# Final Response to Charge Questions Housatonic River

Frank Gobas, Ph.D., Professor

School of Resource & Environmental Management

Simon Fraser University

July 20, 2006

## Response to Charge Questions

## **Charge Question 1**

"Considering the changes implemented in the Phase 2 calibration, does the model as calibrated and validated, based on your technical judgment, reasonably account for the relevant processes affecting PCB fate, transport and bioaccumulation in the Housatonic River to a degree consistent with achieving the goal of the modeling study."

Since the goal of the modeling study is to address 6 model goals (Table 1), I have organized my response to charge question #1 by specifying the various goals of the model.

Re. Model Objectives #1, #5 and #6 on the issue of temporal response:

The main goal of the model is to is estimate the temporal response of the PCB concentrations in the River as a function of various remediation strategies and natural recovery. The model's temporal response is key to (i) the quantification of future spatial and temporal distribution of PCBs (model objective #1), both dissolved and particulate forms) within the water column and bed sediment; (ii) the estimation of the time required for PCB-laden sediment to be effectively sequestered by the deposition of uncontaminated material (model objective #5) and (iii) the estimation of the time required for PCB concentrations in fish tissue to be reduced to levels established during the risk assessment process, that no longer pose either a human health or ecological risk (model objective #6) as well some of the other model objectives.

The temporal response of the model is based (i) on the parameterization of the sedimentwater exchange rate of PCBs (which is the rate determining step in the depuration of the River) and (ii) on model calibration. With regards to the parameterization of the sediment-water exchange of PCBs, there are several model parameters including the depth(s) of "accessible" and "non-accessible" bottom sediments, diffusion rates, bioturbation rates and subduction velocities that are currently difficult to measure or assess. The best strategy for parameterization is to use the best empirical data and best expert judgment possible. I am not convinced that this was achieved in this study. Dr. Lick has provided several papers to demonstrate that the current parameterization of the sediment-water exchange process in the model is not consistent with some key studies and observations. Also, I place considerable weight on Dr. Lick's expert judgment and his lack of confidence in the selection of parameter values. However, that said, it is unknown at this time whether an alternative parameterization of the sediment-water exchange processes will produce a significantly different and better characterization of the temporal response of the PCB concentration in the River. The model calibration has been complicated by the lack of a significant change in PCB concentration data in the River during the calibration period. Hence, the model calibration sheds little light on the issue of whether the model is able to account for changes in PCB concentrations over

time that may occur as a result of remediation. The main conclusion from the calibration is that the temporal response of PCB concentrations in the River is likely slow, but it cannot tell us accurately how slow.

Evidence to indicate that the current temporal response of the model may be flawed was presented by Dr. Connolly, who suggested that the half-life time of PCBs in the River is likely is closer to 36.5 yr (i.e. 0.693/0.019) than the current model prediction of 110 yr (i.e. 0.693/0.006). I think that Dr. Connolly is probably correct, but the uncertainty in the estimates of the half-lives is large and I have not been convinced that the current PCB concentration data in the River allow one to distinguish between these two estimates.

In conclusion, the current characterization of the key temporal aspects of the model is too uncertain to make reliable long term predictions of the concentrations of PCB in water, sediments and biota of the Housatonic River. This said, it is clear from the empirical data and the model calculations that the long term temporal response to changes in PCB loadings is slow. There appears to be very large standing mass of PCBs in the River sediments and its floodplains and the sediment removal rate from the PSA is relatively small. Natural recovery therefore can be expected to take a long time, with a system half-life time in the order of decades. Given this slow response time, the calculation of a more accurate natural recovery time may in some cases be inconsequential. Under certain conditions, the model, as it stands, may already be sufficient to address the long term temporal response of PCB concentrations in the water column and bed sediments (model objective #1).

