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Housatonic River

Model Calibration

Comments

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Many of my concerns have to do with the modeling framework and data needs. The panel addressed this topic in 2001. However, at that time, the modeling framework was quite general, very ambitious, and had little detail. The framework and model details have changed considerably since then. Because of this, in answering the questions on Modeling Calibration, some preliminary comments on the modeling framework are necessary. Since Question 3 is closest to the concerns about the modeling framework, most of my preliminary comments are included as introductory material to Question 3.

Question 3. Does the model, as calibrated, based upon your technical judgment, adequately account for the relevant processes affecting PCB fate, transport, and bioaccumulation in the Housatonic River?

In water quality models, the values for many parameters are commonly determined by parameterization, i.e., by varying the values of each parameter until the solution, however defined, fits some observed quantity. There are serious difficulties with this type of procedure. As a simple example, consider the erosion and deposition of

sediments. In this case, a limiting situation is where there is a local steady-state equilibrium between erosion and deposition. Denote the erosion rate by E and the deposition rate by pw_sC , where p is the probability of deposition, w_s is the settling speed of the particles, and C is the suspended solids concentration. Local steady-state equilibrium then implies that

$$E = pw_sC \quad (1)$$

Rearranging, one obtains

$$C = \frac{E}{pw_s} \quad (2)$$

From this, it is easy to see that a numerical model can “predict” the observed value for C with an almost arbitrary value of E , as long as pw_s is changed accordingly, i.e., such that $E/pw_s = C$. For example, a particular value of C can be obtained by high values of erosion and deposition or by low values of erosion and deposition, as long as they balance to give the observed value of C . For a predictive model, the values of E and pw_s can not both be determined from calibration of the model by use of the suspended solids concentration alone.

As a practical illustration of this problem, consider the sediment and contaminant transport modeling in the Fox River (Tracy and Keane, 2000). Two groups independently developed transport models. Each group calibrated their model based on suspended sediment concentration measurements. Each group believed that the parameters used in their model were reasonable.

However, the results predicted by the two models were quite different, both in the transport of sediments and of contaminants. As an example, the amount of sediment resuspended at a shear stress of 1.5 N/m^2 (a large but not the maximum shear stress in the

Fox) was predicted by one group to be 11.3 g/cm^2 (on the order of 10 cm) while the other group predicted 0.1 g/cm^2 (or 0.1 cm), a difference of two orders of magnitude.

This difference of course has a direct impact on the choice of remedial action. Small or no erosion at high shear stresses indicates that contaminants are probably being buried over the long term and natural recovery is therefore the best choice of action. Large amounts of erosion indicate that buried contaminants may be uncovered, be resuspended, and hence will contaminate surface waters; dredging or capping is therefore necessary. The differences in the model estimates by the two groups make it difficult to decide on the appropriate remedial action.

This may seem like a long and tedious introduction, but I want to make the point that models with many unconstrained parameters and especially models which include processes that are not described correctly as far as their functional behavior is concerned can lead to non-unique solutions; these can then lead to the incorrect predictions of long-term behavior.

For the long-term prediction of sediment and contaminant fluxes, it is essential that the functional behavior of the most significant processes be described correctly. In this regard, the most significant processes are sediment erosion/deposition and the diffusional flux of contaminants between the bottom sediments and the overlying water. Erosion/deposition is significant not only because of the contaminants transported with the sediments, but a major question is whether erosion/deposition during big events will expose deeply buried contaminated sediments **or** deeply bury surficial contaminated sediments. Both are possible during big events and will strongly influence the contaminant flux in the future. Accurately predicting suspended sediment concentrations

under present conditions, although necessary, is not sufficient for an accurate, long-term prediction of contaminant exposure and transport. As far as the diffusive flux between the sediments and overlying water is concerned, the magnitude of this flux is obviously important. However, for the long-term prediction, the depth over which this flux acts is also significant. I will concentrate my comments on the two processes of sediment resuspension/deposition and sediment-water flux of PCBs.

a. Sediment Erosion

The Shaker was developed and used in 1990-94 as a field device to measure the erosion potential of relatively undisturbed sediments in cores. No other device was available at that time. It was calibrated against the annular flume. Both the annular flume and Shaker measure net resuspension, i.e., resuspension of sediments in the presence of deposition. In contrast, Sedflume measures pure erosion, i.e., erosion of sediments with no deposition. Pure erosion is the quantity that is used in sediment flux equations and in water quality models.

