

CapSim 4.2 Basic Users Manual

11/11/23

1. Introduction

CapSim is designed to simulate contaminant transport in sediments. It was primarily developed to model contaminant transport through sediment caps for the purposes of design, but it can also be used to simulate contaminant migration in uncapped sediments (e.g., for the evaluation of natural recovery) and in-situ treatment of sediments. The model is built on a foundation of sediment and cap modeling dating back to 1991 [1], and early versions were described in EPA guidance for capping in 1998 [2]. The model is designed to simulate contaminant transport as a result of processes in both the water and solid phases based upon the interstitial or porewater concentrations of contaminants.

The model breaks the sediment into one or more layers to allow different properties and conditions in each layer. These layers are of arbitrary thickness, and the model manages conditions across the interfaces between layers. Initial conditions (both uniform and variable sediment or water concentrations) can be specified within each layer. Boundary conditions of various types can be specified at the top and bottom layers. The top layer can connect to a completely mixed water volume (e.g., a lake) or a vertically mixed flowing water body (e.g., a river).

The current version is an extremely robust tool that includes capabilities for modeling contaminant transport in sediments under a wide range of conditions, including:

- Dynamics of multiple species with linked equilibrium and kinetic reactions in sediments, conventional and amended cap materials, and sediment amendments
- Biogeochemical processes and reactions
- Multiple layers with widely varying physical and chemical conditions and materials, including commercially available remedial materials
- Advection and diffusion/dispersion in all layers with corrections for tortuosity
- Bioturbation transport of contaminants in water and solids modeled by both uniform mixing over depth or depth-dependent bioturbation and with particle size dependent rates
- Groundwater upwelling and tidal or oscillating flows with both time-dependent and average fluxes or concentrations over oscillating flow cycles
- Hyporheic exchange
- Sediment consolidation with the input of characteristic time and 90% consolidation depth
- Simultaneous sediment erosion and deposition and intermixing of particles by bioturbation
- Linear, nonlinear, and kinetic sorption
- Mass transfer limited sediment and contaminant exchange at the sediment-water interface
- Estimation of water column concentrations for a finite well-mixed waterbody as a function of time
- NAPL can be modeled as either an immobile ("solid") or mobile phase.
Precipitation/dissolution reactions can be used to model immobile NAPL partitioning. Mobile

NAPL is modeled as a reactive aqueous component similar to colloidal organic matter and moves with the aqueous phase.

CapSim is largely menu-driven, and users can select options as needed. The model can estimate a variety of common sediment parameters, or the user can override these estimates with their own inputs. The purpose of this guide is to introduce CapSim and how to use the program. The scientific background and logic structure in programming can be further explored in references [3] and [4].

The current version of CapSim is V 4.2, and recent changes include the addition of hyporheic exchange, particle size dependent bioturbation, sediment exchange at the sediment-water interface, additional commercial materials, enhancements to computational speed, enhancements to equilibrium and kinetic reactions, ability to define initial and boundary conditions with solid or water concentration.

2. Download and install CapSim

CapSim can be downloaded from the webpage:

<https://www.depts.ttu.edu/ceweb/research/reiblesgroup/capsim.php>

Please send a short note to danny.reible@ttu.edu so that we can add you to the list of users to notify you of any future updates.

After downloading, you can launch the self-installing file and install the program by double clicking the .exe installation file. Make sure that you are using the version of CapSim appropriate for your computer (The current version of CapSim is currently only available for 64-bit Windows operating systems). If a Windows protection window pops up after running the installation file, click on “More info” and then click on the button “Run anyway” to process the installation.

You can also download this quick start manual, databases of chemical information, example input files, and example batch files from the above webpage.

3. Getting Started

This session introduces the basic structure of CapSim and an example of running CapSim input files. Session 3.1 introduces the main menu and its provided functions. Session 3.2 to 3.4 discusses three major compartments of CapSim, database, input, and output. Session 3.5 provides the instructions for loading and processing a batch input file for CapSim.

3.1. Main Menu

Upon starting the program, you will be presented with a main menu (Figure 1) which are series of push-button boxes that provide the following options:

- **Create new input file** – CapSim creates an input file that saves all your simulation options. This option creates a new input file and goes through all parameter input windows sequentially to gather information. An input file (.cpism) will be created after all parameters are collected.
- **Load existing input file** – CapSim saves all your simulation options from previous runs, and this option allows users to load information from existing input files. There is a sample input file available.
- **Load existing output file** – if you have output files from previously executed simulations, you can load the exported data file back to CapSim. CapSim will generate an input parameter file from the information in the output data file for future simulations.
- **Plot existing results** – if you have a previously executed simulation, you can load the exported data file and examine plots from that simulation or compare multiple simulations on one plot.
- **Run a batch file** – this is an advanced option to allow you to run multiple simulations without intervention. Two types of batch files are available, “Multi Scenarios” and “Monte Carlo Simulation”. Both types of files can be generated by selecting the appropriate choice of output batch file at the run time of what is presumed to be the baseline simulation. The batch file must be edited to achieve the desired multiple scenarios or a stochastic simulation around a particular parameter or parameters.
- **Edit chemical database** – this is the chemical database that provides CapSim basic data for the simulations. Some databases that include a variety of commonly used compounds are available online with the downloadable model. You can add to that database or create your own. You can also bypass the database and put information on materials and chemicals directly into a simulation as well. The database allows the information to be available for any simulation.
- **Edit material database** – this is the common solid material database that provides CapSim basic data for the simulations.

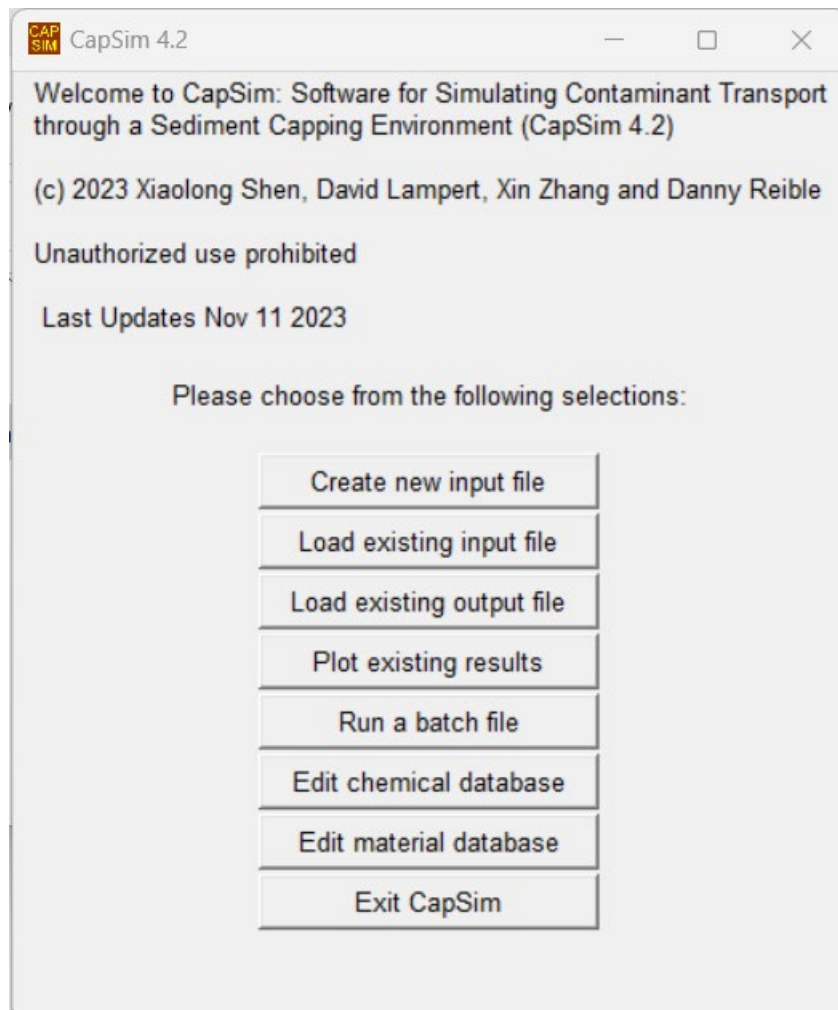


Figure 1 CapSim Main Menu

3.2. Database of Chemicals and Materials

CapSim stores properties of common contaminants and common remedial solid materials in the chemical database file “*capsim3_chemicaldatabase*” and “*capsim_soliddatabase*”, respectively. Both database files are stored in the folder “*database*” under the CapSim file directory and can be viewed in CapSim as shown in Figure 2 using the button **Edit chemical database** and **Edit material database** from the main menu. If you have a database from an old version of CapSim on your computer, you may need to delete that file before installing CapSim to avoid any complications with incompatibility.