The reason for the model's ability to convincingly assess the long term temporal response of the PCB concentrations in water, sediments and biota of the River are twofold. First, no significant long-term-changes in PCB concentrations over time were observed in water, sediment or biota throughout the PSA during the calibration period. Secondly, the key parameters controlling the temporal response of PCB concentrations are difficult to measure or estimate. Based on this, the following recommendations can be made:

#### Recommendations:

The modelers should explore alternate parameterization schemes (possibly with the help of Dr. Lick) of the sediment-water exchange processes with the goal to select model parameterization schemes that are defensible based on available laboratory and field observations.

The modelers should revisit the calibration of the temporal response of the model based on a more in-depth statistical analysis of the available model calibration data. I specifically refer to the sediment concentration data as a function of time. Model calibration schemes should be evaluated in terms of their ability to reproduce statistically validated temporal PCB concentration data.

The modelers should improve the calibration of the model by lengthening the model calibration period. This most likely involves a continuation of monitoring the response of PCB concentrations in the River to the remediation efforts that have recently taken place. Over time, a more definite change in concentration may take place, which can be used to better calibrate the model.

#### Re. Model Objective #1 on the issue of Space:

The model report reveals insufficient information to determine whether the capability of the model to make accurate predictions of spatial differences in PCB concentrations is adequate. The reason is that the calibration of the spatial characteristics of the model revealed that differences in PCB concentrations (e.g. see Fig 6-2-45 and 6-2-46 Model Validation Report) among River sections are small while variability in the PCB concentrations in the sediments at individual river locations is high.

The spatial resolution of the environmental fate and food-web model is unnecessarily complex. A much simpler spatial model is consistent with the empirical data and the current model calculations. The hydrodynamic model does not run on a low spatial resolution. However, it is possible to run the hydrodynamic model on its optimal spatial resolution and aggregate the hydrodynamic data for a much simpler PCB environmental fate model. The latter would also reduce the model run-time from the current, unacceptable 30 to 50 d. This would also make the model more transparent due to greater simplicity. The modelers could argue that in terms of predicting spatially varying concentrations the current multi-compartment model is consistent with a much simpler lower spatial resolution model, so there is no need to develop the simpler model. This is true for the model's current application. However, the modelers should keep in mind that when the current model is applied to make predictions of the impact of remedial actions on PCB concentrations as a function of space (i.e. model objective #1), the model may predict spatial differences in concentrations that have not been "validated" or "ground truthed".

#### Recommendations:

Better spatial statistical methods should be used to explore the current spatial PCB concentration data for spatial trends in the available PCB concentration data.

The modelers should consider developing a simpler spatial representation of the environmental fate and food-chain model by decoupling the hydrodynamic and sediment transport model from the environmental fate and food-chain model. The current high spatial resolution of the model is unnecessary for the environmental fate and food-chain model. Also, the time-step requirement for the hydrodynamic model is too onerous and unnecessary for the environmental fate and food-chain models. This change in model design will make it possible to make many model runs within a reasonable computational time.

### Re. Model Objective #2:

With regards to achieving model objective #2, i.e. ability to quantify the historical and current relative contributions of various PCB sources to PCB concentrations in water and bed sediment, I do not think that the model reasonably accounts for the relevant fate processes. The reason is that the model has difficulty assessing the amount of historical PCB mass that is "accessible" by the River. Difficulties in the selection or determination of an "accessible" sediment layer and decisions regarding the inclusion or exclusion of flood plains as accessible sources of PCBs to the Housatonic River contribute to the overall difficulty in assessing the current mass of PCBs in the River. As a result it is difficult to assess the relative contribution of any current inputs of PCBs into the River. The lack of any significant change in the PCB concentrations in the River over time over the period that significant removal of PCB sources in the immediate vicinity of the GE facility remediation took place may be an indication that historical sources of PCBs throughout the PSA are likely the main contributor to current PCB concentrations in the River.