In 1999 (Lick, et al., 1999; also see chapter 3 of class Notes), a comparison of the Shaker and Sedflume was made and the processes in each (as well as in the annular flume) were carefully examined. It was determined that, because of experimental artifacts in the annular flume (and hence inaccurate calibration of the Shaker), the annular flume and shaker gave qualitatively correct results but did not give accurate quantitative results. Because of this, the use of the Shaker is not recommended.

However, the use of Sedflume is recommended, primarily to determine erosion rates as function of shear stress and as a function of depth in the sediment. As a by-

product, a critical shear stress for erosion as a function of depth is also determined. Sedflume should be used in conjunction with the Density Profiler (Gotthard, 1997; Roberts et al., 1998), which determines the bulk density of the sediments (including solids, water, and air) as a function of depth in the sediment core in a non-destructive manner. This allows the determination of sediment layering before erosion rates are measured (which is destructive) and allows the determination of erosion rates as a function of the bulk properties of the sediment in that layer. This has been done successfully in other places (e.g., the Kalamazoo River, McNeil et al., 2004 and Chapter 3 of Notes). Unfortunately, this was not done for the Housatonic. Because of this, it is difficult to differentiate between the effects on erosion rates of shear stress as compared with variable bulk properties.

In a paper by Lick et al. (2005), approximate equations for sediment erosion rates are examined. It is shown that, for fine-grained, cohesive sediments, a valid formula is

$$E = 10^{-4} \left(\frac{\tau}{\tau_c} \right)^n \quad (3)$$

where E is the erosion rate, τ is the shear stress, and τ_c is a critical shear stress defined as the shear stress at which an erosion rate of 10^{-4} cm/s occurs; τ_c depends on the particular sediment being tested and generally is a measured quantity. This equation is valid for fine-grained, cohesive sediments but **not** for coarse-grained, non-cohesive sediments.

For coarse-grained, non-cohesive sediments, the appropriate formula is

$$E = A(\tau - \tau_c)^n \quad (4)$$

where A , τ_c , and n are functions of particle diameter but not a function of density. This equation is shown to be valid for coarse-grained, non-cohesive sediments but **not** for fine-grained, cohesive sediments.

To approximate erosion rates for all size sediments with a single, uniformly valid equation, the appropriate equation is

$$E = 10^{-4} \left(\frac{\tau - \tau_{cn}}{\tau_c - \tau_{cn}} \right)^n \quad (5)$$

where $\tau_{cn}(d)$ is the critical shear stress for non-cohesive particles and is given by

$$\tau_{cn} = 0.414 \times 10^3 d \quad (6)$$

where d is the particle diameter. Eq. (5) is uniformly valid for both cohesive and non-cohesive sediments. It reduces to Eq. (3) as $d \rightarrow 0$ and to Eq. (4) for large d .

In all the work we've done with Sedflume on the determination of erosion rates as a function of shear stress (the number of cores is on the order of 100), n in Eq. (5) is typically about 2 or more (see Lick et al., 2005 and Chapter 3 of Notes). Because of this, I suspect that the parameters $n = 1.59$ and $n = 0.95$ used in the Housatonic modeling (p. 4 of Attachment B.5) are incorrect.

One reason for this may be (especially for $n = 0.95$) that Eq. (4) was used to describe erosion rates even though the sediments were fine-grained. In our work, when Eq. (4) was used to describe fine-grained sediments, the n determined by regression was quite low (1.31 in our experiments), but at the same time it was also shown that Eq. (4) was a poor approximation. However, Eq. (5) applied to the same data gave an $n \cong 2$ for all particle sizes, and the agreement between data and Eq. (5) was very good.

