PEER REVIEW OF EPA'S HAZARDOUS WASTE IDENTIFICATION RULE RISK ASSESSMENT MODEL

Background Document for the HWIR Aquatic Food Web Module and Supporting Module Input Data

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NOTE

This report was prepared by Eastern Research Group, Inc. (ERG), an EPA contractor, under Contract Number 68-W-99-001. The report presents comments provided by peer reviewers on the *HWIR Aquatic Food Web Module* and *Supporting Module Input Data* documents that are part of EPA's Hazardous Waste Identification Rule risk assessments.

The comments presented in this report have been compiled by topic and by individual peer reviewer. As EPA requested, this report provides the peer review comments exactly as they were submitted to ERG. Also attached are the original comments submitted by each individual reviewer.

Peer Review Charge for the HWIR Aquatic Food Web Module and Supporting Module Input Data

Background

The multi-media, multi-pathway and multiple receptor risk assessment (3MRA) model was designed to establish safe, constituent-specific exit levels for low risk hazardous wastes under the Hazardous Waste Identification Rule (HWIR). Wastes to be assessed under HWIR are those currently designated as hazardous because they were listed, or had been mixed with, derived from, or contained listed wastes. One of the intended outcomes of HWIR is to reduce possible over-regulation arising from application of the "mixture" and "derived-from" rules that were promulgated as part of the first comprehensive regulatory program for the management of hazardous wastes under RCRA in May of 1980. Both of these rules remain important in reducing risk to human health and the environment associated with the management of hazardous wastes; however, because they apply regardless of the concentration or mobility of hazardous constituents in the wastes, they also open the possibility of over-regulation. Therefore, one of the primary purposes of 3MRA is to provide a tool for identifying possible instances of over-regulation, and to provide an avenue for the safe relief from Subtitle C disposal regulations.

In December of 1995, the Agency proposed a methodology designed to identify the exposure pathway associated with the highest predicted risks to both human and ecological receptors. This methodology constituted the first multi-media risk assessment tool developed to support risk-based exit levels (i.e., acceptable chemical concentrations in wastes), and was referred to as the Multiple Pathway Receptor Analysis (MPRA). It utilized the revised EPACMTP modeling approach for the groundwater pathway analysis, and the indirect exposure methodology for other pathways. The MPRA was designed to simulate each exposure pathway independent of other pathways, and the model was parameterized such that the contaminant fate and transport favored one pathway for each simulation. That is, the parameters to which each pathway was most sensitive were set to high end values, and the model was executed to drive risks to one pathway at a time (i.e., contaminant losses to other environmental media were not tracked). During an extensive series of reviews of the MPRA, the EPA Science Advisory Board (SAB) and others urged the Agency to consider using a simultaneous, mass-constrained analysis that would account for dispersal, transport and transformation of contaminant mass through all media and exposure routes. This was perhaps the most important and strongly expressed element in all of the review comments received.

The goal of the 3MRA is to identify wastes currently listed as hazardous that could be eligible for exemption from hazardous waste management requirements. The 3MRA risk assessment predicts chemical-specific potential risks to human and ecological receptors living within a radius of 2 kilometers of industrial nonhazardous waste sites that could manage HWIR-exempted waste. These risk estimates, along with other information, may be used to identify the chemical-specific concentrations for exempted waste that would be protective of human health and the environment at selected sets of risk protection criteria.

The 3MRA assessment strategy provides a methodology to evaluate multiple exposure pathway risks to human and ecological receptors at a statistically representative sample of waste management units (WMUs) and associated environmental settings to estimate the distribution of risk nationally. It is a forward-calculating approach that begins with selected concentrations of a chemical in waste, and estimates the associated hazards and risks to human and ecological receptors.

The risk assessment is designed to produce chemical-specific distributions of cancer risks or hazards to humans and ecological receptors living in the vicinity of industrial waste sites that could manage HWIR-exempted wastes throughout their operating life. For each site and waste concentration, the model generates risks for each receptor location and then sums the number of receptors that fall within a specified risk range (bin) to get the distribution of risks for the population at each site. We can use the distribution of risks for a setting to determine whether the setting is protective based on the percentage of the population protected, a specified cancer risk or hazard level, and the initial concentration in waste. The model then uses these data to generate a percentile distribution based on the number of settings protected at a specified risk level for each waste concentration to generate the national distribution.

The 3MRA model consists of 17 media-specific pollutant fate, transport, exposure, and risk modules; 6 data processors to manage the information transfer within the system; and 3 databases that contain the data required to estimate risk.

As shown in Figure 1, the 3MRA Model incorporates the following interacting modules:

- Source modules, which estimate the simultaneous chemical mass losses to the different media and maintain chemical mass balance of the releases from the waste management unit into the environment

- Fate/transport modules, which receive calculated releases from waste management units and distribute the mass through each of the media to determine the chemical concentrations in air, groundwater, soil, and surface water across space and time

- Food chain modules, which receive the outputs from the fate and transport modules and estimate the uptake of chemicals in various plants and animals

- Exposure modules, which use the media concentrations from the fate and transport modules to determine exposure to human and ecological receptors from inhalation (for humans only), direct contact (for ecological receptors only), and ingestion (for both receptor types)

- Risk modules, which predict the risk/hazard quotient for each receptor of concern.