#### Recommendation:

An alternative to the difficult characterization of the current mass of PCBs in the River, is using the model to investigate under which set of model parameters historical sources are the main contributor to the PCB concentrations in the Housatonic River and judge whether these model parameter sets are reasonable. This would avoid having to characterize the actual current mass of PCBs in the River.

## Re. Model Objective #3:

Due to the heavy reliance on calibration during model development, the relative PCB concentration data in water, sediments and biota that are calculated by the model are overall consistent with the model predictions of the mean concentrations. The model can therefore be used with confidence to address the relative contributions of <a href="mailto:current">current</a> PCB sources to bioaccumulation in target species (i.e. model objective #3). Dr. Connolly argued that the potential underestimation of the overall PCB depuration rate in the River affects estimates of the relative contributions of current PCB sources to bioaccumulation in target species. While this is correct, I do not think that this will have a significant effect on the derivation of current relative sources of PCBs to fish because PCB concentrations did not vary significantly over the time period that calibration was performed.

The application of the model of the model to quantify the <u>historic</u> contributions of various PCB sources to bioaccumulation in target species is dependent on the time dependent capabilities of the environmental fate model, which are more uncertain (see discussions above). The FCM model can be expected to properly estimate the relevant contributions of water and sediment concentrations as sources of PCB bioaccumulation in benthos and

fish species from PCB concentrations in water and sediments delivered by the EFDC model.

### Re. Model Objective #4:

The report indicates that the model reasonably accounts for the role of storm events. The model appears to do a good job in describing the short term temporal response of river flow rates in response to storm events. The comparison of simulated and observed river flows is more than adequate. However, the excellent flow predictions do not translate in equally impressive TSS concentrations. Figures 6.2-19 to 6.2-22 show considerable discrepancies between observed and predicted short term TSS concentrations at Holmes Road, Lennox Road and Woods Pond Outlet. On the other hand, Figures 6.2-39 to 6.2-41 show that the short term PCB concentration variations in the water phase (assuming that the concentration data displayed are water column tPCB concentrations) are reasonably well predicted. The reason for the poor predictability of TSS concentrations, but good predictability of the PCB concentrations in the water column is somewhat surprising and unclear. However, the data presented produce confidence in the model's ability to make reasonable predictions of the effects of storm event(s) on the redistribution of PCB-laden sediment in the study area (model objective #4).

#### Recommendation:

I recommend that the modelers investigate the source of error in the estimation of the TSS.

#### **Charge Question #2**

Is there evidence of bias in the model, as indicated by the distribution of residuals of model/data comparisons?

There is evidence of bias in certain model outcomes in the model validation.

First, in the majority of comparisons between measured and model predicted TSS concentrations, the TSS concentrations are over predicted. This does not appear to have a corresponding impact on the calculation of the PCB concentrations in water. The effect of this bias on the calculation of PCB concentrations under current conditions appears to be low. However, the bias may become important when the model is applied under different conditions. It is therefore important to explore the reasons for the bias in TSS and make appropriate corrections.

Secondly, the combined or linked model (Table 6-4.7) shows a systematic underprediction of the mean PCB concentrations as high as a factor of about 2 for some of the species. Overall, including all species, the underprediction of PCB concentrations in biota is about a factor of 1/0.60 or 1.67. This systematic bias does not appear to be due

to the bioaccumulation model itself. Judging from Table 6-4.6 (Model Validation Report), the bioaccumulation model itself appears to have little or no systematic bias. Judging from Figures 6.3.3 to 6.3.8, the uncertainty in the characterization of the model bias is large. The authors could have calculated the standard deviation of the mean, but did not do this. If they would have done this, they would have found that the standard deviations of the model bias for any of the PCB concentration in fish data sets are quite substantial due to the large variability in the observed PCB concentrations in the biota. This means that while the mean model bias for the PCB concentration predictions in fish is relatively low, the uncertainty of the mean model bias is high. I think that it is important in any model to be upfront about the ability of the model to make predictions of reality. The reporting of the model bias without its uncertainty is misleading in my view. The reality is that PCB concentrations in biota vary substantially and we do not really understand why this is. So, we should not pretend that we can predict PCB concentrations in fish with the accuracy that the mean model bias measures suggest. I therefore suggest that the authors provide a full reporting of the model bias of the PCB concentrations (i.e. report uncertainty in the mean model bias) using the linked model and interpret the findings in terms of model uncertainty when the model is applied.