Another reason for the low values of n determined for the Housatonic is that the above equations are only applicable to sediments which have the same bulk properties. In order to use these equations properly, sediments with similar bulk properties must be grouped together. Properties of sediments in a single sediment core generally vary with depth due to consolidation but also because of layering due to deposition after big events. Because of consolidation with depth, Sedflume measurements on one core will bias the value of n since cores at depth will be more consolidated, more difficult to erode, and will be measured later in the measurement cycle. Because the Density Profiler can give continuous density profiles as a function of depth with as little as 1 mm resolution, the use of the Density Profiler is important in determining the sediment structure and in interpreting sediment properties as a function of this structure.

The values of n are crucial for extrapolating to and determining the effects of large storms (large stresses). The data as shown seemed to have large variability. Eq. (5) is probably a better equation to approximate the data and may reduce this variability. In any event, the fact that $n \cong 2$ or more is a very strong experimental fact and hence must be considered seriously.

Whatever was done, Fig. 4-19 on p. 4-35 showing critical shear velocity as a function of grain size is incorrect. In all measurements that I am aware of (e.g., see Roberts et al., 1998; Lick et al., 2004, 2005; and Chapter 3 of Notes), the critical shear velocity (or critical shear stress) increases as grain size decreases beyond a minimum at about 100 to 200 μm .

b. Flocculation and Deposition

Extensive work has been done on the flocculation of cohesive sediments including a simple model of time-dependent flocculation and measurements of settling speeds (Lick and Lick, 1988; Burban et al. 1989, 1990; Lick et al., 1993; for a summary, see Chapter 4 of Notes). Experimental results show quite clearly that the steady-state median diameter of flocs is inversely proportional to CG (where C is sediment concentration and G is fluid shear) and inversely proportional to C when fluid shear is negligible. Since settling speeds are proportional to the floc diameter, this also demonstrates that settling velocities are also inversely proportional to CG and C . In general, flocculation is time-dependent as well as dependent on CG and C .

Eq. B3-34 on p. B.3-31, which is the formula for settling speed used in the modeling, has no dependence on time or fluid shear and has the incorrect dependence on sediment concentration. Fig. B.3-33 on p. 31 of B.3 Figures is completely inconsistent with experimental results.

Despite what EPA says in their response to my initial comments, I did not recommend or suggest a “flocculation formulation based on local instantaneous conditions”. That is EPA’s misinterpretation. On the other hand, EPA’s model of flocculation and settling speed, since it has no dependence on time, does depend only on local instantaneous conditions. As EPA states, that is incorrect.

For the correct determination of the flocculation and settling of cohesive sediments, a simple model of time-dependent flocculation is necessary and is available (Chapter 4 of Notes). This model reproduces all of our experimental results on the steady-state floc diameter as a function of sediment concentration and fluid shear and

also the time-to-steady-state behavior as a function of time, fluid shear, and sediment concentration. Together with experimental results on settling speeds, this will give a correct and quantitative prediction of flocculation and settling.

The flocculation model is quite simple and is simply a single conservation equation for the average diameter of the flocs (which replaces the conservation equation for cohesive sediments already in the model) with a source term which determines the increase or decrease in the size of the floc. The increase in computational time is negligible.

c. PCB Flux and Depth of Mixing Layer in River

In the model as described (and in most water quality models), the depth of the mixing layer is absolutely crucial in the prediction of the long-term behavior of the PCB flux between the sediments and overlying water. In the absence of sediment resuspension/deposition, the time for natural recovery is directly proportional to the depth (thickness) of the mixing layer. Increasing the thickness by a factor of 2 increases the time for recovery by a factor of 2; decreasing the thickness by a factor of 2 decreases the time for recovery by a factor of 2, etc.