The default chemical database only contains one contaminant but could be edited to include more contaminants. A full CapSim database, including the properties of all common organic and inorganic contaminants such as PCBs, PAHs, DDx, and heavy metals, are available on the CapSim webpage, named “Specific Chemical Database Files”. To load the properties of desired chemicals to the current database, you need to download the “Specific Chemical Database Files” .zip file from the webpage and extract the files to a known location. You could then use the button **Import database file** to import the desired chemicals from the full database provided online.

If you can’t find the corresponding properties for the chemicals, sediments, or auxiliary conditions in the existing database or prefer to use your own data, you can enter these directly for a simulation or you may want to edit the chemical or material database. For chemical properties, you generally need at least MW (molecular weight), K_{ow} (octanol-water partition coefficient), D_w (molecular diffusion coefficient), K_{oc} (organic carbon partition coefficient), and K_{doc} (dissolved organic carbon partition coefficient) under the same temperature. You can have data at multiple temperatures for a single contaminant if desired. These parameters can be estimated by CapSim from K_{ow} for hydrophobic organic compounds such as PAHs or PCBs using correlations in previous literature[5-8]. For metals, the K_{ow} , K_{oc} and K_{doc} may not be relevant, and you might leave these blank and simply specify a partition coefficient, K_d , during the simulation. Note that since these parameters are normally entered in log units, 0 should not be entered but instead small values such as -10 (log units) might be used. For material properties, porosity, bulk density, particle size, and organic carbon fraction are needed, and you can choose the form of sorption model, you would like to use for that material (“Linear specified- K_d ”, “Linear Kocfoc” (for organics), “Langmuir” or “Freundlich”). You have the option of changing these for a particular simulation, but the database contains default values.

CapSim 4.1

Please provide the following fundamental properties for the chemicals:

	Chemical name	Formula	Type	Temperature °C	Diffusivity in water cm ² /s	OC partition coefficient log(L/kg)	DOC partition coefficient log(L/kg)	Reference
Add Edit Delete	phenanthrene	C ₁₄ H ₁₀	Solute	0.0	7.47e-06	4.22	3.48	TCEQ

[Add new chemicals](#)
[Import database file](#)
[Save](#)
[Cancel](#)

Figure 2 CapSim Chemical Database

3.3. Input Parameter Summary

An input parameter summary window is shown after entering all parameters for a new input file or loading a previously created case using **Load existing input file** or **Load existing output file** from the *Main Menu*. The column of buttons on the right-hand side of the *Input Parameter Summary* window will lead to the parameter windows.

Most of the CapSim parameters are self-explanatory and follow standard usage. Some important parameters and their definitions within the program are summarized below,

- Concentration and total aqueous concentrations – concentration refers to truly dissolved porewater concentration (e.g., C_{free} as measured by partitioning passive samplers). Total aqueous concentrations include truly dissolved plus colloiddally associated contaminants, i.e., contaminants associated with dissolved organic matter or fine particulate matter. You can also set your initial conditions with a total concentration (e.g., concentrations measured by extraction of filtered water samples which would include colloiddally associated contaminants). In the latter case, you should set dissolved organic carbon concentrations to 0 and use measured site-specific partitioning coefficients since theoretical models of partitioning are based upon truly dissolved concentration.
- Solid concentration – Solid concentration is the concentration on solids in contaminant mass per mass dry solids.
- Bulk density – solid phase density of porous medium on a dry basis, i.e., dry solid mass/total volume
- Sorption– modeled as equilibrium partitioning using linear- K_d specified, linear-Kocfoc, Langmuir, or Freundlich models. In the absence of specific data, it is recommended that inorganic contaminants be modeled with an effective K_d specified. Similarly, the sorption of hydrophobic organics would normally be modeled as Kocfoc on sediments containing natural organic matter, K_d specified on organophilic clay, and with Freundlich models for activated carbon. Kinetics is modeled as a first-order rate constant times the *porewater concentration* and is normally of concern with a strongly sorbing porous material such as activated carbon. The sorption rate constant can be approximately estimated from the characteristics of the sorbent as described in the advanced topics.
- Upwelling Velocity – is a Darcy or superficial velocity based upon total flow area. If U is the Darcy velocity and v is the seepage velocity based upon void area, ϕ , $U=v\phi$. The velocity is positive upward from sediment to water.
- Diffusivity – molecular diffusion coefficient in water. The coefficient will be corrected for the porosity and tortuosity of the medium within the program.
- Hydrodynamic dispersivity – dispersion is modeled as αU , where α is the dispersivity (units of length), and U is the Darcy velocity. The dispersivity α is largely associated with the length scale of heterogeneities in the sediment layers and is not easily characterized. A common choice of dispersivity is an approximation of 5-10% of the travel path of groundwater flow. In the sediment system modeled by CapSim, the thickness of the sediment layer is used. Due to uncertainty in this parameter, it might be used as a basis for a sensitivity analysis.

- Bioturbation – bioturbation is the normal life-cycle activities of benthic organisms that cause movement of both particles and interstitial water. The process is modeled as the particle intermixing between layers (over the depth of bioturbation) and contaminant movement near the benthic surface. The strength of bioturbation is characterized by effective diffusion coefficients entered by the user. This manual includes some guidance for selecting the depth and magnitude of bioturbation. Bioturbation can be modeled as dependent upon particle size.
- Hyporheic exchange – water movement across the sediment-water interface as a result of the flow over the sediment surface and encourages mixing of interstitial water in the near-surface sediment. The depth and intensity of hyporheic exchange depend on the friction velocity in the overlying water and the particle size of the surficial sediment layer.
- Erosion and deposition can be modeled simultaneously to simulate sediment exchange or to represent a combination of depositional and erosional events over time (e.g., annually)
- Reaction kinetics – normal reactions are modeled as occurring in the porewater only. CapSim could simulate common reaction kinetics, including coupled reversible, precipitation/dissolution, and equilibrium reactions. The simulation time may increase greatly for complicated reaction networks.

A note about coordinates:

- The vertical (z) coordinate is usually defined from the sediment-water interface *downward* into the sediment
- The origin of the vertical coordinate can either be the original sediment-water interface or follow the sediment-water interface upward in the case of deposition (i.e., always at the current sediment-water interface)
- Although the vertical coordinate is positive downward, flux and velocity are defined as positive upward because these are typically of primary concern. For clarity, the flux is termed upward flux, and the velocity is termed upwelling velocity. Note that in previous versions of CapSim, flux was defined according to the coordinate direction that is positive downward.

A more detailed description of the use of the model and the simulation parameters is in Section 4.

CapSim 4.2

The following summarizes the information you have provided for this simulation. Please verify that it is correct and update as necessary.

System:	Length unit:	cm	Time unit:	yr		Edit System Parameters
	Concentration unit:	µg/L	Diffusion unit:	cm²/s		
Chemicals:	Mercury	Methylmercury	phenanthrene			Edit Chemical Properties
Equilibriums:						Edit Equilibrium Properties
Reactions:	Methylation	Hg ==> MeHg				Edit Reaction Properties
	Demethylation	MeHg ==> Hg				
	phenanthrene decay	C ₁₄ H ₉ NO ₂ Decay				Edit Reaction Coefficients
Layers:	Deposition	Sediment	0.1 cm/yr	No DOC	1.0 cm	Edit Material Properties
	Layer 1	Sand	10.0 cm	No DOC	1.0 cm	
	Layer 2	Activated Carbon	2.0 cm	No DOC	1.0 cm	Edit Sorption Properties
	Layer 3	Sediment	10.0 cm	No DOC	1.0 cm	
						Edit Layer Properties
Processes:	Advection flow: None					Edit Sediment Processes
	Bioturbation depth: 5.00 cm	Particle bioturbativity: 0.00 cm²/yr				
	Consolidation: None					Edit Boundary Conditions
	Hyperheic exchange: None	Erosion: None				
	Bioreaction model: TEA inhibition	Ionic activity: None				Edit Initial Conditions
Solver:	Simulation duration: 20.0 yr	Output time steps: 100				Edit Solver Options
	Total number of grids: 220	Time step size: 0.1 yr				
	Input file name: input_example					Edit File Options
	Batch file: None					
<div>OK</div> <div>Return to Main Menu</div> <div>Exit CapSim</div>						

Figure 3 CapSim Parameter Summary Window

3.4. Output

The default model output is the concentration profile of the first contaminant as a function of position at different times. You can also show “Total Aq. Concentration” (the sum of truly dissolved and colloiddally associated contaminants in the porewater), “Solid Concentration”, or the “Upward Flux”. For time-varying plots, you can also show the mass in the system (to check the material balance of the simulation to aid in ensuring adequate time and space resolution in the simulation).

