Summary

This technical note summarizes the practical use of models for the design of contaminated sediment caps comprising both conventional cap layers (comprised of largely inert sandy materials) and active caps (typically composed of more sorbing or more reactive materials). The focus is on a particular model, implemented in an Excel spreadsheet which is appropriate for preliminary design or final design when a more sophisticated model is not required. Processes that must normally be considered in design of a sediment cap include advection (groundwater upwelling), diffusion, sorption, and reaction. Deposition of fresh sediment at the cap water interface may also be an important process. The models considered include an analytical steady state model and an analytical transient model, both implemented in the Excel spreadsheet. Together they represent a complete model of a cap capable of meeting the typical design questions for capping, namely 1) how long is a cap completely protective?, and, 2) what is the maximum concentration or flux in or through the near surface layer of a cap at any time?

To maintain simplicity, the active cap layer thickness is converted to an equivalent sand cap thickness using the transport and sorption characteristics of the active cap layer. Both models are conservative in that they assume that the contaminant source in the underlying sediment is essentially constant (constant underlying sediment concentration). The steady state model is the most conservative in that it estimates the maximum concentrations and contaminant fluxes that can ever be observed in and through the cap. The transient model is primarily designed to predict the time before any significant concentration or flux is detected in the near surface biologically active zone but also is useful for estimating concentrations versus depth in the cap prior to that time. Together, the two models provide a nearly complete description of cap behavior since the time between when significant concentrations are first observed in the near surface biologically active zone and the attainment of steady state conditions is typically short.

Description of the period between the onset of significant concentrations in the biologically active zone and steady state or the analysis of multiple layers of cap material with the full suite of potentially applicable processes normally requires a numerical model. In particular, explicit modeling of the transport characteristics of the active cap layer or simulation of depletion in the underlying contaminated sediment generally requires a numerical design model. A numeric model is typically pursued when the conservatism in the analytical models give rise to an unfeasible design. The better representation of fate and transport processes available from the numerical model can provide a more accurate final design. Both the analytical and numerical models are available from www.ce.utexas.edu/reiblegroup/index.htm .

Model Description

The model includes both a transient model to predict the time until significant concentrations or fluxes of contaminants are observed in the near-surface biologically active zone and a steady state model which describes maximum concentrations and fluxes. The transient model only predicts the concentration as a function of time and position in a single layer, the cap isolation layer. The cap isolation layer is the placed layer of sand or other capping material minus the portion of the cap compromised by consolidation of the cap or underlying sediment (which expresses porewater into a portion of the cap) or by bioturbation of the near surface biologically active zone. The transient model simulation is valid as long as significant concentrations have not yet penetrated into the overlying biological active zone. The model is based upon the solution to the advection-diffusion equation referenced in Van Genuchten (1981). Since the model simulates behavior in only a single layer, assumed to exhibit uniform properties, the different physical properties and transport conditions in the biologically active zone are not simulated. An active layer with strong sorptive properties or retarded transport properties is represented by an effective thickness with the same properties of the rest of the chemical isolation layer. That is, the effective thickness of the chemical isolation layer is increased to account for the specific properties of the active layer.

The steady state analytical model evaluates the long time behavior of the cap, after both the biologically active layer and the underlying cap layer are influenced by contaminant migration from below. It estimates the maximum concentration or flux that can ever be expected from a cap assuming that the underlying concentration is constant. The model implemented in the spreadsheet is a two layer steady state model which predicts concentrations and fluxes in a chemical isolation layer or in the near surface biologically active zone. The model is described in detail in Lampert and Reible (2008). Because the model explicitly models two distinct cap layers (the chemical isolation layer and the biologically active layer), it can describe a variety of conditions that the transient model cannot. To incorporate spatial variations in parameters in a transient model, a numerical model is normally required   Because an active cap layer is potentially a third layer, it is simulated in the spreadsheet by an effective cap thickness. The steady state effective active layer thickness is not identical to the transient layer thickness, however, due to the fact that sorption-related retardation is strictly a transient property.

Model parameters and their definitions are shown below. Although the parameters are used to define both the steady state and transient model, note that many are not applicable in the transient model since it describes migration in only a single capping isolation layer (as modified by the effective thickness of an active cap layer). Parameters shown in the spreadsheet in blue are normal model inputs that the user is free to change as needed. Parameters shown in red are calculated and normally these values should not be changed unless different calculation procedures are desired or there exist site or contaminant specific data that are believed to lead to better parameter predictions than the embedded model.