Aquatic Food Web Module

The Aquatic Food Web (AqFW) module calculates chemical concentrations in aquatic organisms that are consumed by human and ecological receptors (e.g., fish filet; aquatic macrophytes). These concentrations are used as input to the human and ecological exposure modules to determine the applied dose to receptors of interest. The module is designed to predict concentrations in aquatic organisms for coldwater and warmwater aquatic habitats.

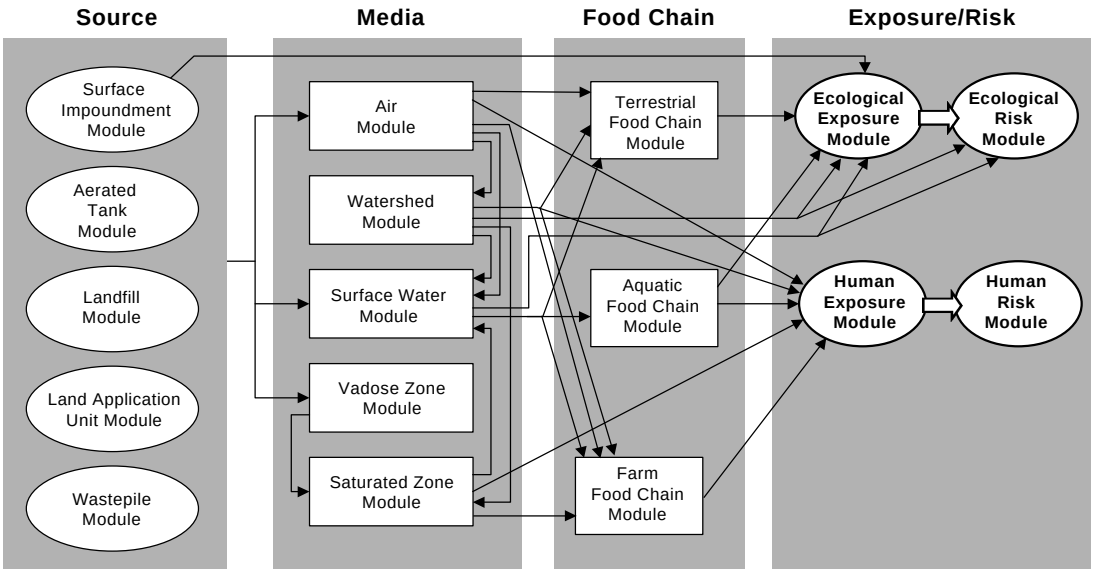


Figure 1. Source, fate, transport, exposure, and risk modules of the 3MRA Model

The underlying framework for the AqFW module is the development of representative freshwater habitats for warmwater and coldwater systems. Four basic types of freshwater systems were included for the two temperature categories: streams/rivers, permanently flooded wetlands, ponds, and lakes. As described in Section 3.1of the Aquatic Food Web Module review document, simple food webs were constructed for each of the eight freshwater habitats (four coldwater and four warmwater) that specify: (1) the predator-prey interactions, (2) the physical and biological characteristics of the species that are assigned to each habitat (e.g., size, lipid content), and (3) the dietary preferences for fish in trophic levels 3 (TL3) and 4 (TL4).

Aquatic Food Web Module Databases

Two primary databases were constructed to support the Aquatic Food Web Module: the aquatic food web chemical properties and the fish attribute database. The chemical properties database contains two types of parameters: (1) equation variables used in estimating the bioconcentration and bioaccumulation of organic chemicals using chemical-specific properties and (2) experimentally-derived bioconcentration and bioaccumulation values for compounds such as metals. The fish attribute database contains data that characterizes the physiological traits and dietary preferences of aquatic biota within the Aquatic Food Web Module.

Materials to be Reviewed According to the Charge:

US EPA, 1999. Aquatic Food Web Module: Background and Implementation for the Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) For HWIR99
U.S. EPA, 1999. Data Collection for the Hazardous Waste Identification Rule, Section 11.0 Aquatic Food Web Data

Peer Review Charge

While reviewing the documents, please address the following general issues:

1. Comment on the organization of the review documents. Do the documents present the information in a clear, concise, and easy to follow format? If not, please provide suggestions to improve the presentation.

2. Is there an adequate description of the purpose and context for the Aquatic Food Web Module and its companion Data report? If not, please explain.

3. As with any risk assessment, there are always additional data and method development efforts that could be undertaken to reduce the level of uncertainty. Are you aware of any major methodological limitations or data gaps in the aquatic food web module or supporting database that have not been identified? If so, how could they be addressed in the near-term (for example, less than six months) and the longer-term?

In addition, the following specific issues should be addressed.

4. Do you agree with the selection and application of the uptake models to estimate tissue concentrations in aquatic biota and, when lacking suitable models, using empirical data on uptake and accumulation?

5. It is implicitly assumed that the eight aquatic habitats developed for this assessment (Section 3.1) provide adequate representation of the major types of

freshwater systems within the constraints of available data and modeling tools. Do you agree with these and their food web structures; if not, can you suggest alternative systems or structures that are appropriate for a national-scale assessment?

6. Although the Gobas (1993) model was calibrated for coldwater lakes (i.e., Lake Ontario), it was determined that this model construct was appropriate for use on other aquatic systems under the general assumption of steady-state conditions. Do you agree that it is appropriate to apply this model (as modified) to different types of aquatic habitats? If not, can you suggest more suitable approaches?