Note that if you input a total concentration, including the contaminants in porewater and DOC, as the contaminant concentration in the auxiliary conditions and set the dissolved organic carbon to 0, the “Concentration” plot will be equivalent to the “Total Aq. Concentration”. Note that there is a subtle difference between this modeling approach versus the approach using truly dissolved concentration and DOC levels. DOC molecules are relatively large and typically have much lower diffusion coefficients than dissolved contaminants. If you input truly dissolved concentration and the dissolved organic carbon in each layer, the dissolved organic carbon is not assumed to diffuse but remains as defined in each layer (but any advection will transport both DOC-associated and truly dissolved contaminant). Suppose you input total concentration and set DOC = 0. In that case, however, the DOC-associated contaminant is assumed to diffuse just as if it were the dissolved contaminant (as well as be transported by advection).

When plotting time profiles, you have the option of plotting the spatial axis with 0 relative to the initial sediment-water interface or the sediment-water interface that may change with time due to deposition. For the latter, click **Edit plot** and choose “*Time profile*” and “*New benthic surface*” and depth of interest of 0. If you wish to see concentration within the surface layer, you can choose any depth relative to the initial or current sediment-water interface. A common choice is the middle of the bioturbation layer (e.g., 2.5 cm in a 5 cm bioturbation layer). This concentration represents the middle of the biologically active zone. It is more representative than the top surface, which is typically controlled by the surface water conditions regardless of the sediment conditions.

You can also view other plots if desired. You can select **Edit plot** and any desired spatial or time plots for porewater concentrations, fluxes, total concentrations, and solid concentrations in various solid materials. You can change the figure size, legend location, axis limits, and label font sizes by using the **Edit figure**.

If you see things you wish to change in the simulation, push **Modify system**. If you are happy with the simulation, you should export the result, and a pop-up window will allow you to choose a name and location. Note that if you do not export the results, the input file and the output results are still saved under the default simulation name. The saved output file has values for all parameters used in the simulation, so it is invaluable in defining the specific simulation conditions. When generating a batch file, the exported file will contain the baseline parameter values that will be changed in the batch file. The default location for exported files is the output subdirectory in the CapSim directory. This data can be brought back to the same plot and compared to other files using the Main Menu option **Plot existing results**. The plot options are the same as in the output screen, except you can import multiple result files and plot them all together.

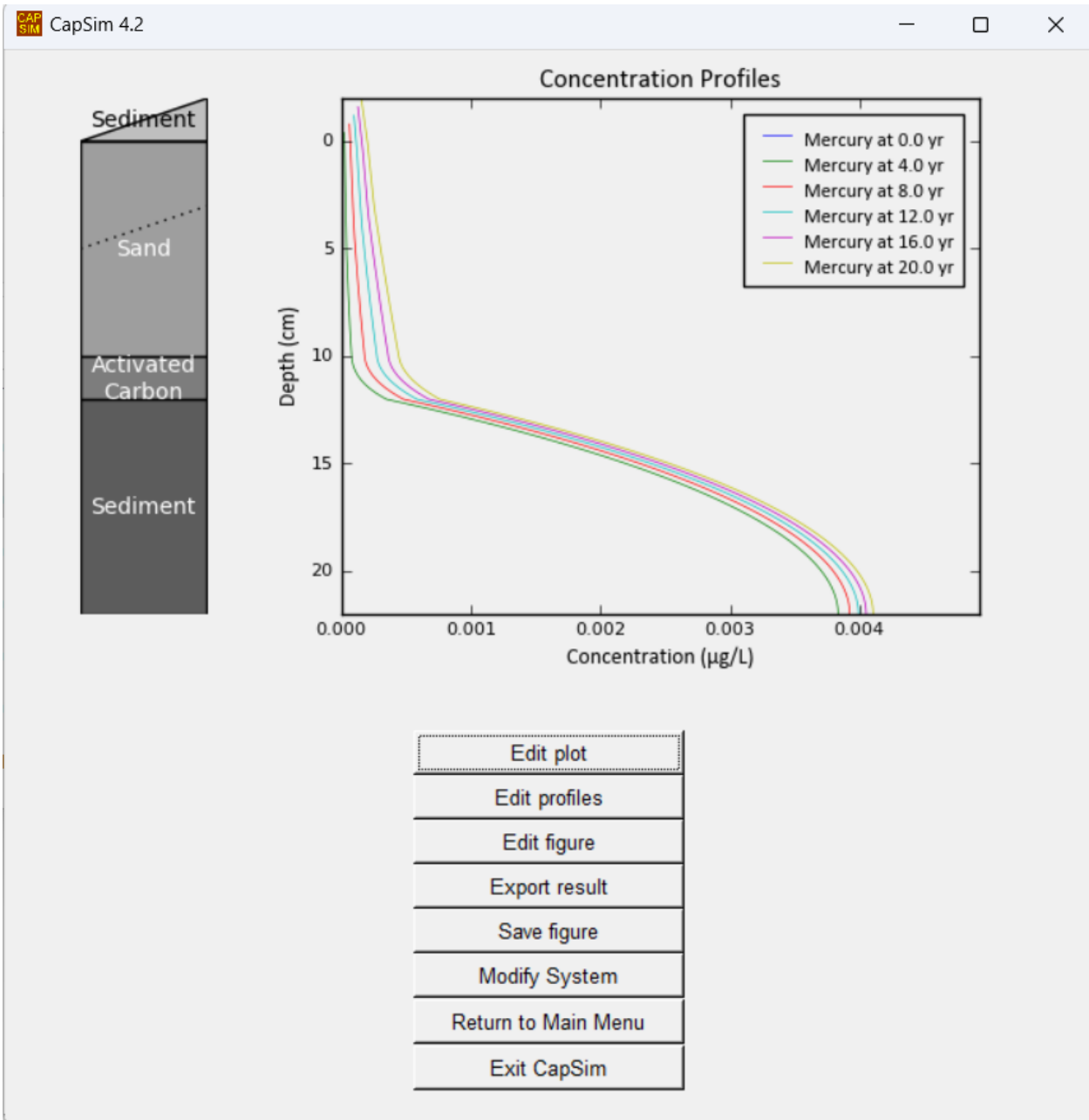


Figure 4 CapSim Output Plot Window

3.5. A Simple CapSim Simulation Example

Going over a simple example will give you a better understanding of what data you need and what output is expected. Click on **Load existing input file** from the Main Menu, and open "Hg_MeHg_PHE_Example.cpsm". A summary of the example simulation will appear with push button boxes on the right-hand side of the screen. You may need to expand the box or move the slider up or down on the right-hand side to see the primary simulation parameters. Other parameters can be viewed by clicking on the buttons on the right-hand side, which opens a menu with related parameters.

The contaminants in the sediment in this example are phenanthrene, mercury, and methylmercury. The example system contains three layers, namely, 10.0 cm of sand, 2.0cm of activated carbon, and 30.0 m of sediment from top to bottom. Mercury and phenanthrene are initially present in the underlying sediment layer, and methylmercury is formed in the lower layers while phenanthrene degrades (at a rate of 0.1/yr). Each layer also exhibits a dispersivity, α , equal to 10% of the thickness of the layer. Sediment processes include a steady Darcy upwelling velocity of 10 cm/yr, and the effective dispersion coefficient is this velocity times α . The system includes bioturbation by benthic organisms in the upper 5 cm of the sediment at an effective particle biodiffusion rate of 10 cm²/yr. To illustrate its use, the kinetics of uptake onto the activated carbon by phenanthrene are simulated assuming 1.5 mm granular carbon with an estimated half-life for sorption of 8.5 days. The simulation is for a period of 10 years, and the output will be saved in a file with the indicated name, and an Excel output file will automatically be created with the same name.