Thirdly, the analysis presented by Dr. Connolly during the June 28 Public Meeting indicates that there may be a bias in the temporal response of the model, i.e. it appears that the rate of temporal response of PCB concentrations in the River is underestimated by the model. However, there is considerable uncertainty in the data on which the calculations are based and it is unclear whether the uncertainty in the data is sufficiently small to distinguish between the temporal response rates calculated by the model and Dr. Connolly's analysis. A bias in the temporal response of the model could have large implications for model projections of remedial actions. More detailed evaluations of the bias in temporal response need to be conducted. This should involve the calculation of PCB concentration response times from observed data and the comparison of the measured response times to the calculated response times to determine whether a bias exists. Alternative model parameterization schemes may need to be explored to investigate whether the model bias (if it exists) can be reduced.

#### Recommendations:

I recommend that the modelers explore model parameterization schemes that remove bias in the TSS model predictions.

I recommend that the authors calculate the standard deviations of the mean model bias of the linked model and make appropriate corrections to account for the systematic underprediction of the mean PCB concentrations in the biota by the model. The systematic underprediction of the mean PCB concentrations in fish by the model needs to be either corrected or recognized when the model is applied.

The possible bias in the model's temporal response of the PCB concentrations in the River needs to be investigated by comparing observed and predicted PCB concentration

decline rates over time. In case, significant bias exists, alternative model parameterization schemes need to be explored to improve the long term temporal response of the model.

### **Charge Question #3**

Are the comparisons of model predictions with data sufficient to evaluate the capability of the model on the spatial and temporal scales of the final calibration and validation

With regard to the temporal scale, the comparisons of model predictions with data are not sufficient to evaluate the capability of the model to make accurate estimates of the temporal response of PCB concentrations in the River. As discussed under charge question #1, this is largely due to the considerable variability in observed PCB concentrations and the lack of a significant decline in PCB concentrations over the calibration period. Hence, a temporal trend is difficult to discern from the data and the lack of temporal trends makes it very difficult to evaluate the temporal characteristics of the model. With regards to the spatial scale of the model, a similar conclusion can be reached at. The small-scale spatial variability in the PCB concentration in the sediments is so great that spatial differences in PCB concentrations among River sections are difficult to discern. The comparison between observed and predicted concentrations therefore provides little information with regards to the capability of the model to make accurate predictions of PCB concentrations as a function of time or space.

#### Recommendations:

Dr. Connolly's analysis suggests that with the application of suitable statistics it may be possible to use the current data sets to better characterize temporal and spatial PCB concentration trends. Spatial statistics and the application of geographical averaging methods may help to better characterize spatial trends in the data that can be used to evaluate the applicability of the model. Temporal trend analysis can be used to discern temporal trends. I recommend that this is done as it may provide better data for a comparison of observed and predicted concentrations.

A second suggestion is to lengthen the model's calibration period. The calibration period for the current model was too short for an evaluation of model capability. This would involve the continuation of monitoring programs with the objective to develop PCB concentration data over a longer period of time.

## Charge question #4

Have the sensitivities of the models to the parameterization of the significant state and process variables been adequately characterized?

The modelers have done a good job describing parameter sensitivities. The latter is not easy as there are many parameters and the sensitivities of each of them depend on the values chosen for the others.