7. For chemicals that have not been shown to be readily metabolizable (e.g., other than PAHs), the module estimates tissue concentrations by multiplying empirical bioaccumulation factors by chemical concentrations in water. Given the wide variety in uptake observed across different species and under different conditions, is it reasonable to use empirical data to support a national-scale analysis? If not, what alternative would you recommend?

8. Several essential metals are likely to be included in the database of the 3MRA. Bioconcentration of essential metals is not linear and modeling approaches that account for nonlinearity are beginning to be available (e.g., see Bergman and Dorward-King, 1997). Given the generally low surface water concentrations expected from the 3MRA system, would the use of such models substantially change the estimates for tissue concentration in aquatic biota from the method currently used based on measured data?

9. Although we recognize that biota sediment accumulation factors (BSAFs) are frequently used in predicting fish tissue concentrations of highly hydrophobic, persistent chemicals (e.g., dioxins), we currently do not use BSAFs due to limitations in the 3MRA system. Rather, we use a mechanistic model (Section 3.2.1) based on Gobas et al. (1993) using BAFs and water concentrations to predict tissue concentrations in fish. Do you agree with this approach and, if not what alternative would you suggest?

10. Although parts of the module have been validated against certain types of systems, the module has not been validated for a wide range of systems and chemicals. Extensive research and review of current models and methodologies was conducted prior to the selection of the models used in the Aquatic Food Web module. Is the underlying theory sufficiently developed to allow us to predict tissue concentrations in aquatic biota in a variety of systems for a variety of chemicals for a national assessment with reasonable confidence?

11. We recognize that the approach developed in the module document to determine prey preference fractions (Section 3.2) simplifies a relatively complex set of

predator-prey interactions. For purposes of a national assessment, are there refinements you can suggest to the random sampling algorithm for estimating dietary preferences for upper trophic level fish?

12. For a national assessment, do you support the approach of using a single value, either calculated or measured, in the aquatic chemical properties database to represent bioconcentration and bioaccumulation into aquatic biota while in the fish attribute database trying to capture some of the variability of parameters that vary significantly across different waterbodies, water temperatures, and habitat structures (e.g., fish weight, fraction lipid)?

13. Are there data sources or references that you are aware of that we could use for information in either the aquatic food web chemical properties and the fish attribute databases?

14. Currently for chemicals for which BAFs are not available, a default value of one is assumed. For certain chemicals, this assumption is stated to be simply a placeholder and will be identified in the characterization of results as such. Can you recommend alternatives to this approach that would be scientifically defensible?

General Comments

Dr. Barnthouse: The approach taken in developing the HWIR food web module appears reasonable, but I believe a substantial amount of additional work is needed to support the use of the module in regulatory risk assessments. The data document does not contain any actual ecological data. Instead, it provides input parameter values for the various food web components; the sources of these values are not documented. Many of them apparently are assumed values based on the authors' professional judgment. Given the heavy reliance on assumptions, thorough sensitivity analyses and comparative evaluations of the eight alternative food web structures should be performed and documented in an appendix to the main report. I suspect that such evaluations would show that the module could be substantially simplified by reducing the number of food webs and by eliminating some food web components. On the other hand, I think the data report significantly underestimates the actual variability of many of the model parameters, e.g., lipid fractions and body sizes of different fish species. Sensitivity analyses would be very useful for determining whether or not it is important to spend additional effort in characterizing this variability

Dr. Gobas: Summary of functionality. This section is unclear. In particular the sections on time series management and module loops. They are insufficiently explained in the report. It is unclear how time issues (e.g. seasonal variations, the effect of remediation efforts) are dealt with. The reference to simulations suggests that the model is applied in a dynamic (i.e. non-steady-state) fashion. However, the equations presented later do not indicate that this is done. The application of the model as explained in this document is limited to situations where ambient concentrations are relatively constant.

I-3 Spelling OK? "all reach order 3 streams".

2-1 First assumption. This assumption is dubious. For example, we are dealing with an aluminum smelter which due to its aerial emissions produces higher concentration several kilometers away from the source than within the first 2 kilometers.

2-2 First sentence. I suggest to rephrase this sentence to "that, considering the error and variability in the estimates of the two models, the BAF estimates of the two models are not significantly different."

Section 2.2. In the report, it is not made clear which substances will be treated by the BAF model, and which substances are special substances. For example, ionizing organic substances, surfactants or organometallic complexes, are they going to be treated by the model or are they special substances? This needs to be clarified.

2-3, 2nd paragraph. Typically, some empirical data, like BSAFs, are available for "problem systems", to which the model may be applied. Perhaps a national-scale analysis can accommodate some degree of model calibration and the usage of high quality empirical data, like the BSAF. It should be possible to present the model in such a fashion that instead of equation 3-10 an empirical BSAF is used. This may help to make the analysis more acceptable to scientists, regulators and the public. In other words, only rely on a model to fill in data gaps and to make future predictions.