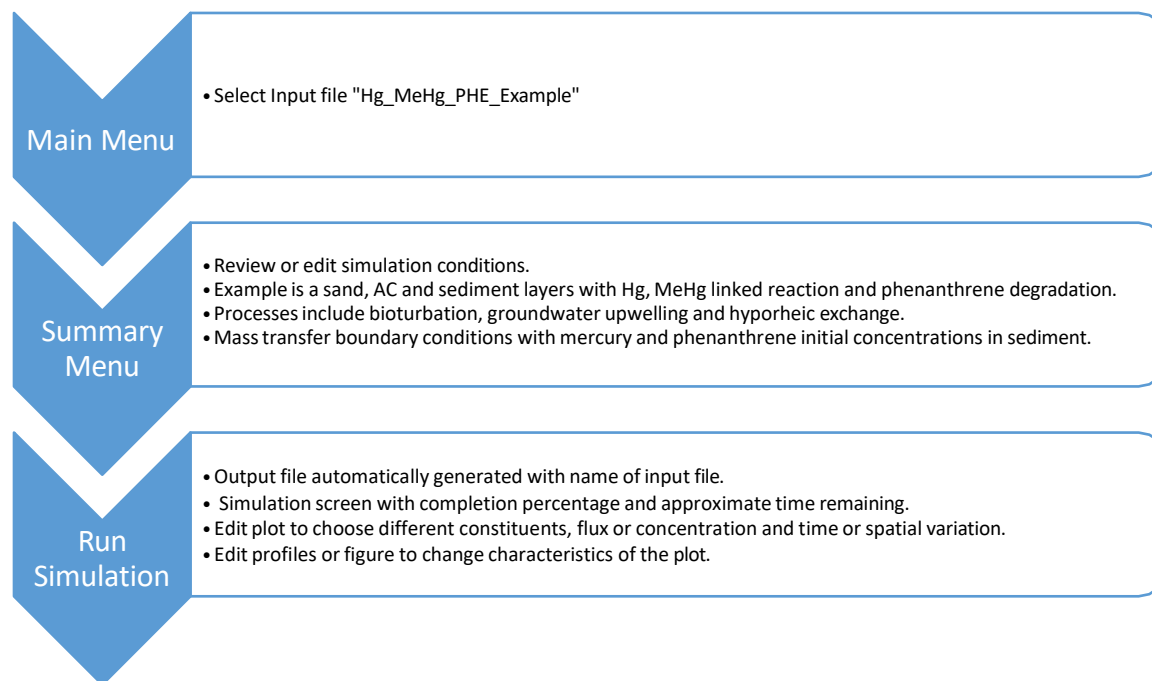


Figure 5 CapSIM Simulation Process for the Included Example File

After examining the input parameters, click **OK**, and you will be given another opportunity to change

the name (to avoid overwriting a file you wish to save). A window will be open to show the amount of the simulation completed and the approximate time remaining. When the simulation is completed, a figure showing one of the contaminants will automatically be generated. Use **Edit Plot** to add another contaminant or clear plots to make a different plot for a different contaminant, phase, or parameter (flux, mass balance) and to show a spatial profile or changes with time. A variety of plotting parameters and characteristics (log scale, color changes, turn on or off depiction of sediment layers, etc.) can be chosen from the **Edit figure** or **Edit profiles**.

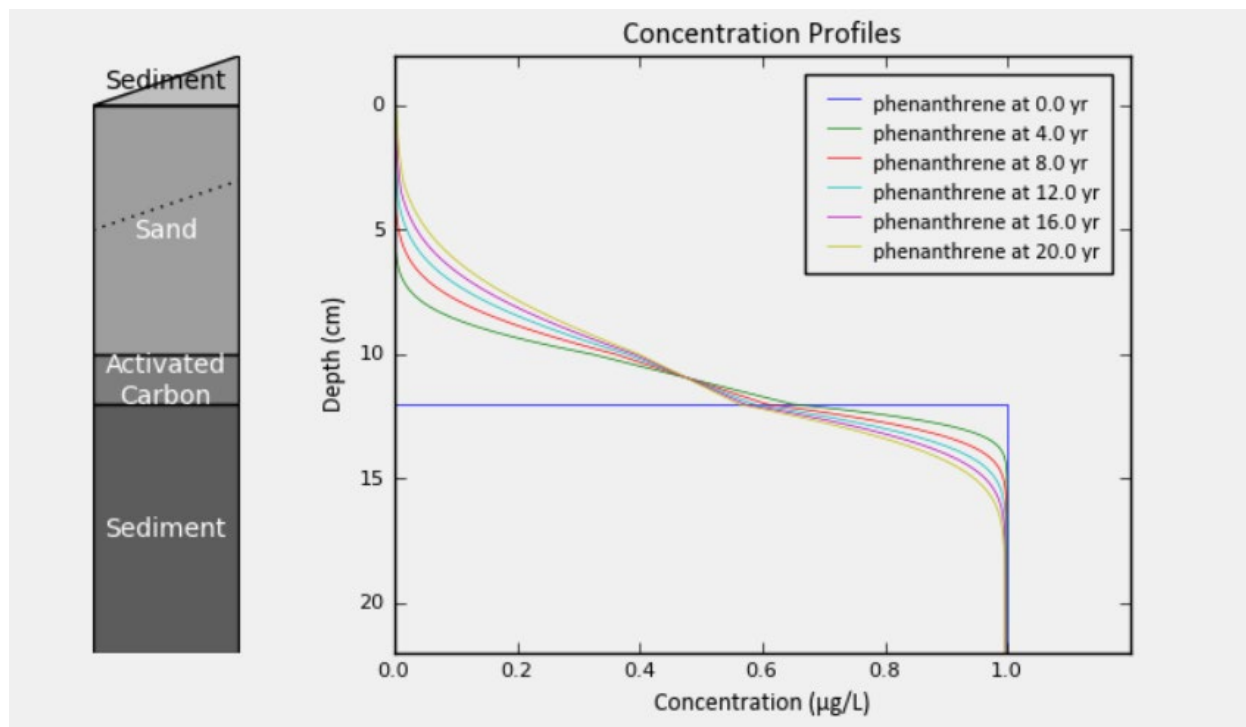


Figure 6 Simulated Phenanthrene Concentration Profiles as a Function of Time.

Figure 6 shows the simulated phenanthrene interstitial water concentrations at different times. The initial concentration (time 0) shows a concentration of 100 $\mu\text{g/L}$ in the entire sediment layer. As time progresses, phenanthrene is depleted at the surface of the sediment layer, and upwelling and diffusion move phenanthrene into the activated carbon layer, where rate-limited sorption occurs. Transport continues into the surficial sand layer, where hyporheic exchange and bioturbation keep the near-surface concentration relatively uniform.

4. CapSim Parameters

A more detailed description of the use of the model and the simulation parameters is included below.

4.1. System Parameters

This menu allows the selection of units for all parameters and the density and viscosity of water. If you have already loaded a simulation, selecting new units will automatically update all units in the simulation. Additionally, any property or parameter values in the old units will be converted to the corresponding values in the new units. For example, if you change the concentration unit from “mg/L” to “μg/L”, the input concentration values will be multiplied by a factor of 1000 to convert their values from “mg/L” to “μg/L”.

4.2. Chemical Properties

You can enter properties or retrieve properties for a number of compounds from the database. You can also edit existing properties. Key properties include molecular diffusivity of the compound and organic carbon partition coefficients (for sediment organic carbon and dissolved organic carbon), which apply to organic compounds. Negligible partition coefficients should not be entered as 0 if the parameter requests log units but instead as a small value (e.g. -10 log units). When entering values, pay attention to the units requested, which are the most common units for these parameters.

4.3. Equilibrium and Reaction Properties and Coefficients

These options allow the inclusion of equilibrium and kinetic reactions and coefficients. Buttons allow the addition of reactants and products using their stoichiometric coefficients (molar units). Chemicals that appear as reactants or products must have been previously defined under *Chemical Properties*. CapSim can simulate quite complicated reaction networks, although simulation time may increase as the number of coupled reactions increase. An example describing surficial sediment biogeochemistry is available to examine how such a simulation is created.

4.4. Solid Materials

Materials can be added from scratch (add materials) or loaded from past materials. Common commercial sediment remedial products can also be added, including Aquagate®, Reactive Core Mats® with activated carbon or organophilic clay, Sedimite® and Tektoseal® with activated carbon, organophilic clays, or arbitrary slurries. The default properties of these materials are shown, but alternative formulations can be entered by choosing different constituent materials or material fractions. The combined properties are estimated assuming linear additivity. Note that the fraction of organophilic clay can be a source of confusion in that it represents the fraction of the clay, not the fraction of organic carbon in that clay.

To edit an existing material (load component), you can select the material by pushing the name button, selecting the appropriate component, and then entering the weight fraction of that component in the mixture. The physical properties of the selected component will be automatically loaded. If

adding a new component, you should enter the material properties, including porosity, bulk density, and organic carbon content. This information is used to estimate the mixture properties assuming an ideal mixture of the components (that is, the total volume is the sum of the volume of the individual components- this may not be true for mixtures of substantially different particle sizes and in such cases, you should calculate or measure the mixture characteristics separately and define it as a new material for CapSim).