In the model, a six inch depth is prescribed. Why? This seems extraordinarily thick. GE says three inches would be better (thereby halving the time to natural recovery). Is there any theoretical or rational basis for 6 inches or 3 inches or any number?

The depth of the mixing layer is a crucial parameter that determines the long-term behavior of natural recovery/remediation (basically it's the answer that you're looking

for). Because of this, it should be a non-calibratable parameter. As much as possible, this parameter should be based on scientific evidence and reasoning. Otherwise, as on the Fox and probably other locations, there will be different opinions and interminable arguments about the correct value for this parameter.

To introduce some science into this argument, let me briefly review some information about PCB fluxes and the depth of the mixing layer.

The flux of PCBs between the sediments and overlying water occurs primarily due to sediment resuspension/deposition, molecular diffusion, and bioturbation. Pore-water convection and gas transport are generally less important but may be significant in some cases.

The flux of PCBs due to sediment resuspension/deposition is modeled **as a separate process** by calculating sediment resuspension/deposition and assuming equilibrium partitioning of the chemical. This modeling includes changes in sediment thicknesses due to resuspension/deposition.

The flux due to molecular diffusion is generally ignored but it can be a significant process in itself and interacts with and modifies all the other processes. It is always present. Molecular diffusion of hydrophobic organic chemicals (HOCs) has been and is being investigated fairly thoroughly (Deane et al., 1999; Luo, 2005). For HOCs with large K_p 's, it is known that (1) rapid changes in chemical concentration profiles are limited to a few millimeters near the sediment-water interface and (2) the magnitude of the flux is relatively constant for periods of 50 to 500 years and more. The profiles are limited to a few millimeters near the surface because in this region the diffusion is balanced by non-equilibrium sorption and only changes slowly with time. This leads to

large gradients and hence high fluxes. Experiments give a mass transfer coefficient ($h \equiv q/C_o$) of approximately 10^{-5} cm/s or 1 cm/d. This is much higher than would be expected for a non-sorbing chemical. **This number is comparable to the 1.5 cm/d reported by the Housatonic modelers for their overall mass transfer coefficient.**

Over time, the diffusion does penetrate into the sediments away from the interface, but at a very slow rate. As a first approximation, this rate can be shown to be h/K_p . For a $K_p = 10^5$ (approximately that for the Housatonic), this rate would be $10^{-5}/10^5$ or 10^{-10} cm/s = 10^{-5} cm/d = 4×10^{-3} cm/yr = 4 cm/1000 yr. It would take approximately 4000 years to diffuse through the 6 inch layer assumed in the modeling. Even for $h = 1.5$ cm/d as assumed in the model, it would take over 2000 years. If $h = 1.5$ cm/d and the mixing layer is 6 inches thick, this says that (except for resuspension/deposition) we can ignore natural recovery; it takes far too long.

A lot of work has been done on bioturbation, but the process is complicated because of many different organisms acting in different ways. As a result, bioturbation is not well understood quantitatively. An important group of organisms is oligochaetes which burrow in the sediments. Their burrows generally extend 2 to 4 cm into the sediment; when disturbed, they may go deeper, up to as much as 10 cm, but only occasionally. They induce a contaminant flux by (1) diffusion of the chemical into and out of the burrow, (2) transporting fecal material to the sediment-water interface, and (3) slow mixing of the sediments due to their burrowing activities. Because of finite sorption rates, these processes are modified by molecular diffusion throughout but especially at the sediment-water interface, just as when molecular diffusion acts alone. The overall mass transfer coefficient is greater than that due to molecular diffusion alone by as much

as a factor of 5 to 10, but only for the highest concentrations of oligochaetes as enumerated in the Great Lakes (EPA, 2004), and generally should be less than that. The magnitude of the mass transfer coefficient depends on the concentration of the organisms and decreases as the concentration decreases.