Contaminant Properties

Contaminant – identification of contaminant for easy reference.

Organic Carbon Partition Coefficient, log K_{OC} – tabulated K_{OC} used in the calculation of the partition coefficient through the formula $K_d=K_{OC}*f_{OC}$ where f_{OC} is the fraction organic carbon of the layer of interest. Note that inorganic contaminants can be simulated by including an effective Log K_d as the Log K_{OC} entry and choosing $f_{OC}=1$ as the layer of interest.

Colloidal Organic Carbon Partition Coefficient, log K_{DOC} – dissolved organic matter can increase the mobile fraction of contaminant. For PAHs, Burkhard (2000) has suggested log K_{DOC} = log K_{OW} – 0.58 where K_{OW} is the tabulated octanol-water partition coefficient.

Water Diffusivity, D_W – diffusivity of the pure contaminant in water, cm^2/s.

Cap Decay Rate (porewater basis), λ_1 – contaminant degradation rate in cap interstitial waters, yr^1.

Bioturbation Layer Decay Rate (porewater basis), λ_2 – contaminant degradation rate in interstitial water of surficial biologically active layer in yr^1.

Sediment/Bioturbation Layer Properties

Contaminant Pore Water Concentration, C_0 – interstitial concentration in the near surface layer of the underlying sediment, µg/L.

Biologically Active Zone Fraction Organic Carbon, $(f_{OC})_{bio}$ – surficial layer organic carbon content (as a fraction of sediment dry weight), assumed to apply to both the underlying sediment before capping and the surficial cap layer at steady state (after deposition of new sediment).

Colloidal Organic Carbon Concentration, ρ_{DOC} – dissolved organic carbon in sediment and cap interstitial waters, mg/L.

Darcy Velocity, V – volume of upwelling water discharging into overlying water body per unit surface area per time, $cm^3/(cm^2\text{-}yr)$. V is forced $\geq$ 0, that is, losing bodies of water (downward velocity) are conservatively estimated as diffusion only.

Depositional Velocity, V_{dep} – rate of deposition of new sediment in cm/yr. The deposition velocity is used to estimate an effective Darcy velocity using the sorption characteristics of the chemical isolation layer.

Bioturbation Layer Thickness, h_{bio} – thickness, in cm, of the biologically active layer that will develop at the surface of the cap. Figure 1 shows the probability distribution for this parameter in freshwater (median = 4.8 cm) and estuarine systems (median = 7.9 cm).

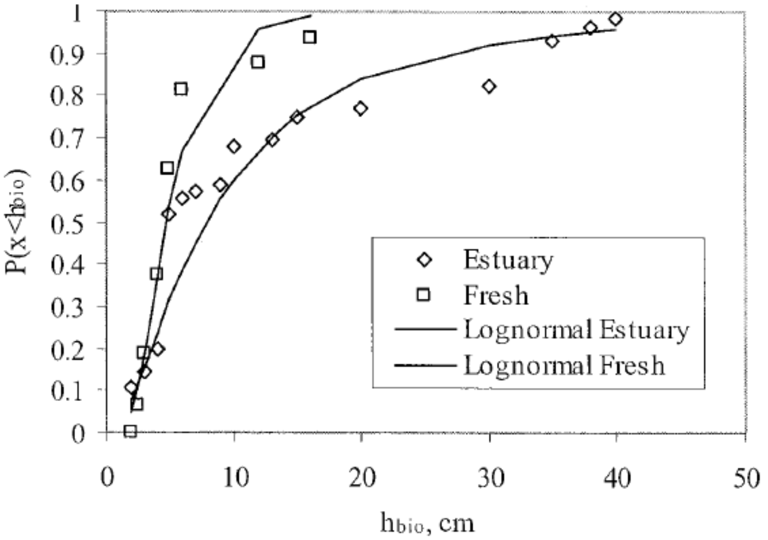

Figure 1. Distribution of measurements of h_{bio} (adapted from Thoms et al. 1995)

Pore Water Biodiffusion Coefficient, D_{bio}^{pw} – effective diffusion coefficient in biologically active layer based upon interstitial water, cm^2/yr. There is very little guidance for this parameter although measurements have shown 10^{-3}-10^{-5} cm^2/yr as reasonable estimates. Since the parameter also characterizes organism behavior, using a multiple of the particle diffusion coefficient below (e.g., 100 x D_{bio}^p) might be a reasonable estimation method. Note that although the numerical value of this parameter may be larger than D_{bio}^p, particle boidiffusion is typically more important due to contaminant sorption on the particles.