In recent versions (including 4.2), the mass fraction of each material is entered into a mixture. A 50-50 mixture means 50% by mass. Volume is assumed additive, although you can enter a mixture bulk density if you have information that the volume is not additive. For example, consider a 50-50 mixture of two materials, one with a dry density of 0.5 g/cm^3 and one with a dry density of 1 g/cm^3 . If we consider 1 g of the lighter material (2 cm^3), the mixture will also contain 1 g of the heavier material (1 cm^3). Thus, the bulk density of the mixture is calculated to be $2 \text{ g}/3 \text{ cm}^3$ or 0.67 g/cm^3 . You can change the bulk density of the mixture if you know it to be different. The actual loading (in mass per unit area) of a component of a mixture will also be calculated based upon the mass placed and layer thickness. Normally this loading would be used to define the placement of a sorbing material in a sediment cap or treatment system rather than the thickness since the thickness would change depending upon the settled bulk density.

You also have alternative ways to introduce mixtures to achieve the actual amount of sorption expected in a system. As an example, consider a 50-50 mixture (by weight) of sand (bulk density of 1.25 g/cm^3) and Aquagate® containing 10% activated carbon (bulk density of mixture 1.09 g/cm^3 from 90% aggregate of 1.35 g/cm^3 and 10% activated carbon, 0.4 g/cm^3). You have two options:

- Input the mixture as being 50% sand, 45% aggregate, and 5% AC (10% of the mass of the aggregate/AC mix) with their respective pure component bulk densities and sorption properties.
- Input the mixture as being 50% sand and 50% Aquagate® with the Aquagate® density being 1.09 g/cm^3 . In this case, you must specify the sorption in this layer as though it is 10% of the sorption of a pure activated carbon layer. For example, specify the Kf in the Freundlich isotherm to be 10% of pure activated carbon.

4.5. Sorption

Sorption properties can be added for each material by selecting from a specified partition coefficient (Linear-Kd specified) entered as a numerical value in L/kg or an organic carbon partition coefficient which uses the organic carbon fraction to estimate the partition coefficient. Freundlich and Langmuir isotherms can also be employed. As previously noted, the linear Kd-specified model is typically most appropriate for inorganic contaminants and hydrophobic organics on organophilic clay (with $K_d \sim K_{oc}$ or K_{ow}). The “Linear- Kocfoc” model is most appropriate for organic sorption onto natural organic matter. Freundlich isotherms are typically most appropriate for activated carbon or so-called “black carbon” in soils or sediments. All parameters are entered directly in the chosen units except for the organic carbon-based partition coefficient, which is entered in log (L/kg) units. Local equilibrium or

sorption kinetics can be assumed. If sorption kinetics are applied, a first-order sorption rate constant must be entered or estimated using the tool provided. If you want to modify any of the default or database properties, click on the sorption properties or layer properties to edit either.

If you add new materials or change the material properties, the sorption pop-up box will automatically appear, allowing you to change both the type and parameter values for sorption in each material. Sorption relationships that can be used include a specified linear partition coefficient, the classic model of a partition coefficient as the product of the fraction organic carbon and the organic carbon partition coefficient, a Langmuir isotherm, and a power law Freundlich isotherm. Database files are available that have sorption data on a variety of organic contaminants. Local equilibrium or transient sorption kinetics can also be assumed. Transient sorption is assumed to follow first-order kinetics if chosen.

CapSim offers a valuable tool that can be used to estimate the sorption kinetic coefficients of HOCs and three heavy metals in activated carbon with varying particle sizes and under different local hydrodynamic conditions. To access this tool, simply click on the button **Estimate AC rate coefficients**, and you will be directed to the AC kinetic estimator window. The particle sizes of the activated carbon and the local Darcy velocities will be automatically updated based on the values entered in the solid material parameter window and sediment process window. However, you also have the option to enter these values manually.

You can choose HOCs or any of the three metals. CapSim provides three levels of estimates for the internal AC particle kinetics (intraparticle mass transfer resistances) to account for uncertainty. You can also choose to include or exclude external (interparticle) mass transfer resistances. In general, you should include external mass transfer resistances, and CapSim provides an empirical correlation based on thin-film mass transfer theory, provided by [9]. For conservative design purposes, it is recommended to use the “Low estimate” for the internal resistance option and the “Wakao model” for the external resistance option.

The details of the first-order kinetic sorption and the determination of its coefficient are given in section 5.2.

4.6. Layers

The sediment layers to be simulated are defined like a layer cake with the defined materials applied to each one. Typically, you would use at least one sediment layer and a layer for each cap layer if simulating a cap. You can also eliminate the sediment layer if you wish to model the sediment as a constant concentration boundary. However, it is normally better to model the sediment explicitly because there is typically depletion over time in the contaminated sediment. You can model multiple sediment layers if you have measured concentration profiles as a function of depth. You would then specify the initial concentration in each layer from the known depth profile (see auxiliary conditions below). You can also specify an arbitrary concentration profile in each layer, although typically, you would reserve this capability for the sediment layer.

A special layer is the deposition layer if you have sediment deposition. It can be selected from the

pull-down menu defining the layers, and one of the materials (typically sediment) can be applied to that layer as well as the average rate of deposition. The deposited material is assumed to exhibit sorption equilibrium with the conditions of the overlying water. A rate of erosion can also be specified (under *Sediment Processes*), which can offset part or all of the deposition. There is a net contaminant exchange across the sediment-water interface with erosion and deposition in that the depositing layer is in equilibrium with the overlying water. The sediment erosion loses whatever contaminants are associated with those solids.

Before defining the solid material of layers, the materials used must be loaded from the materials database or created in the material window. Note that if you want to have layers of the same material with different physical properties (e.g., a depositing sediment layer that has a porosity of 0.8 and a consolidated sediment layer that has a porosity of 0.5), you should define the two different sediment types in the solids database and give them names that you can use to distinguish between them (e.g., surface sediment and consolidated sediment).

Layers are laid out top to bottom using the materials that you have defined. The thickness of the layers, dispersivity, and dissolved organic matter can be different in each layer. The dispersivity is a difficult parameter to estimate, but it is essentially the scale of heterogeneities in the layer. In general, it is best to use a fraction of the layer thickness (e.g., 5-10% of the layer thickness). For thin layers such as a reactive core mat, the entire layer thickness (1 cm) might be used as a conservative approximation. Dispersivity is only a parameter relevant to an advective component such as groundwater upwelling. In summary, the recommended dispersivity values without site-specific information are as follows.

For regular layer (thickness ≥ 10 cm): dispersivity $\approx 10\%$ thickness

For thin layer (thickness < 10 cm): dispersivity ≈ 1 cm

The tortuosity correction also appears in the layer definition. This is the ratio of the flow length to the straight-line length through the layer, and two models are recommended. Two models are provided. The Boudreau model[10] is recommended for consolidated materials such as sediment, and the Millington and Quirk model[11] is recommended for granular materials like sand. Either can be selected by editing a particular layer and clicking on the appropriate push button.

4.7. Sediment Processes

If you have a system with groundwater flow and consolidation, you can incorporate that information under the window "Sediment Processes". You can click on the slide-down menu "Upwelling groundwater" to enter an upwelling (positive) or downwelling (negative) groundwater flow or oscillating (tidal) flow. Both can be selected for a flow with a mean and oscillatory component. The oscillatory flow is specified by selecting a maximum amplitude and a period. Note that the input flow velocity is the Darcy velocity in the sediment resulting from tidal or other oscillations, not the tide itself. If the tidal amplitude is 1-2 ft, this may result in a flow amplitude in the sediment of 1-2 cm or less, depending upon the permeability of the sediments. For example, we have measured an oscillation of approximately 1 cm/day (365 cm/yr) in fine-grained surficial sediments due to a tidal amplitude of 1 ft in the Anacostia River in Washington, DC. In a coastal area with two tidal cycles

every 24 hours and 50 minutes, the period would be 0.0014 years. Other oscillating flows, such as periodic flood events, can be simulated using a longer “tidal” period. Note that the time step of the simulation will be modified to ensure adequate resolution of whatever periodic flow is chosen. The periodic flood event may lead to long run times for simulations of long duration with a short tidal period.

For oscillating groundwater upwelling, the model output can be either instantaneous values (flux or concentration) or values averaged over the period of oscillation. This option is selected from solver options (below). Average would be the preferred choice for simulation periods that are much longer than the oscillation period. Instantaneous would only be of interest when evaluating the variations through an oscillation cycle (for example, an annual simulation with seasonal variations in flow).