For other benthic organisms, the effects of bioturbation on the flux are probably smaller. Chironomids disturb the sediments to only 1 to 2 cm and the mass transfer coefficient seems to be smaller than that for oligochaetes. Hyallela cause even a smaller effect.

In summary, benthic organisms disturb sediments primarily to a depth of 2 to 4 cm with some much smaller disturbances to as much as 10 cm. The mass transfer coefficient is on the order of 1 to 10 cm/d depending on the types and concentrations of organisms.

These numbers are approximate and subject to change, but they are the right order of magnitude. They suggest that the depth of a well-mixed layer due to molecular diffusion and bioturbation is on the order of 2 to 4 cm; some lesser disturbances may extend to as much as 10 cm. Sediment resuspension/deposition probably acts to depths greater than this; but this process is considered separately and should not be included when considering the depth of the mixing layer.

Neither pore-water convection nor gas transport has been shown to be significant in the Housatonic.

d. PCB Flux on the Floodplain

In the calculation of the PCB diffusive flux on the floodplain, since nothing else was said, the parameters such as depth of mixing layer and PCB mass transfer coefficient are the same as those in the river. I assume there are minimal benthic organisms on the floodplain (even if present at any time, they wouldn't survive dry conditions), and therefore PCB diffusion should be primarily due to molecular diffusion. For hydrophobic organic chemicals, such as highly chlorinated PCBs, the magnitude of molecular diffusion is comparable to but generally less than diffusion by benthic organisms; however, molecular diffusion behaves quite differently compared to bioturbation and certainly does not act over a mixing depth of 6 inches (Deane et al., 1998).

e. Grid Size and Number of Cells in River

With the present grid, the width of the river is generally approximated as one cell. In most rivers (and this includes the Housatonic; see cross sections in BBL report), there are large differences in erosion between the deeper parts and the shallower parts along a cross-section of a river. In particular, erosion/deposition in the deeper parts is not the same as the erosion/deposition averaged across the river.

Predicting the dissimilar amounts of erosion in the deeper parts and erosion/deposition in the shallower parts is crucial in predicting the long-term exposure of PCBs by erosion in the bottom sediments and/or natural recovery by deposition. Averaging across the channel does not describe the erosion/deposition processes accurately. A minimum of three cells across the river (two shallow, near-shore cells and one deeper, center cell) should be used.

Quite extensive and high quality work has been done on the modeling. However, as described above, the model has serious deficiencies as far as the descriptions of (a) erosion at high shear stresses, (b) flocculation and deposition, (c) PCB flux and depth of mixing layer in the river, and (d) PCB flux and depth of mixing layer on the floodplain. In addition, the spatial scale of the model in the river is inadequate to even approximately describe the variability of erosion/deposition across the river, and hence any remediation activities in the river. For these reasons, the model as is does not adequately account for the relevant processes affecting PCB fate, transport, and bioaccumulation in the Housatonic River. However, because of the extensive work already done and existing work done elsewhere, the model can be modified so that it can adequately predict PCB fate, transport, and bioaccumulation.

Question 1. Are the comparisons of the model predictions with empirical data sufficient to evaluate the capability of the model on the relevant spatial and temporal scales?

The variations in sediment erosion/deposition between shallow and deep waters of a cross-section of a river can be and generally are quite large. Averaging the data and comparing it with the present model which only has one grid cell in it may give a good comparison but will not accurately predict erosion/deposition patterns now and over the long term.

The thickness of the well-mixed sediment layer is an extremely difficult parameter to determine by calibration. Due to its assumed thickness, variations in

contaminant concentrations are very slow (see numbers in Question 3) and will be difficult to detect. A determination based on scientific reasoning may be the only way to go.

Question 4. Based upon your technical judgment, have the adequate methodologies been employed to evaluate the sensitivity of the model to descriptions of the relevant processes, and to evaluate the uncertainties of model predictions?

As described in the introductory material for Question 3, rates of erosion and deposition are both questionable. The fact that the model predicts suspended sediment concentrations fairly accurately does not imply that the rates of erosion and deposition are correct.