2-3 I do not agree that the model has not been validated. This needs to rephrased. There have been several model validation studies. Other than the Gobas 1993 study, I think of the work of Thomann and Connolly 1984 (Lake Michigan), Thomann 1989 (Lake Ontario), which use a comparable modeling

approach. Also see Thomann et al. 1992, and in 1991 for a review of model application/validation studies, e.g. Hudson River. Also, model validation work has been done by Morrison et al. (1996, 1997) in Lake Erie and Campfens and Mackay (1997) in Lake Ontario, Gobas et al. 1998 for the Fraser River, and Burkhard 1998 in his model comparison work. Also, reports may exist on the Green Bay modeling and the Lake Michigan modeling studies. In my opinion, the level of model validation is adequate to recommend it for a more general application. In terms of model validation, you may wish to know that several validation studies are in progress. I am involved in on-going model validation studies for 4 of the Great Lakes, the Kalamazoo River, San Francisco Bay and Burrard Inlet as well as the Bay of Fundy for mercury. I know that Menzie&Cura and Limnotech Ltd. are also applying the model as part of their work. I think that the combined data can be useful in assessing the model's predictive ability and uncertainty and provide further support for applying it on a general basis.

3-2 What was the rationale for using the Bertelsen 1998 approach? As you will see later on, I do not recommend the use of the regression models. However, if you want to include this, I would recommend the correlations presented in Meylan et al. 1999 because of their recognition of chemical specific factors in the correlation.

3-18 Reference to Gobas et al. (1993) should be Gobas (1993) throughout the text.

3-20 When listing the units of k1 it is better to use: L/kg.day rather than l/kg-day.

Eq. 3-9. We have moved away from using the lipid content for most phytoplankton/macrophyte calculations. The reason is that the lipid content is small and the majority of the chemical is in many cases is not primarily or exclusively contained in the lipids but in the other organic carbon fractions of the organisms as well (See also Skoglund & Swackhamer 1999). We now suggest:

$$C_P = \phi L.C_{WD}.K_{OW} + \phi_{NLOM}.C_{WD}.0.033.K_{OW} + \phi_W.C_{WD}$$

where ϕL is the lipid content, ϕ_{NLOM} is the non-lipid organic carbon content (i.e. the organic carbon content minus the lipid content, TOC-L) and ϕ_W is the water content.

Eq. 3-10 is a reasonable model but in Morrison et al. (1996) we suggest a different, more complex model. This model makes better predictions, but requires significantly more data which are not that easy to find. I think that for this model the equilibrium model should be sufficient assuming its weaknesses are recognized.

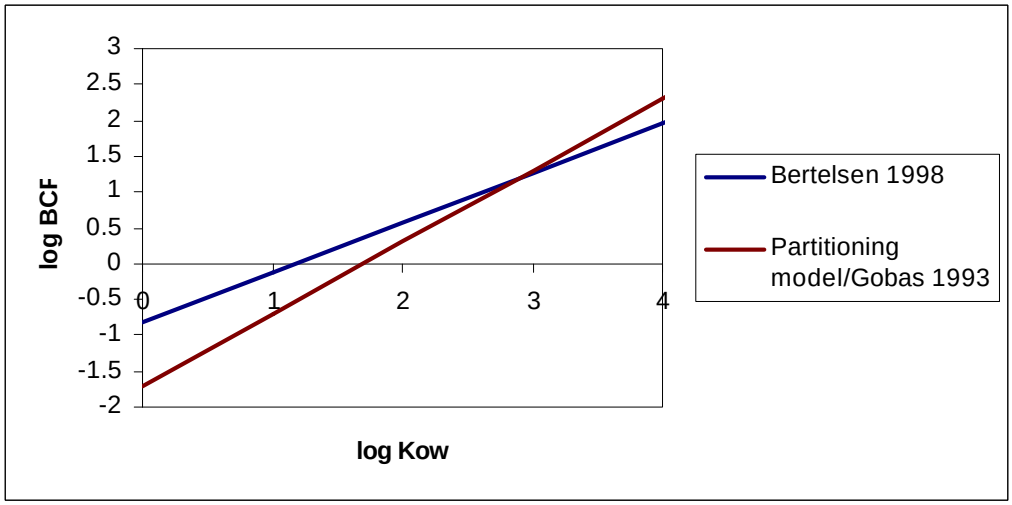
Section 3.2.2 I have to caution against the use of regression equations. Regressions models have a number of weaknesses, i.e.

The BCF data used in empirical BCF regression models are subject to experimental error that typically tends to underestimate the true value of the BCF. The most important errors originate from (i) the short exposure period in most bioconcentration tests compared to life time exposure of organisms in the field, (ii) preparation of water concentrations under laboratory conditions that are constant over time, below the water solubility and represent a bioavailability similar to that in the field.

The "training set" of chemical substances has a large effect on the estimated values for the BCF. For example, the inclusion of metabolizing substances in empirical BCF models based on correlation of the

BCF with Kow will tend to reduce the estimation of the BCF even for substances that do not metabolize and are bioaccumulative. The inclusion of BCFs in the training set that exhibit metabolic transformation in the test species, will result in an underestimation of the BCF of the same substance in an organism which can not metabolize the substance.

Another problem with the regression models is that they typically include chemicals in the higher Kow range and few chemical in the low Kow range. The high Kow chemicals typically exhibit lower BCFs than predicted from a linear relationship because essentially the linear correlation breaks down at high Kow because of a number of factors including experimental error (short exposure time, a reduced bioavailability in the water), the role fecal elimination, growth dilution and others. When this is not considered, a linear regression will actually increase the intercept at the cost of a lower slope, resulting in an overestimate of the BCF for the lower Kow substances (for which this regression is used) and an underestimate of the BCF for the higher Kow chemicals. The difference can be substantial (see figure below).