You can also incorporate upwelling velocities that change with time by providing these in a batch file. This is normally employed for velocities that change over long periods of time (e.g., seasonally or over the years) and is not well represented by a constant amplitude periodic model. An example batch file with arbitrary velocity changes is available from Texas Tech University. In principle, a similar batch file could be developed, allowing arbitrary changes over time in other parameters used in the model.

Other sediment process options in the model include hyporheic exchange, erosion, depth, and intensity of bioturbation (mixing via and consolidation. Hyporheic exchange can be modeled by porewater bioturbation or directly using a model developed by [12]. Significant hyporheic exchange extends 50-100 particle diameters into the sediment by this model. Hyporheic exchange is limited to the depth of the surface layer or the depth of bioturbation, whichever is greater. If multiple layers are influenced by bioturbation, the geometric mean particle size is used to estimate effective hyporheic exchange.

The model can incorporate erosion and deposition either separately or together. Normally, either erosion or deposition might be chosen, but using them together allows for a sediment exchange process that can be used to simulate sediment resuspension and settling as a result of flow dynamics. Long-term erosion without deposition would result in the loss of the entire sediment layer. It is balanced by deposition, and if the speed of deposition and erosion are equal, there is no net change in sediment thickness but a net exchange of sediment and contaminants (deposition in equilibrium with the water column but erosion carrying any contaminants in the eroding layer). If deposition is faster than erosion, there is both deposition and sediment exchange. The latter case is common when there is net deposition long term, but erosive events remove part of that deposition layer during high flow events. For example, 2 cm/yr deposition and 1 cm/yr erosion would yield 1 cm/yr net deposition, but the sediment exchange would yield somewhat different results than modeling just the 1 cm/yr deposition.

Bioturbation, the mixing process associated with benthic organisms, is modeled as an effective diffusion process (biodiffusion) and can be assumed uniform over a fixed depth or depth-dependent where the intensity is assumed to drop off a Gaussian distribution with input standard deviation in depth. In the latter case, 95% of the bioturbation occurs over a depth of about 2 standard deviations. Thus, the biologically active zone (BAZ) might be approximated by the defined depth of bioturbation in the fixed depth model and 2 standard deviations in the Gaussian model. The intensity of biodiffusion of a contaminant in both porewater and solid materials depends on the local

concentration gradient. It is scaled by the porewater biodiffusion coefficient and particle biodiffusion coefficient, respectively. Typical values of bioturbation are a depth of 5-15 cm and an intensity of particle reworking of 1-100 cm²/yr. [4] summarized literature reported values of bioturbation depth and intensity. It indicated an average bioturbation depth of 5.3 cm and intensity of 3.9 cm²/yr in freshwater systems and 12.3 cm and 125 cm²/yr, respectively, in estuarine systems. The model will move both particles and the contaminants associated with them. Note that these depths are associated with the layer thickness where there is active particle reworking. Isolated deeper interactions from individual organisms may occur, but the area's average intensity may not be significant. Organisms also pump water back and forth, but the magnitude of this value is more uncertain and is typically not important if you have a sorbing sediment contaminant. If the particle size of the surface sediment is provided to the model, you can use particle size dependent biodiffusion in which the intensity of bioturbation is reduced for particles of sizes greater than 10 µm using the data of [13]. Particles 100 µm in diameter exhibit about 20% of the bioturbation of 10 µm particles, which bioturbation is effectively zero for particles of 10000 µm (10 mm) and larger. Bioturbation cannot penetrate a commercial geotextile layer if this is placed within the set bioturbation depth.

Consolidation due to the weight of a cap tends to be rapid initially but slows considerably over time—consolidation results in an effective upwelling velocity due to porewater expression. The process of consolidation is not modeled explicitly within CapSim, but the effects of consolidation are modeled by assuming the process is an exponential process that is characterized by inputting the expected magnitude of consolidation and the time to 90% of that consolidation. For example, a cap may lead to 6 in (15 cm) of consolidation, with 90% occurring in the first year. The inputs would then be 15 cm and 1 year.

The final options in *Sediment Processes* (ionic activity and biotic reaction model) are associated with modeling biogeochemical processes and are beyond the scope of this manual. An example input file is available with a detailed biogeochemical model of surficial sediments. Cap Sim can be employed to explicitly model the surficial biogeochemical reactions such as oxygen, iron, and sulfate reduction and contaminant reactions that result.

4.8. Auxiliary Conditions (boundary and initial conditions)

The boundary and initial conditions (concentrations or fluxes) are set in each layer and at the top and bottom boundaries. Concentration profiles within a layer can be defined arbitrarily by setting depth and concentration.

When providing initial or boundary concentration data, the truly dissolved porewater concentration (typically measured by passive partitioning samplers), which defines thermodynamic partitioning, is expected as input. If equilibrium sorption is assumed, solid information can be provided, and the partitioning parameters can be used to estimate the truly dissolved porewater concentration. Often the available porewater concentration might be the result of extraction of porewater (either directly or centrifugation), and the total contaminant concentration rather than the truly dissolved concentration might be measured. In this case, the input concentration should be the measured total porewater concentration, and the DOC concentration should be set to 0 (since it is already included in the measured contaminant concentration).

Special consideration should be given to the surface boundary condition and the bottom boundary condition. If the surface boundary condition is set to 0 concentration, the concentration at the surface is always forced to be 0, even if the contaminant is moving through the surface. Contaminant migration into the overlying water can be monitored by examining flux, which is much less sensitive to the boundary condition at the surface.

Setting the surface boundary to 0 concentration can also lead to some unusual behavior with deposition. The deposition is simulated by adding a grid cell after a sufficient period of deposition to justify making a new grid cell, reflecting that there is a rapid change in the condition at the top boundary. It can lead to oscillations if the boundary condition is forced to 0. The oscillation can be moderated or eliminated by setting a more realistic mass transfer boundary condition.

Typically, a better upper boundary condition might be to employ a mass transfer boundary condition at the surface with the overlying water concentration. The mass transfer coefficient can be estimated using the characteristics of the overlying water and is typically of the order of 1 cm/hr. CapSim includes two classic correlations for estimating the mass transfer coefficients in rivers and lakes (Page 342 in [4]) and an analysis based on analogy theory and friction velocity. Note, however, that the surface mass transfer typically does not control the rate of migration from the sediment. So, this may simply be equivalent to setting a 0 concentration at the surface.

CapSim offers the "Fixed Volume Water Column" boundary condition for simulating natural systems with a limited overlying water volume. This condition allows for the modeling of changes in water concentrations due to the migration of contaminants from the sediment. When you opt for this boundary condition, it establishes a mass balance of contaminants in the overlying water by accounting for flux from the underlying sediment, inlet flow, and outlet flow. The flux at the sediment-water interface is determined by a mass transfer model with user-defined coefficients. Users have the flexibility to customize hydrodynamic parameters for the overlying water body to align with their specific requirements. These parameters include water depth, horizontal velocity, and dissolved organic carbon (DOC) levels. If you define a deposition layer in the layer property window, it's essential to specify a settling velocity. Simulated water concentrations can be visualized by plotting them in the output window and are also included in Excel output files for further analysis.

The bottom boundary is normally set at the bottom of a contaminated sediment layer. The most common conditions would be to set this layer at a measured deep sediment porewater concentration (if known and presumed constant) or at the concentration of the sediment layer above it (if not known). The flux matching condition is recommended and ensures that the flux at the bottom boundary is defined by the lower sediment concentration times the groundwater upwelling velocity. This condition is commonly used to model advective, reactive transport [4]. Note that setting a zero concentration or zero velocity with flux matching will define a zero-flux boundary at the simulated bottom, while choosing just a zero concentration (or any fixed concentration) will allow diffusive transport through the bottom of the simulated sediment. If the modeled sediment layer is sufficiently deep, the bottom boundary conditions will have little effect on the modeled solution.

4.9. Solver Options

Solver options allow the user to set the simulation duration in the time units that were selected, as well as discretization and numerical solver options. If your simulation involves multiple contaminants that are not linked to other contaminants (e.g., compounds exhibiting no degradation), you can speed the simulation by using multiple processors if available. If your compounds are linked to each other, this option is not available.