The well-mixed layer is very thick and insensitive to diffusional flux processes. I think it will be almost impossible to determine by calibration; some scientific reasoning is necessary.

Question 5. Is the uncertainty indicated by model-data differences sufficiently inconsequential to permit use of the model to predict differences among remedial options?

No.

Question 6. Are the processes in the model calibrated to the extent necessary for predicting future conditions including future concentrations of PCBs in the environment under natural processes and under potential remedial options for

sediments and floodplain soils in the Housatonic River in the reach below the confluence? If not, what additional work needs to be done to calibrate the model?

The model has serious deficiencies as far as the descriptions of (a) erosion at high shear stresses, (b) flocculation and deposition, (c) PCB flux and depth of mixing layer in the river, and (d) PCB flux and depth of mixing layer on the floodplain. In addition, the spatial scale of the model in the river is inadequate to even approximately describe the variability of erosion/deposition in the river and hence any remediation activities in the river.

Suggestions for improvements are as follows.

(a) Erosion at high shear stresses. Because of the low values of n used in the erosion equation, the erosion rate at high shear stresses and big events is not predicted properly. A re-examination of the data with a grouping of the data for similar sediments and use of Eq. (5) should be helpful. In any event, the fact that $n \cong 2$ or more is a very strong experimental fact and hence must be considered seriously.

(b) Flocculation and deposition. As described in the response to Question 3, a simple, time-dependent model of flocculation is available and should be used. This, along with experimental results on settling speeds, should give a better and more rational description of settling as compared with making up an equation for settling.

(c) PCB flux and depth of mixing layer in river. Based on existing information, the depth of the mixing layer is much less than 6 inches (15 cm) and is probably more like 2 to 4 cm. A thorough review of the literature and on-going work should be done to ascertain this. Some evidence of this layer from field observations and measurements on the Housatonic would be useful. Field tests of PCB diffusive fluxes from the sediment to

the overlying water should be made. These have been done elsewhere, so that it's not a new procedure.

(d) PCB flux and the depth of the mixing layer on the floodplain. Although some work has been done on sediment-water fluxes in a river, sediment-water fluxes on the floodplain are quite different in character. A more detailed investigation of this process is necessary including (a) field tests of the diffusive flux and (b) some evidence for a mixing layer.

(e) Grid sizes and number of cells in river. Because of the dissimilar amounts of erosion in the deeper parts and erosion/deposition in the shallower parts of the cross-section of a river, a minimum of three cells across the river (two shallow, near-shore cells and one deeper, center cell) should be used in the calculations. This of course increases the computational time. However, the computational time can be greatly decreased by (a) separating the hydrodynamic and sediment transport calculations, (b) for small and moderate flows, approximate and calculate the hydrodynamics as a sequence of steady-state flows at discrete values, and (c) only treating big events in detail. This will greatly decrease the computational time – more than sufficient to offset the increase in the number of grid cells.

It is not clear to me at this time how the model deals with erosion/deposition together with molecular diffusion and bioturbation. To do this properly, the sediment bed should be vertically divided into layers no more than a centimeter thick with additions and subtractions of mass from the surface layer as erosion/deposition occurs. Adding on the order of 10 to 20 layers of this type in the sediment bed does **not** appreciably increase computational time. These are layers which have essentially no computations associated

with them and are only there until needed; in essence, their presence only requires minimal bookkeeping and no significant computation.

These suggestions are not radical, untried, unproved, new ideas. A sediment and contaminant transport model, SEDZLJ, already exists (Jones and Lick, 2000, 2001, 2002; Lick et al., 2004) which incorporates most of these ideas. It uses Sedflume data and includes multiple size classes, a unified treatment of suspended load and bedload, bed armoring, an active layer due to physical mixing at the surface, HOC flux and transport, and fine layering in the vertical in the sediment bed to adequately describe sediment bulk properties and HOC flux. SEDZLJ is presently being incorporated into EFDC.

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