However, there is one area in the model where conducting a thorough sensitivity analysis is crucial because of the lack of good calibration data and difficulties in model parameterization. This is in the component of the Environmental fate model that controls the long term temporal response of the model. The selection of the thickness of sediment layers, diffusion rates, and bioturbation rates are all very difficult. Hence, a thorough sensitivity analysis is crucial to determine the bounds within which temporal changes in concentrations can be expected to occur. This analysis is not presented in the current reports and supports my conclusion that the long term temporal response of the model is too uncertain to make meaningful predictions.

#### Recommendations:

Given the lack of calibration data, the sensitivity analysis is probably one of the few things that can be done to increase confidence in any estimates of the temporal response in PCB concentrations calculated by the model. I recommend that it is considered and added. For this sensitivity analysis to be doable and convincing, the modelers could just focus on the part of the model that controls the long term temporal response of the model.

## Charge question #5

*Are the uncertainties in the model output(s) acknowledged and described?* 

1. While the report presents several efforts to calculate uncertainty, the model uncertainties are not fully acknowledged. In essence, the report presumes that the model's ability to calculate mean concentrations is sufficient to address the goals of the study. I think that this is a flaw in the study design because the goal of the model is to compare PCB concentrations resulting from different remedial scenarios. Such an application involves the comparison of mean concentrations. However, comparing mean concentrations alone is insufficient to determine the significance of the differences in mean concentrations. The calculation of the statistical significance of a difference in the means is required. The latter is a well established practice in scientific and engineering studies. I do not think that a convincing rationale is presented for why this practice is not applicable in this study. The authors argued that ecological receptors (including fish), due to their continuous movement, tend to be exposed to a large variation in concentrations, which get "averaged out" to produce an internal concentration in the fish that corresponds to the average or mean exposure concentration rather than the variation in concentrations (l. 10-14, p.15 Responsiveness document). Figures 6-2-35, 6-2-56, 6-3-3 to 6-3-8 (Model Validation Report), and similar figures in the calibration documents demonstrate a one-to two order variability in predicted concentrations of PCBs, which does not differ substantially between fish and sediments (i.e. the variability in fish concentrations does

not appear to be any less than that in suspended solids). This indicates that the original assumption that PCB concentrations in fish may be less variable than the sediment concentrations may not hold.

The model's capability to estimate only mean concentrations, makes it difficult to apply the model to some objectives. For example, when the model is applied to address model objective #6, it can only calculate at what point in time the mean concentration falls below a target level that no longer poses a human health or ecological risk. This means that roughly (depending on the frequency distribution of the concentrations) half the concentrations are still above the target level. Risk assessment calculations typically depend on the distribution of the concentration and set limits based on a percentage of individuals exceeding a particular concentration. Hence, a frequency distribution of the concentrations is essential. Perhaps it is assumed that the risk assessment calculations can deal with the distribution of the concentration. However, in the application of the model, it is the model that has to generate the distribution of concentrations (since there are no data for the future) and at this point, none of the model components can do this. A comparable argument can be made for the application of the model to model objective #1, i.e. quantify future spatial and temporal distribution of PCBs (both dissolved and particulate forms) within the water column and bed sediment. The mean concentrations that will be produced by the model do not provide information on the statistical distribution of the predicted concentrations. Hence, as the model stands, it is impossible to determine whether any calculated difference in concentration (e.g. as a result of a remediation strategy) is significant and can be treated as a difference in effectiveness among remediation strategies.

I agree with the EPA that it is not necessary to understand the processes causing small scale variability in concentrations (1.3-4, p.15 Model Validation Report). This is normal is any scientific observation. However, when interpreting the observation or the model calculation (in this case), it is then important to recognize the uncertainty that is associated with the lack of understanding, so that it can be taken into account in the decision analysis.