3-26. Reference to Eq. 3-18 should probably be 3-13.

11-6 The text below the equation is missing.

Table 11-3. Correlations with a slope a of 0.69 and 0.74 are suspicious. Theoretically the slope should be 1.0 and some of the better BCF data sets do show the coefficient to be much closer to 1.0 than the values used in the table. As before, the correlations have a tendency to overestimate the BCFs of low Kow substances & underestimate the BCFs of high Kow substances (the latter is not an issue as the regression model is not used for this purpose). A good method to get to better empirical values and more meaningful correlations is to screen the BCF data for data quality.

My recommendation is to use the BAF model for low Kow substances as well. The model will make the uptake of low Kow substances from the diet insignificant and essentially convert to a partitioning model. Given the range of Bertelsen-type regression models in the literature (see Gobas and Morrison 1999), the partitioning model is in good agreement with the regression models. Also, the often assumed negligible intake of low Kow substances from food may not always apply. In her thesis and in an upcoming publication, MacLean found very large disequilibria (up to 10,000 fold) between sediment and water especially for lower Kow substances in 4 of the Great Lakes. The impact of these disequilibria is that

uptake through the consumption of benthic invertebrates becomes more important relative to uptake from water. This process can be easily accounted for if the BAF model is used (since it relies on water and sediment concentrations as input parameters) but not if the BCF model is used (BCF only relies on the water concentration).

For low Kow substances the Gobas 1993 model makes a small theoretical error by not accounting for the chemical in the water fraction of the organism. This can be fixed up by simply adding (1-lipid content) to the BCF calculated by the model.

The report lacks guidance in terms of selecting high quality, i.e. reliable, BAFs, for special chemicals and metals. Thisis important as there is in many cases a large variability in reported BAFs for metals, special chemicals and even simple hydrophobic organic chemicals alike.

Dr. Jacobson: The modeling approaches described in the reviewed documents appear to be generally scientifically sound. The documents do a good job of clearly and concisely describing the Aquatic Food Web Module and the data bases supporting implementation of the models. The project team has made substantial progress toward the goal described in the Peer Review Charge.

More detailed information on the way(s) in which the models will be applied would facilitate evaluation of the models, as would detailed descriptions of the Source, Media, and Exposure/Risk modules.

My specific comments fall into three categories:

- Point by point responses to each of the questions posed in the Peer Review Charge,
- Comments relating to specific locations in the documents, and
- Marginal notations in the review documents.

I would be happy to discuss these comments with the project team, if any of them feels there is a need to do so.

Responses to Specific Charge Questions

1. *Comment on the organization of the review documents. Do the documents present the information in a clear, concise, and easy to follow format? If not, please provide suggestions to improve the presentation.*

Dr. Barnthouse: The documents are well organized and the information that is presented is clearly explained and easy to follow. The main problem, as noted above, is that much essential information is missing. The validity of the approach cannot be properly assessed without additional documentation.

Dr. Gobas: The review documents are well organized and easy to read for the expert. However, section 1.2. is unclear. The sections on time series management and module loops are insufficiently explained in the report. It is not clear how this is done and how the model is used to accomplish this as the model is not a dynamic (i.e. non-steady-state) model. An overview, perhaps presented as a flow diagram of the larger model, of how inputs and output of the various submodels are related would help.

Dr. Jacobson: The report is well written and generally easy to understand. Sections 3.2 and 4.0 would benefit from expanded treatment of the material.

2. Is there an adequate description of the purpose and context for the Aquatic Food Web Module and its companion Data report? If not, please explain.

Dr. Barnthouse: The purpose and context of the module is well-described.

Dr. Gobas: Yes, the description is accurate with the exception of the time series management and how the issue of time is dealt with when the AqFW model interacts with the SW model.

Dr. Jacobson: Generally speaking, yes; however, the adequacy of any model can only be evaluated in the context of its intended application. Additional information on how the model will be applied would be beneficial. Furthermore, a more thorough job of evaluating the adequacy of the Food Web Module could be undertaken if detailed descriptions of the Ecological and Human Exposure Modules had also been provided.

3. As with any risk assessment, there are always additional data and method development efforts that could be undertaken to reduce the level of uncertainty. Are you aware of any major methodological limitations or data gaps in the aquatic food web module or supporting database that have not been identified? If so, how could they be addressed in the near-term (for example, less than six months) and the longer-term?

Dr. Barnthouse: As noted above, there are many gaps and limitations in both the module and the data base. The ecological components of the food web model are not well-supported. Most of the food web parameters are based on assumptions, or are only indirectly derived from empirical data. It is not clear how much additional data are needed, because the relative influences of the various assumptions on the model results are unknown. To further support the development of the module, the following steps should be performed:

- To the extent possible, calibrate the food web models to data from ecosystems other than the Great Lakes. MacIntosh et al.(1994, *Risk Analysis* **14**:405-419) and Connolly et al. (2000, *Environmental Science and Technology* **34**:4076-4087) have developed and validated food web models of other freshwater ecosystems (Watts Bar Reservoir, Tennessee, and the upper Hudson River, New York). Predicted fish body burdens from the HWIR models could be compared to predictions from these models, given the same input parameters.

- Compare predictions from the eight food web models to each other, given the same input parameters. The range of predictions may not be great enough to justify retaining eight models.

- Perform sensitivity analyses to identify the most important input parameters; obtain additional information on variations in these parameters across regions or ecosystem types.