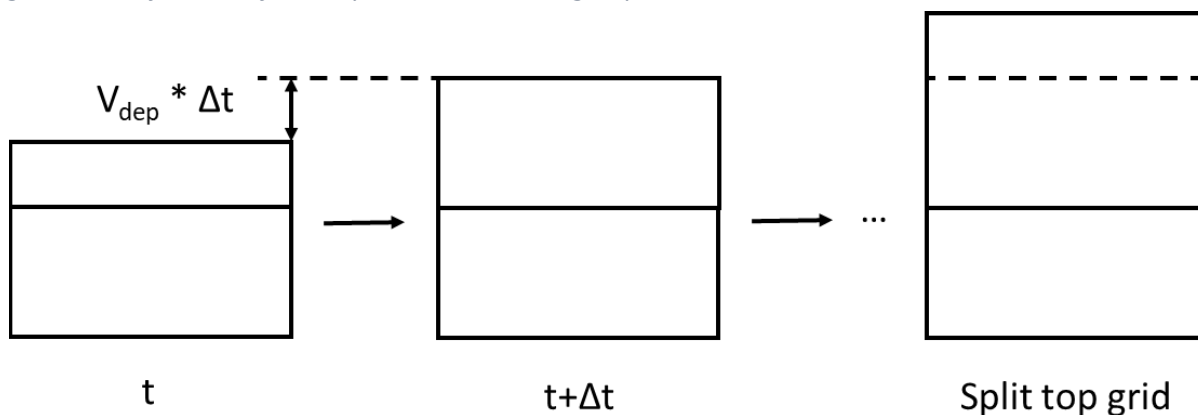
By default, the system employs a stable implicit finite difference method to solve the differential equations describing the system and chooses grid sizes and time steps as appropriate for the simulation. The default numerical options are very stable and likely to lead to a result with minimal numerical errors. It may, however, require a long time to run in some simulations, particularly with a combination of thin and thick layers, rapid tidal oscillations, multiple species and reactions, and nonlinear sorption or reaction. The model run times can be shortened using manually defined discretization options but note that model instability may result. The fastest solutions to generate are those that are run with a uniform number of grid cells in each layer and use the fastest layer to set the time step. Any simulations with minor oscillations observed in the output can be improved by changing the spatial grid and time step. In all simulations, reducing time and spatial grid sizes is recommended until no changes are observed in results versus the decreasing grid sizes or time steps.

The user should be especially cautious of results using nonlinear sorption or reaction/sorption kinetics. With nonlinear systems, the results may be sensitive to modeling parameters. A user should always check the results in such a problem by refining the time and spatial discretization (smaller time and distance step sizes) and/or by reducing the error tolerance in the iterative solver and make sure the results don't change significantly (that is, an important change in your desired output, e.g., time to contaminant breakthrough in a cap). If they do change with the refined time and distance steps, the step size or error tolerance should be reduced further, and the simulation should be attempted again. An indication that you may have a problem in this regard is the calculation time displayed during the simulation repeatedly increasing. The growing time means convergence problems exist in the iterative solver, and CapSim is taking corrective action. However, you still may need to reduce error tolerance or time and space steps to achieve the most accurate results.

For cases with deposition, the size of the top grid continuously increases at the deposition rate until it is larger than 1.5 times the grid size set by users, when then the top grid is split into two grids, a bottom one of size equal to the set grid size and the top one with leftover subtracted size. In case of erosion, the size of the top grid continuously shrinks at the erosion rate until the grid is removed.

Note that the input for grids in the deposition layer is the number of deposition grids that are added in the time units of the simulation. If a deposition rate of 1 cm/yr is modeled and the time unit in the simulation is years, then 1 in the deposition grid is 1 /yr (and the grid size will be 1 cm), 0.5 is 1 per 2 years (grid size 2 cm), and 10 is 10 grids per year (grid size 0.1 cm).

Figure 7 Modification of the Top Grid in Simulating Deposition Cases.



The mass tracking system checks and records the mass of contaminants during the simulation. By selecting the mass tracking option, the users could track the fate of the contaminants in the remediation system and check the quality of the numerical simulation from the conservation of mass.

4.10. File Options and Execution

The final input screen is the “Edit File Options”, allowing you to name files. By default, the name is not changed, and your results will write over your previous results unless you change the name. Note that the system does not trap the error if you try to write to an output file that you have opened in another program. It will simply run the simulation but not show the output and instead generate an entry in the error log file (located in the CapSim directory by default). Close the output file or change the name and rerun the simulation.

The file name screen can also be used to output a batch file of a type of either “Multi Scenario” or “Monte Carlo Simulation”. The conditions used to generate this batch file will be the baseline conditions in the batch file. In particular, the parameter values for this baseline run should be saved so that all baseline conditions can be saved. The batch file will need to be edited to indicate what runs are desired. Instructions in the batch file indicate how to modify the batch file to automate any run that might be desired. This would include changing a parameter in the batch file, i_num , which indicates the number of simulations and the parameters changed in each simulation for the “Multi-Scenario” batch simulation or a function that includes a random variation about the baseline in each simulation for Monte Carlo Simulation. In the Monte Carlo Simulation, only the mean and standard deviation of the Monte Carlo Simulation runs are produced as output. Again, it is important to save the results of the baseline simulation at the same time as the batch file is generated for a record of the baseline output.

The completion of inputs is noted by pushing the OK button and then running the simulation on the following menu.

5. Advanced Topics

5.1. Problems with using the sediment-water interface for evaluation of concentration

As noted previously, the concentrations calculated at the sediment-water interface are often dominated by the conditions in the overlying water. The deposition will also affect the concentration at the surface since a new grid cell, when sufficient deposition has occurred, causes fluctuations over time as grid cells are added. Thus, evaluating concentrations right at the surface should be avoided. A better option would be to evaluate the concentration at a layer deeper into the sediment, e.g., the middle of the biologically active zone. You could also use the model to show flux at the sediment-water interface, which is typically not significantly affected by conditions at the surface or in the overlying water.

5.2. Sorption kinetics

Sorption can be modeled as a local equilibrium process or as a kinetically limited process. This may be particularly important for strongly sorbing media such as activated carbon and strongly hydrophobic contaminants such as PCBs. Kinetic sorption is selected by editing sorption properties and making the appropriate choice at the equilibrium/transient push button.

To simulate the sorption kinetics of a sorbing phase, we use the first-order sorption kinetic model, which predicts uptake by the product of an intrinsic rate (specified by a rate coefficient) and the deviation from equilibrium in the sorbing phase. A kinetic rate coefficient can be entered based upon site-specific information or estimated from a sorption model.

Sorption kinetics for activated carbon (AC) is particularly important due to the complex internal pore structure of this sorbent, and CapSim provides a tool to estimate the kinetic coefficient. CapSim models the adsorption rate of COCs onto AC with the equation below where C_w is the freely dissolved concentration in water K_{ac} is the AC-water partition coefficient corresponding to that concentration (if concentration-dependent sorption isotherm is selected, e.g., a Freundlich isotherm)

$$\text{Sorption rate} = \lambda_{ac} \left(C_w - \frac{q_{ac}}{K_{ac}} \right)$$

The overall kinetic coefficient λ_{ac} is the harmonic average of an internal kinetic coefficient $\lambda_{ac,i}$ representing intraparticle diffusion and an external kinetic coefficient $\lambda_{ac,sl}$ representing interparticle mass transfer resistances.

$$\lambda_{ac} = \frac{1}{\frac{1}{\lambda_{ac,i}} + \frac{1}{\lambda_{ac,sl}}}$$

The external coefficient can be estimated by

$$\lambda_{ac,sl} = Sh \frac{6D_w}{d_{ac}^2} \frac{6}{d_{ac}} T$$

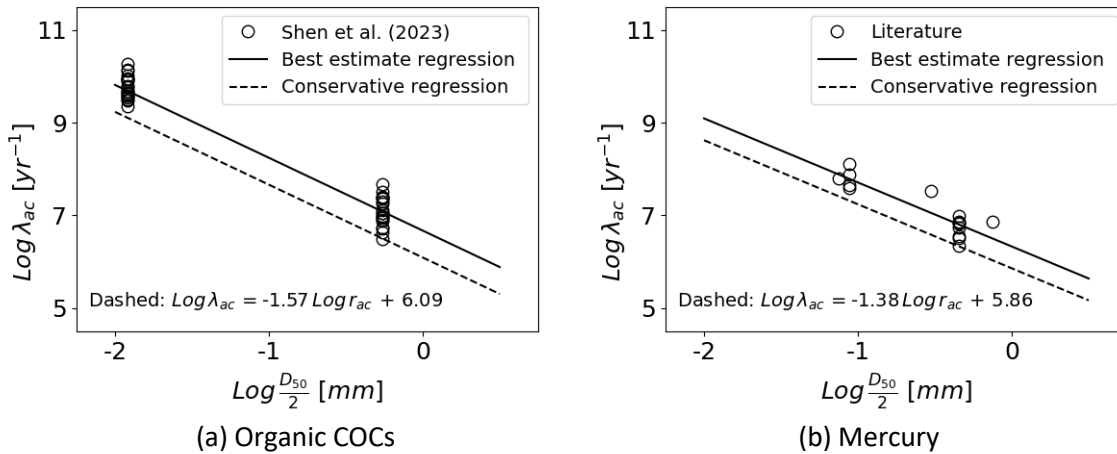
The correlation between the Sherwood number and flow and contaminant conditions follows a classic correlation published by [9],