2. The calculation of model uncertainty in the report is seriously flawed. The report includes several references to this. For example, based on findings that the uncertainty in the calculated PCB concentrations is greater than the variability in the sampling data, the authors conclude that "the results should not be interpreted to mean that the uncertainty in model predictions renders the model predictions too uncertain to be usable" (p.5-56 Model Validation Report). The authors further "acknowledge that a true statistical analysis of uncertainty, particularly when uncertainty is propagated through the modeling framework, can produce bounds that may not be possible (or likely) based on an understanding of that system. (p.5-57 Model Validation Report). I think that these are important points. I agree that in models of this complexity, it is virtually impossible to meet some key criteria for a meaningful Monte Carlo Simulation, namely (i) that the model parameters included in the simulations are independent, and (ii) there is insufficient data to properly characterize the variability/uncertainty/error in the many

parameters used in the model. Also, it should be recognized that the MCS method does not recognize error in the functional relationships of the model. The KS method is subject to the same limitations as the MCS method and the failure of 4 out of the 56 runs may be due to implausible parameter selections causing the model to crash for these runs due to the problems outlined.

In conclusion, the conditions for a meaningful MCS or KS uncertainty analysis are not met in this study. The calculated uncertainty values are therefore seriously flawed. It is unclear what the meaning of the calculated uncertainty is. The lack of a meaningful uncertainty analysis is a major flaw of the current model because model projections are very difficult, if not impossible to interpret.

To include uncertainty and better characterize it, the modelers could consider using the formidable empirical data set to calculate frequency distributions for the model predicted mean concentrations. To formalize this method, the authors could further develop the MB method described on p. 6-118 (Model Validation Report) by calculating the standard deviation of the mean (i.e. MB). What this will do in the case of PCB concentrations in the sediments is simply project the observed variation in PCB concentrations on the model predicted concentrations. The result is now a distribution of predicted concentration that is grounded in empirical data. This is not a major job, and could be done with little extra work.

#### Recommendation:

My recommendation is to ignore the MCS and KS results and remove it from the model framework when the model is to be applied in the next phase of the study. Instead I recommend that the modelers use the discrepancy between model predicted concentrations and observed concentrations as a measure of model uncertainty. This is simpler, easier to understand and avoids current computational problems. For example, the data depicted in Figures 6.3.3 to 6.3.8 (Model Validation Report) can provide a reasonable description of the overall model uncertainty. This can be achieved by calculating the confidence limits of the MB used in the report. See Environ. Toxicol. Chem. 23, 2343-2355 for additional details on this method. The application of this method will also generate frequency distributions of model outcomes that can be used in risk assessments. The method that I recommend is not complicated and can be carried out in little time. The main drawback of the application of this method is that it relies on the assumption that the uncertainty identified in past application of the model is a good measure for uncertainty in future model applications. I think that this is a reasonable assumption for some model applications. However, if river functioning is drastically altered by the remediation efforts, this assumption may not apply.

#### **Charge Question #6**

Upon review of the model projections of changes in PCB concentrations in environmental media in the example scenarios, are such projection reasonable, using your technical judgment, and are they plausible given the patterns observed in the data.

The patterns in the data indicate a slow temporal response of the PCB concentrations in the River. The example scenarios also indicate a small decline of somewhere between 0 to 5% (it is hard to spatially average the concentrations depicted without additional information) over 26 years in response to the assumed loading reductions. I think that this is consistent with the observations.

The data illustrate large small-scale spatial variability in PCB concentrations in sediments. The model appears to capture this to some degree as changes in concentrations relative to the control vary between grid cells within many transects.

I have trouble understanding why PCB concentrations in so many cells of the lower part of the River (Figure 7-1b and 7-3b) increase in concentrations as a result of the loading reductions. This is not what I would expect to happen intuitively given the long history of the PCB contamination problem and the slow response time of PCB concentrations in the river. I would expect concentrations to go down throughout the river, but at higher rates at some locations and lower rates at others.

Comparing scenarios 1 and 2, one would expect that elimination of additional PCB loads in scenario 2 would produce a greater change in PCB concentration over time in scenario 2 than 1. Perhaps, this is the case. It is hard to see from the graphs. However, even if this is not the case, it is possible that concentrations decline over the 26 years are comparable for scenarios 1 and 2. Without more information, it is hard to be more definite.