Dr. Gobas: There are several improvements that can be made to the model.

a. When using a linear regression model, I recommend that the data quality of the data used for the regression is evaluated before the regression is done. We did this recently on behalf of Environment Canada and we found that removing poor data had a large impact on the linear regression. This can be easily done and it is expected that the results of the regression model will move closer to those of the BAF model.

b. As stated earlier, I recommend to omit the regression model and use the BAF model exclusively. I expect that it will improve the accuracy of the model as the regressions models are subject to experimental error and other artifacts described earlier. The other reason is that the often assumed negligible intake of low Kow substances from food may not always apply. In her thesis and in an upcoming publication, MacLean (1999) found very large disequilibria (up to 10,000 fold) between sediment and water especially for lower Kow substances in 4 of the Great Lakes. The impact of these disequilibria is that uptake through the consumption of benthic invertebrates becomes more important relative to uptake from water. This process can be easily accounted for if the BAF model is used but not if the regression model is used. Eliminating the regression model is easy.

c. The model for bioaccumulation in plankton (i.e. eq. 3-9) provides underestimates of the actual concentrations. I think that this is now generally recognized (see Skoglund & Swackhammer 1999). The main reason is that the lipids are not the only medium in these organisms to contain hydrophobic organic chemicals. Because of the low lipid content in many plankton samples, the non-lipid organic matter in these organisms contains a significant fraction of the total concentration of hydrophobic organic chemicals in these organisms. I suggest the following eq.

$$C_P = \phi_L.C_{WD}.K_{OW} + \phi_{NLOM}.C_{WD}.0.033.K_{OW} + \phi_W.C_{WD}$$

where ϕL is the lipid content, ϕ_{NLOM} is the non-lipid organic carbon content (i.e. the organic carbon content minus the lipid content, TOC-L) and ϕ_W is the water content. I suggest to use 0.01 for ϕ_L, 0.32 for ϕ_L and 0.67 for ϕ_L. This model will double the concentrations compared to equation 3-9. This can be done with little effort.

d. The issue of uncertainty is not addressed in the report. I recommend that the uncertainty of the model is assessed. In my view, this can be best achieved by comparing the model predictions to actual data. This should not be a major task and can be done within 6 months. I do not recommend that Monte Carlo Simulations are attempted as they provide little information about the uncertainty of the model.

e. The model does not include a method to assess concentrations of disassociating substances like chlorinated phenols. For more discussion on this, I would refer to Gobas and Morrison 1999. If the model is applied to dissociating substances, I would recommend to explore relationships that express this process.

f. Another source of error lies in the temperature dependence of Kow, which is not recognized in the model. If the model is applied in cold systems with temperatures of 8^{o}C and in systems with 25^{o}C, different Kow values should be used. This said, the temperature dependence of Kow is not

particularly large and there is often significant uncertainty about the correct Kow value to use and the Kow - temperature relationship is often not accessible. This issue can be addressed in the longer term.

Dr. Jacobson: See below.

4. *Do you agree with the selection and application of the uptake models to estimate tissue concentrations in aquatic biota and, when lacking suitable models, using empirical data on uptake and accumulation?*

Dr. Barnthouse: The uptake models used to estimate tissue concentrations are appropriate. The use of empirical data when models are unavailable is appropriate. It should be noted, however, that the Bertelsen et al. (1998) model used to predict uptake of hydrophilic chemicals was actually developed for weakly hydrophobic chemicals (i.e., log K_{OW} between 1.5 and 4). It may not be valid for truly hydrophilic chemicals.

Dr. Gobas: Yes, I agree subject to the constraint that when empirical data are used, the data meet certain guidelines for data quality, i.e. only good quality data are used. The latter is very important as BCF data for the same substance can vary by orders of magnitude.

Dr. Jacobson: Yes; however, validation of the models is needed for each of the waterbody types to which the models will be applied.

5. *It is implicitly assumed that the eight aquatic habitats developed for this assessment (Section 3.1) provide adequate representation of the major types of freshwater systems within the constraints of available data and modeling tools. Do you agree with these and their food web structures; if not, can you suggest alternative systems or structures that are appropriate for a national-scale assessment?*

Dr. Barnthouse: None of the habitats and food webs appear unreasonable (as in infeasible or unrealistic), but it's not at all clear that they adequately represent the variability of bioaccumulation-related chemical exposure potential across all freshwater ecosystems. It's possible that the variations in food web structure within a given habitat type (e.g., between different reservoirs) may be greater than the variations between types, as represented in the food web module. As noted above, this issue should be addressed through additional model comparisons and sensitivity analyses. It's also unclear whether all of the important food-chain pathways are included. As noted below, some aquatic biota, e.g., snails and mussels, bioaccumulate chemicals such as metals and PAHs that do not bioaccumulate in fish. The module, as currently formulated, would underestimate doses of these chemicals to animals that prey on mollusks. Moreover, birds such as tree swallows that feed on emergent insects have been found to accumulate high body burdens of PCBs. This pathway, like the mollusk pathway, is not currently included in the module.

Dr. Gobas: I think that the food-chains are adequate when used in a general sense. Often, there is much uncertainty about the structure of the food-chain and the feeding preferences of the organisms in question. In that case it is not productive to tinker with the food-chains too much. The model will only be affected if one or several trophic levels are forgotten. There are probably examples of this, but when generalizing on a national level the food-chains are reasonable.