Particle Biodiffusion Coefficient, D_{bio}^p – effective particle diffusion coefficient in biological active layer, cm^2/yr. Figure 2 shows the probability distribution for this parameter in freshwater (median = 3.3 x 10^{-8} cm^2/sec= 1.06 cm^2/yr) and estuarine systems (median = 3 x 10^{-7} cm^2/sec= 9.4 cm^2/yr)

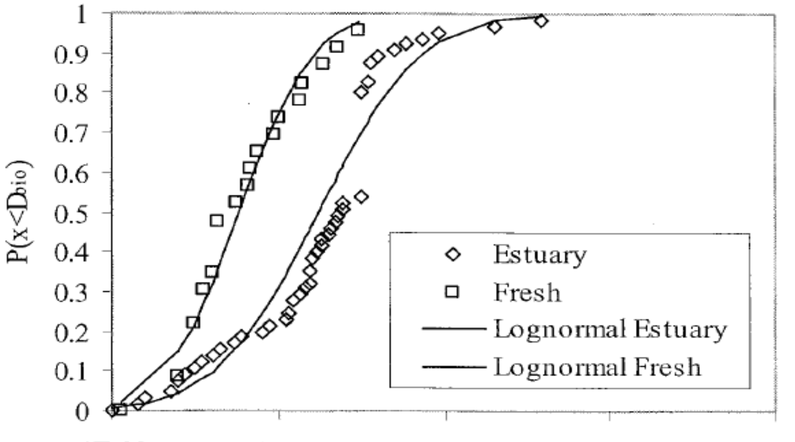

Figure 2. Distribution of measurements of D_{bio} (adapted from Thoms et al. 1995).

Boundary Layer Mass Transfer Coefficient, k_{bl} – benthic boundary layer mass transfer coefficient, cm/yr. A typical value is 1 cm/hr. A useful model for this parameter is:

$$k_{bl} = \frac{\sqrt{\nu_w} u_*}{Sc^{2/3} y_0^{1/2}}$$

Where v_w is the viscosity of water (~0.01 cm^2/hr), u is the friction velocity characterizing the shear stress at the sediment-water interface (typically 1-5 cm), y_0 is the hydrodynamic roughness of the sediment-water interface (typically 1-10 cm) and S_c is the Schmidt number, the ratio of kinematic velocity of water to the molecular diffusion coefficient of the contaminant in water (on the order of 1000 for most contaminants in water).

Note that the bioturbation layer and the benthic boundary layer do not normally influence the time over which a cap is protective nor the flux through the cap since the rate of chemical transport is much faster in these layers than in the chemical isolation layer. They are important, however, in assessing the steady state contaminant concentration that will be achieved in these layers.

Active Layer Properties

Layer Thickness - thickness of the active layer (enhanced sorbent) in cm. This can range from 1 cm (a typical active layer in a mat) to a thicker layer placed in bulk.

Steady state ratio of transport in active layer relative to conventional layer – Although the primary purpose of most commercially available active layers is to enhance sorption related retardation (a transient phenomena), it is also possible that an active layer may exhibit reduced transport rates under steady conditions. This would normally be a reduction in effective diffusion coefficient relative to the conventional sandy cap layers, for example, diffusivity in clay relative to that in sand. Since many active cap layers are also composed of granular media, this parameter should be assumed equal to one (transport in active layer equal to transport in sandy layer) without specific information to the contrary. This parameter should also normally be set equal to one in advection dominated systems.

Equivalent Active layer thickness (steady state equivalent) –Calculated thickness and is the actual layer thickness divided by the steady state ratio of transport in the active layer to the conventional layer.

Effective Partition Coefficient – Effective partition coefficient in (mg/kg sorbed)/(mg/L in porewater).

Active adsorbent loading – Mass of sorbent in active layer in kg/m^2 per cm of layer thickness.

Effective retardation factor, active layer – Calculated parameter given by effective partition coefficient times active adsorbent loading times layer thickness.

Equivalent sandy cap thickness (transient equivalent) – Calculated parameter indicating equivalent cap thickness under transient conditions. The greater sorption of the active cap layer (a transient phenomena) will cause the cap to have an equivalent thickness much greater than its physical thickness. If sorption in the active cap is identical to the conventional cap, this transient thickness will be identical to the steady state equivalent thickness.