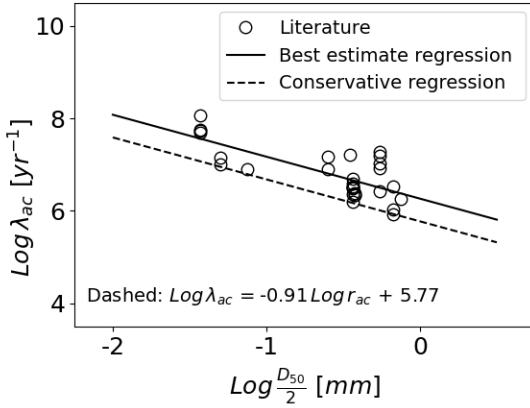
$$Sh = 2 + 1.1 Sc^{1/3} Re^{0.6}$$

The internal coefficient of HOCs onto AC was measured in batch experiments and correlated to the particle radius of AC r_{ac} using a log-log function [14]. The correlation is expressed in the following equation, which includes a slope coefficient α and an intercept coefficient β . To determine the coefficients for different COCs, the correlation is fitted to sorption experiment data from the literature (see Figure 8). To ensure the conservation, the slope coefficient α is obtained through linear regression (represented by the solid black line) of all data, while the intercept coefficient β is derived by requiring the dashed line to either pass through or lie below all experimental values (represented by the dashed line).

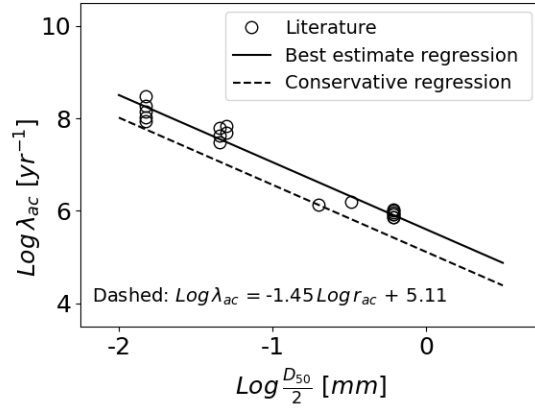
$$\log \lambda_{ac,i} = \alpha \log r_{ac} + \beta$$

The correlation for organic COCs in Figure 8 was obtained by fitting the data from [14]. The measured coefficients showed little connection with the hydrophobicity of PCB congeners and were consistent with kinetic coefficient values reported for PAHs in other literature. These findings suggest that the correlation can be applied to estimate kinetic coefficients for other organic compounds when sorption kinetic data are unavailable. Therefore, we apply this correlation to calculate the kinetic coefficients of all organic COCs for the CIL design. The correlation was fitted to the sorption kinetic coefficients evaluated from the literature for metal COCs, including mercury [15-19], copper [20-32], and lead [30, 33-37].





(c) Copper



(d) Lead

Figure 8 Log-log correlations between the mean particle size of ACs and the first-order sorption kinetic coefficients for (a) organic COCs, (b) mercury, (c) copper, and (d) lead. The circles represent the literature values used for regression. The black regression line reflects the best-estimated regression for all literature values. The dashed line reflects the low estimate with the same slope as the best estimate regression line and the intercept to keep all the experimental values on or above the line.

5.3. Reactions

The default model for a reaction is first order. You can choose “user-defined” and input the index value for the rate equation. For organic decay, you don’t need to worry about products.

Changing the reaction rate index value will mainly cause the variation of concentration and flux of the specific chemical and probably have little influence on the other chemicals. But by increasing the index value, the system’s nonlinear properties will be increased, which will decrease the stability.

You can also input multiple compounds that are linked through reactions and products. The more complicated the reaction network, however, the slower the model simulation and potentially the greater the likelihood of increased instability. CapSim is probably best used for relatively simple reaction networks for no more than 3-5 reactants and products that are linked. In principle, however, there are no limits on the complexity of the problem you wish to solve.

Fast reactions may also cause the same phenomena as indicated for fast sorption processes. That is, a smaller time step may be required than would otherwise be the case.

5.4. Effect of deposition and oscillating velocities

After increasing the deposition velocity, the grid numbers will automatically change back to defaults, so you may need to change it. If the system being simulated is a complicated nonlinear system, increasing deposition velocity will increase the system’s instability, which could lead to a failure to achieve convergence to a solution. You can modify the grid number and time step to decrease the instability of the system. Deposition is modeled by adding a grid when sufficient deposition has occurred. This leads to some oscillations, although the model output is automatically averaged, so they may not be important.

By increasing oscillating velocity, the calculation time will increase, and the flux versus time curve will fluctuate more obviously if the instantaneous option is selected. This does not, however, mean that the system is unstable. It may simply be tracking the fluctuations that are occurring in the system.

Note that a high-frequency fluctuation (e.g., twice per day tidal fluctuations) may not be synchronized with your output file (e.g., 1000 output values, for example, means that the output times saved are 1/1000 of the total simulation time). In such cases, the output may catch different parts of the fluctuation cycle and show fluctuations that do not accurately capture the frequency or amplitude of the fluctuations. If capturing the fluctuations are desired, the values should be output at a greater frequency than the actual fluctuations.

Frequency of output > Frequency of fluctuations desired to track.

In general, for simulation times that are long relative to the oscillation period, the averaging option should be selected in the solver options.

5.5. Unstable solutions

According to the central differencing scheme, the maximum Pe number based upon grid size should be less than 2 in case of overcoming instability, but the system is designed to modify Pe automatically, so users don’t need to worry about this. If users observe unstable model results (i.e., oscillating

solutions or solutions that “blow up”) for a nonlinear system (including Langmuir sorption or Freundlich sorption), decreasing the time step is the most useful method to try, at the same time, they can also increase grid number to shorten grid size and let the system have more points to do the calculation for nonlinear system. Switching to the implicit method for the solution can also be helpful.

As indicated above, too large a time step may also lead to a failure for nonlinear simulations to converge, and the system seems to “hang”. In such cases, the first step is again to abort the simulation and reduce the time step.

If you conduct nonlinear simulations (e.g., with nonlinear sorption such as a Freundlich isotherm), the model uses Newton-Raphson iteration. The error tolerance will appear as a solver option, and problems with the solution (such as non-physical results) may be corrected by reducing the error tolerance. The system will automatically use a different iterative solver if the Newton-Raphson iteration fails, for example, for extremely nonlinear problems. As indicated previously, users should be especially cautious when conducting simulations involving nonlinear sorption or reaction. Reduction in error tolerance (this option only appears in nonlinear simulations) or reductions in time step size may be required to get the most accurate results.

5.6. Speeding up CapSim for Complex problems

Sometimes, CapSim will take hundreds or thousands of seconds to finish a particular simulation. To speed up CapSim for complex problems, we can decrease the grid number and thus enlarge the grid size, and at the same time, we can increase the time step and lower the simulation duration to shorten the calculation time. There is a lot of flexibility in CapSim to speed up the simulation. It is always a good idea to test a complicated simulation by ensuring that decreasing the time step and decreasing the spatial grid size does not appreciably change the results. If that is the case, you can use the larger time step and spatial grid to solve the problem routinely.

5.7. Addressing special processes

As partial activities of benthic organisms, the burial process should be included in the particle bioturbation term with its depth and intensity calibrated by burial depth and frequency. Particle bioturbation mixes the solid materials and contaminants near the benthic surface, which is equivalent to the burial process in long-term behavior.

Resuspension and recontamination could be modeled using the finite water column boundary condition, which treats the overlying water body as a fully mixed container with inlet and outlet streams as well as evaporation and decay processes. The transient and steady-state behaviors of contaminants transported from sediment to the overlying water body could be simulated with a benthic mass transfer coefficient calibrated to the resuspension/recontamination strength.

In CapSim, consolidation is modeled as a process happening underneath the modeling layers that increases the upwelling groundwater flow from there. In such cases, the users should only include the capping layer in the simulation domain and use a fixed concentration bottom boundary condition to represent the contaminated sediment.

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