Based on the current information presented, there is no basis for concluding that the patterns provided in the example scenarios are not plausible given the patterns observed in the data. But more data is needed to support a more positive and definitive conclusion. The example scenarios in the validation report provide little information about the functioning of the model. To address the charge question properly, it is important that the model outcomes of the example scenarios are further analyzed. In particular, it is important to average model outcomes over space and time such that the model predictions can be compared to available data.

#### Recommendation

I recommend that the behavior of the combined model is explored in greater detail than is presented in the validation report. I recommend that the model outcomes in the model scenarios are aggregated to depict the overall response of the PCB concentrations in the River. This will provide the opportunity to better compare model projections to available data sets and judge whether the model projections are plausible.

## Charge question #7

Is the final model framework, as calibrated and validated, adequate to achieve the goal of the modeling study to simulate future conditions 1) in the absence of remediation and 2) for use in evaluating the effectiveness of remedial alternatives?

The model is the only available tool to simulate the future response of PCB concentrations in response to remediation efforts. The model framework represents a suitable approach to estimating the future time response of PCB concentrations in the River and the calibration and validation of the model have involved significant efforts. The most valuable information for the calibration and validation of the model is a change in PCB concentrations in the River in response to a known reduction in PCB loading. This kind of information was not obtained in the current study as concentrations of PCBs in the River showed little or no significant variation with time. The current model therefore has to rely on the characterization of a number of key state variables for the estimation of the long term temporal response of PCB concentrations to remedial scenarios. The key parameters include the amount of "available" River and floodplains sediments and rates of resuspension, diffusion, bioturbation and subduction. All of these model state variables are either currently unmeasurable or very difficult to measure or estimate. As a result the model's outcome with regards to the long term time response of PCB concentrations in the River is uncertain. The model uncertainty translates in considerable uncertainty about future PCB concentrations in the River resulting from remediation efforts or the absence of remediation.

Any model has inherent uncertainty. So, this is normal. But where the model framework is inadequate is in the recognition of this uncertainty and in the development of adequate methods to characterize or estimate this uncertainty. Without the inclusion of uncertainty in the current model framework, I do not think that it is possible to convincingly distinguish between the effectiveness of different remedial options.

The model as it currently stands is incomplete. A lot of excellent work has been done but there are some major gaps that need to be addressed before the model is ready for application. This may sound disappointing to some, especially for those living in the immediate vicinity of the River. However, the remediation options that can be expected to be considered have very large and long lasting impacts on the River and its ecology. Therefore, caution should be exercised and there should be confidence in the outcome of remediation efforts before such remediation takes place.

#### Recommendations:

I have several recommendations for the completion of the model:

- 1. Include model uncertainty in the model framework and provide guidance about how the results from the uncertainty analysis are to be used when comparing outcomes resulting from different model scenarios.
- 2. Do not use the MCS or KS method for calculating model uncertainty.
- 3. Include an uncertainty analysis that takes full advantage of the empirical data that have been collected. As discussed earlier, this can be achieved by comparing observed and model predicted PCB concentrations.
- 4. Reduce the model run-time from an unacceptable 30 to 50 days to 1 d (at most), such that different model parameterization schemes can be explored for making model projections.
- 5. Conduct sensitivity analyses with the goal to (i) further investigate the parameterization of the sediment-water exchange of PCBs, on which the temporal response of PCB concentrations in the River largely depends and (ii) improve the parameterization of the key processes if possible (see under charge question #1 for additional details on this issue).
- 6. Continue existing PCB concentration monitoring programs to measure the changes in PCB concentrations over time as a result of the recently completed remediation. Use the data together with calculations of PCB source reductions due to remediation to extend the calibration period and improve the calibration and/or validation of the long term temporal response of the model.
- 7. Apply a staged and adaptive approach in the planning of River remediation. Plan to gauge the river's response to remedial efforts at certain locations in the River throughout the River remediation. A PCB concentration monitoring program can detect the effect of remedial actions on PCB concentrations over time and space. These data can then be used in the model to further optimize the model, such that the effects of newly planned remedial efforts can be better estimated.