Conventional Cap Properties

Depth of Specific Interest below cap-water interface, z – If performance (as indicated by porewater or bulk solid phase concentration) at a particular distance below the cap surface is desired, this depth can be entered here, in cm.

Fraction organic carbon at depth of interest, $f_{oc}(z)$- Fraction organic carbon at the depth of interest which is used to estimate the bulk solid phase concentration from the porewater concentration with the relationship $W=K_{oc}\, f_{oc}\, C_{pw.}$

Conventional Cap placed depth – The depth of placed sand or other conventional cap material, in cm. The effective depth will be less due to bioturbation or consolidation.

Cap consolidation depth – Depth that the cap consolidates (typically small for a sandy cap), in cm. This does not include the consolidation of the underlying sediment.

Underlying sediment consolidation due to cap placement – Underlying sediment consolidation, in cm. This indicates the total volume of porewater expressed into the cap layer. The migration of a contaminant expressed with this porewater may be considerably less than the total consolidation due to sorption-related retardation in the cap material.

Porosity, $\tilde{\varepsilon}$ - Void fraction in conventional cap material.

Particle Density, ρ_P - Conventional cap grain density, in g/cm^3.

Fraction organic carbon, $(f_{oc})_{eff}$ – Fraction organic carbon in conventional cap material.

Effective Sand Cap thickness, *h_{sand}* – Calculated quantity of effective thickness of conventional cap, in cm considering placed thickness, consolidation of cap and underlying sediment.

Steady State Equivalent Cap thickness, h_{cap} – Calculated effective thickness of overall cap for steady state calculations including both sand cap and active cap layer, in cm.

Transient Equivalent cap thickness, h_{equiv} - Calculated effective thickness of overall cap for transient calculations including both sand cap and active cap layer, in cm.

Effective cap partition coefficient – Calculated effective cap partition coefficient in L/kg.

Output-Steady State Model

Pore Water Concentration at Depth, C(z) – Model calculated steady state porewater concentration in porewater at the specific depth of interest, in µg/L.

Solid Concentration at Depth of Interest, W(z) – Model calculated steady state bulk solid phase concentration in µg/kg.

Average Bioturbation Layer Loading, $(W_{bio})avg$ – Model calculated steady state average bulk solid phase concentration in the biologically active zone, in µg/kg.

Flux to Overlying Water Column, J – Model calculated steady state flux to overlying water, $\mu g/m^2 \cdot yr$.

Cap-Bioturbation Interface Concentration, C_{bio}/C_0 – Steady state porewater concentration at the cap bioturbation layer interface, in % of concentration in underlying sediment.

Cap-Water Interface Concentration, C_{bl}/C_0 – Steady state porewater concentration at the cap water interface, in % of concentration in underlying sediment.

Average Bioturbation Concentration, $(C_{bio})avg/C_0$ – Steady state average porewater concentration in the biologically active zone, in % of concentration in underlying sediment.

Time to Containment Breakthrough, tadv/diff – Time before significant concentrations are expected in the biological active zone. Also the time after which the transient analytical model (2nd tab) may begin to overestimate concentrations in the biologically active zone.

Output - Transient Model (Transient Model Tab)

The model inputs summarized above are used to calculate key parameters for the transient model in the chemical isolation layer, i.e. the conventional sand layer as modified by the effective thickness of the active cap layer. These parameters include Peclet number (relating advection to diffusion, Dahmkohler number (relating reaction to diffusion), and a parameter u which is affected by both diffusion and advection. The final parameter needed for the model is the simulation time. The time until significant concentrations are noted in the biologically active zone is $t_{adv/diff}$. This would normally be the simulation time although if the the bioturbation rate in the biologically active zone is small or the concentration in that zone as predicted by the model at $_{tadv/diff}$ is small, the simulation time can be extended to give estimates of concentration in the capping isolation layer over a longer period of time. This may be especially important with an active sorbing layer in that the concentrations in much of the capping isolation layer are very small and essentially uniform for long periods of time after some penetration of contaminants are noted in the biologically active layer. If a longer simulation time it can simply be entered in the identified cell. The output from the simulation is shown on a figure showing both transient curves at various times and the long-time steady state curve for comparison. The results are also shown as concentrations (as the ratio of concentration to underlying sediment concentration) as a function of depth (in cm) and time. Note that the output will provide increased resolution in the sorbing active cap layer as appropriate.

The final tab in the spreadsheet model is designed to conduct sensitivity analyses on the steady state model only in that a variety of model parameters can be modified in each column and the steady state output values for those parameters are shown in that column.

References

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