Dr. Jacobson: Reservoirs differ from both rivers and lakes, both in terms of their physical/chemical limnology and their foodwebs. Consequently, they may warrant separate treatment. Tidal freshwater wetland and stream habitats should also be considered. Food webs for the existing habitats types seem to be appropriate; however, lack of a trophic level 4 piscivore for warmwater ponds needs to be rectified.

6. *Although the Gobas (1993) model was calibrated for coldwater lakes (i.e., Lake Ontario), it was determined that this model construct was appropriate for use on other aquatic systems under the general assumption of steady-state conditions. Do you agree that it is appropriate to apply this model (as modified) to different types of aquatic habitats? If not, can you suggest more suitable approaches?*

Dr. Barnthouse: The Gobas (1993) model represents biological processes in a generic way, and so it is in principle applicable to other aquatic systems. Similar models have been implemented for other systems (e.g., Watts Bar Reservoir and the Hudson River; there probably are other examples as well). If possible, the Gobas model should be calibrated to data for one or more other ecosystems.

Dr. Gobas: The model was designed to be applied to different types of food-chains. We have applied the model to different systems, i.e. 4 of the Great Lakes and several marine systems in the North West. The model produced the same degree of agreement with empirical data as in Lake Ontario. Others, e.g. Menzie/Cura and DePinto/Bierman have applied the model to US River systems and found good agreement with empirical data. One of the shortcomings when applying the model to warm water systems is in characterizing growth rates of fishes. This can be overcome by using empirical data on growth rates, which are often available.

Dr. Jacobson: The Gobas model structure appears to be appropriate; however, the models as modified need to be validated for each of the habitat types.

7. *For chemicals that have not been shown to be readily metabolizable (e.g., other than PAHs), the module estimates tissue concentrations by multiplying empirical bioaccumulation factors by chemical concentrations in water. Given the wide variety in uptake observed across different species and under different conditions, is it reasonable to use empirical data to support a national-scale analysis? If not, what alternative would you recommend?*

Dr. Barnthouse: The bioaccumulation factor approach is certainly appropriate. However, Table 11A-2 lists only a single BAF for each chemical. Multiple published values must be available for many of these chemicals. Examination of the range of values could reveal differences in BAF between ecosystem types. The published values could also be used to develop probability distributions for BAFs, for use in Monte Carlo analyses.

Dr. Gobas: I think that using empirical data is an acceptable alternative. The other method that could be used, which also relies on empirical data, is to derive metabolic transformation rate constants from laboratory studies and enter the rate constants in the model. Given the objective of broad national level type of assessment, I think that it is reasonable to extrapolate metabolic transformation between other species of the same classification and between environmental conditions. An alternative to this method is to use a range of values for metabolic transfromation rates, representing species that do and do not metabolize the substances, giving values between 0 and the rate of metabolic transfromation that is now considered. This will produce a range of concentrations, including a worst-case calculation, which in the Risk module can be further interpreted.

Dr. Jacobson: It is, provided that the observed variation (site-specific uncertainty) is propagated through the analysis.

8. Several essential metals are likely to be included in the database of the 3MRA. Bioconcentration of essential metals is not linear and modeling approaches that account for nonlinearity are beginning to be available (e.g., see Bergman and Dorward-King, 1997). Given the generally low surface water concentrations expected from the 3MRA system, would the use of such models substantially change the estimates for tissue concentration in aquatic biota from the method currently used based on measured data?

Dr. Barnthouse: I think bioaccumulation of essential metals is a non-problem. Basing the tissue concentrations on measured data rather than on a model is acceptable. Since essential metals are regulated by most vertebrate and invertebrate species, the probability of a predator receiving a toxic exposure to essential models via any of the food webs included in the module is pretty low. There is, however, one significant exception. Mollusks, including snails and mussels, do not regulate metal concentrations and do not metabolize PAHs. They can accumulate very high body burdens of these chemicals. Because these organisms can be important prey items for some wildlife species, they should be included in the model.

Dr. Gobas: One would expect that the model will be in agreement with the observed data. Hence, there should not be a disparity between the model calcuated values and the observed BAFs. However, one should be cautious when extrpolating the empirical BAFs beyond the range of ambient concentrations at which the measurements were made, e.g. from high to low or low to high ambient concentrations. If this practice is considered then there could be a substantial difference between model calculated and empirical BAFs.

Dr. Jacobson: I don't know if it will or not. Non-linearity suggests it ***might*** be important to incorporate temporal variation in surface water concentration. I suggest using one or more of the models (e.g., Berman and Dorward-King (1997)) outside of the AqFW module to examine this issue.

9. Although we recognize that biota sediment accumulation factors (BSAFs) are frequently used in predicting fish tissue concentrations of highly hydrophobic, persistent chemicals (e.g., dioxins), we currently do not use BSAFs due to limitations in the 3MRA system. Rather, we use a mechanistic model (Section 3.2.1) based on Gobas et al. (1993) using BAFs and water concentrations to predict tissue concentrations in fish. Do you agree with this approach and, if not what alternative would you suggest?

Dr. Barnthouse: The BSAF approach makes no sense here and should not be used. Many poorly understood environmental variables affect the bioavailability of sediment-bound chemicals, so that BSAFs measured in one ecosystem cannot be directly extrapolated to other ecosystems. Moreover, in the 3MRA model, it would be necessary to predict the sediment concentrations from water concentrations and then apply a BSAF. It's obviously preferable to predict the concentrations in biota directly from the surface water concentrations, as is done in the current version of the module.

