Appendix E: Food Web Model and Biota-Sediment Accumulation Factor (BSAF) Development

Page 10, Section 3.2, Model Development and Methodology: The text here clearly states some general assumptions with regard to the model use here which are that the system is in steady state and that the flux between different media are governed by fugacity relationships. Based on Gobas, with these assumptions the following is true:

-The steady state assumption is reasonable for applications to field situations where organisms have been exposed to the chemical for a long period of time. It applies best to chemicals that are subject to relatively fast exchange kinetic (e.g. lower Kow substances, small organisms), as steady state will be achieved rapidly in these situations. It should be used with caution in situation where the exchange kinetics are very slow (e.g. slowly metabolizable chemicals of high Kow in large lipid rich organisms) because steady state takes a long time to achieve.

Page 14, Section 3.2.5.1, Selection of Model Parameter Values and Distributions Used for Calibration:
Gobas does not recommend calibrating the food web model as long as the model is used with its application domain. Tables 3-5 to 3-9 show calibrated environmental and biological parameters. Unless we have enough information on these parameters to represent them as a robust distribution or unless we have conducted additional site specific studies to justify a change to the value, we should not be changing the values in order to get better agreement between the model and tissue. This is especially true since you aren't always sure the data you are trying to calibrate the model to is correct or without its own inherent uncertainties (such as the limited and highly composited tissue dataset we are currently working with).
However, there is a need to check whether the model calculations are consistent with available empirical data such that confidence in the model is gained. This has the same objective of calibration, but it is more of a hypothesis testing scenario, where the model outcomes are compared with independent data (data not used in the construction of the model). In this case, the preferred model outcome is the chemical concentration in a particular species, and involves the comparison of observed and predicted concentrations in different aquatic species.
Instead of Table 3-7 presenting "calibrated values" for weight, lipid content, etc. for each species, it should be presenting a rigorous evaluation of how well the model outcomes match tissue observations in the harbor. In order to evaluate how well the model outcomes match the observations, Gobas uses the mean model bias MB to express the central tendency of the model. MB is the geometric mean (*assuming a log-normal distribution*) of the ratio of predicted and observed concentrations. The LWG includes a similar equation on page 13, which appears to not use a log-normal distribution, and does not appear to use information from a number of observations from each species (it looks like one average is used).
Where $C_{P,i}$ and $C_{O,i}$ are the concentrations of the chemical in a particular species that are respectively predicted by the model and observed in the field and i can refer to the

number of observations (i.e. for a particular chemical in a particular species), number of chemicals (in a particular species) or a number of species (for a particular substance).

**In the calculations of MB, over-and under predictions have a tendency to cancel out, and therefore it describes the central tendency of the model outcome. Variability in the over- and under-estimation of measured values should be represented by the 95% confidence interval of MB. *This is something that should be added to the LWG analysis.*

Page 47, Table 3-8, Calibrated values for species specific dietary parameters: **Dietary parameter assumptions should not be calibrated, but rather a sensitivity analysis should be run to better understand how much of a difference a range of prey assumptions would make.**

Page 48, Table 3-9, Calibrated Kow and Water Concentration Values: **Empirical data such as chemical concentration in water should not be calibrated, but rather represented in the model as a distribution (in addition to a distribution of sediment concentrations).**

Page 20, Section 3.2.5.5., Uncertainty Assessment:
The role of any uncertainty analysis should be to assess the error in the model calculations, which is important because the magnitude of the model needs to be considered when interpreting the results of the model calculations for management purposes. The comparisons of predicted and observed results in an uncertainty analysis, and can be plotted as a distribution of predicted and observed ratios. The *wider the range* of predicted versus observed values is not good. We should be relying on a rigorous analysis of observed versus predicted data variability to give us an estimate of uncertainty.
In an uncertainty analysis, many parameters are correlated, so it is difficult to apply Monte Carlo simulations of uncertainty. One of the key requirements is that the model state variables are independent. Examples of related state variables are animal size, growth rate, lipid content and feeding rate. In addition, in order to do this analysis correctly, you have to characterize uncertainty in each model parameter, which is hard to do, especially since we may not know how they vary over time.

For uncertainty analysis, the parameters you can include and still maintain independence include lipid content, temperature and Kow. He does not recommend conducting an uncertainty analysis on prey composition, but can use a sensitivity analysis to see how much of a difference prey assumptions would make (see above comment).

Model Application, Forward Calculation:
We should be using a distribution of PCB concentrations in sediment (frequency over long SUM PCB (ug/kg dry wt) in sediment) and adding the model distribution of BSAFs from the model (using individual paired data) to give us a distribution of tissue predictions.

For PCB modeling, Gobas has found that you should be able to get within a factor of 2 to 2.5 – these factors shouldn't be any higher. Also, all PCBs should be calculated as congeners – don't try and model total PCBs!!!