## **Additional Comments**

## **DOC-water partitioning**

The model assumption that the sorptive capacity of DOC is two orders of magnitude less than that of POC (1.27-28, p.6-67 Model Validation Report) seems out of touch with the literature. The lowest value I have seen to characterize the sorptive capacity of DOC compared to octanol was 0.08, i.e. DOC has 8% of the sorptive capacity of octanol (Burkhard, L.P. Estimating dissolved organic carbon partition coefficients for nonionic organic chemicals. *Environ. Sci. Technol.* 2000, *34* (22), 4663-4668. – Note that in response to p. 2-72 of EPA response, Burkhard states that K<sub>DOC</sub> = 0.08.Kow, not K<sub>DOC</sub> = 0.08.K<sub>POC</sub>). In comparison, the sorptive capacity of POC is approximately 35% of that of octanol (Seth, R.; Mackay, D.; Muncke, J. Estimating the organic carbon partition coefficient and its variability for hydrophobic chemicals. *Environ. Sci. Technol.* 1999, 33 (14), 2390-2394.). Following these papers, the difference in sorptive capacities between DOC and POC is approximately a factor of 35/8 or 4.38. Burkhard et al. did report 95% uncertainty limits of a factor of 20 for the 0.08 value, hence the 0.01 value used in the model is plausible, but it is very low.

Much higher values of the sorptive capacities of DOC in relation to octanol have also been measured. For example, Macintosh et al. report  $1.16 \pm 0.49$  for spiked and  $61 \pm 47$  for native PCBs and phthalates. This compared to  $35 \pm 19$  for POC (Sorption of Phthalate Esters and PCBs in a Marine Ecosystem, Mackintosh et al. Environ. Sci. Technol.; 2006; 40(11); 3481-3488.). The latter results indicate no significant differences between sorptive capacities of DOC and POC and also evidence of DOC-water disequilibria.

The assumed two orders of magnitude difference in sorptive capacities of POC and DOC in the model is, albeit plausible, a very low value. Given the variation in literature data, I recommend that empirical data are used to calibrate this model input requirement. The recent EPA response document suggests that the latter has indeed been done.

#### **Diffusive Flux**

The importance of a diffusive flux of PCBs from sediments to the water between Holmes Road and New Lennox Road during low flow periods is surprising (p.6-72 Model Validation Report) given the otherwise dominant roles of erosion and deposition (Fig 6.2-62 Model Validation Report). I have never seen a system, especially a riverine system, in which diffusion played such an important role. I think that it was necessary to invoke a high diffusion rate to explain the concentration data. I am not sure if there is any precedent for such a high diffusion rate though. This may be perhaps point to another parameterization problem in the model. I recommend the authors investigate this process in more detail and explore other options for calibrating the model.

## **Tables**

## Table 1: Model Objectives

## Model objectives:

- 1. Quantify future spatial and temporal distribution of PCBs (both dissolved and particulate forms) within the water column and bed sediment
- 2. Quantify historical and current relative contributions of various PCB sources to PCB concentrations in water and bed sediment
- 3. Quantify historical and current relative contributions of various PCB sources to bioaccumulation in target species
- 4. Quantify relative risk(s) of extreme storm event(s) contributing to the resuspension of sequestered sediment or the redistribution of PCB-laden sediment in the study area
- 5. Estimate the time required for PCB-laden sediment to be effectively sequestered by the deposition of uncontaminated material (i.e., natural recovery)
- 6. Estimate the time required for PCB concentrations in fish tissue to be reduced to levels established during the risk assessment process, that no longer pose either a human health or ecological risk, based upon various response and restoration scenarios