Dr. Gobas: I think that the model provides reasonable predictions. Also, see DiToro et al. 1991, for further rationale of the application of the sediment-benthos accumulation model. In Morrison et al. 1996, we provide a more accurate model. It requires more input data. But, when parameterized properly, it will produce better estimates of concentrations in benthic invertebrates. Another alternative is to use

empirical BSAFs instead of equation 3-10 but keep the rest of the model intact. This will provide the benefit of both using empirical data and applying theoretical knowledge.

Dr. Jacobson: It is unclear from the information provided what would be required to use BSAFs within the 3MRA framework. Given the data limitations that exist for BAFs, it may be beneficial to make use of BSAFs in the situations for which they exist.

10. *Although parts of the module have been validated against certain types of systems, the module has not been validated for a wide range of systems and chemicals. Extensive research and review of current models and methodologies was conducted prior to the selection of the models used in the Aquatic Food Web module. Is the underlying theory sufficiently developed to allow us to predict tissue concentrations in aquatic biota in a variety of systems for a variety of chemicals for a national assessment with reasonable confidence?*

Dr. Barnthouse: This question is impossible to answer. The underlying theory is certainly adequate. The important question is whether the available data are sufficient to support development of credible models of the full range of systems included in the module. As noted above, it does not appear that the calibration and validation studies needed to demonstrate the adequacy of the approach for representing national-scale variability in food-web bioaccumulation have been performed.

Dr. Gobas: I think that the BAF/BCF model in eqs. 3-1 to 3-14 provides estimates with a reasonable confidence for poorly or non-metabolizable non-dissociating hydrophobic organochlorines. Also, see my earlier comments (re. 2-3) on the state of model validation, which is quite good. Perhaps, the report could outline a range of chemicals or chemical properties that could be modelled by the BCF/BAF model and which substances should be treated as special substances. The empirically based models 3-15 and 3-16 for special chemicals can produce significant uncertainty. For example, fishes exhibit a wide variation in metabolic capacity for PAHs. Hence, it is best to apply the model without having to extrapolate the model from species to species. Because of the lack of non-linearity in the model for metals, there is a potential for considerable uncertainty (I am uncertain of the magnitude). I recommend that this issue is further explored if BAF data for areas with low metal concentrations are used to assess concentrations in more contaminated areas.

Dr. Jacobson: The underlying theory supports the structure of the module; however, validation of the module is needed for the range of habitat types, food webs, and chemicals.

11. *We recognize that the approach developed in the module document to determine prey preference fractions (Section 3.2) simplifies a relatively complex set of predator-prey interactions. For purposes of a national assessment, are there refinements you can suggest to the random sampling algorithm for estimating dietary preferences for upper trophic level fish?*

Dr. Barnthouse: The dietary preference algorithm appears unnecessarily complicated, given the simplistic way in which the food webs have been defined. The diet of all fish species changes with the age and size of the individual fish, and is strongly influenced by the array of prey types and sizes available. Moreover, even for a single species of fish, average sizes vary greatly across ecosystems. Yet, in the model, each species is characterized by a single size. A great deal of effort appears to have been spent in massaging the available data on fish diets to obtain input parameters for the dietary preference calculations. The results of those calculations clearly cannot be viewed as realistic representations of the actual variability in fish diets. If the ultimate objective is to characterize the variability of hydrophobic

chemical concentrations in fish, it would be more reasonable to (1) develop size distributions for all predator and prey fish species, and then (2) assign size-related diet compositions to each species, based on the published literature. I do not have access to all of this literature myself, but I know that it exists and I know the names of a number of experts who could provide assistance in locating and interpreting this information.

Dr. Gobas: This methodology combined with the matrix solution is an appropriate method.

Dr. Jacobson: If I understand the method for generating dietary preferences, it is statistically flawed. In any case, the description of the algorithm and its implementation are inadequate. The algorithm appears to assign diet fractions in a sequential manner, such that the range of possible diet fractions is progressively reduced. As a result, the diet fractions generated through the Monte Carlo method may be more strongly influenced by the order in which the assignments are made than by the ranges in the input database.

It is unclear from the description of the algorithm what time scale is used to vary the diet composition. Diet composition may vary from water body to water body, driven by population dynamics of the predators and the prey within a given water body. An inappropriate choice of temporal and spatial scale for simulation of variation in diet composition can, to some extent, amplify or obscure important spatio-temporal variation in tissue contaminant concentration. While the objective is to develop a national assessment, ecological variation should be propagated through the analysis, and synthesis to the national scale should occur as a final step.

12. *For a national assessment, do you support the approach of using a single value, either calculated or measured, in the aquatic chemical properties database to represent bioconcentration and bioaccumulation into aquatic biota while in the fish attribute database trying to capture some of the variability of parameters that vary significantly across different waterbodies, water temperatures, and habitat structures (e.g., fish weight, fraction lipid)?*

Dr. Barnthouse: I think that EPA should pay much more attention to variation in the bioaccumulation and bioconcentration factors. Measured values of BAFs are, in my experience quite variable. The observed range of these values could be used to quantify this variability. In addition, as discussed above, I think EPA may have significantly underestimated the variability of the ecological factors that affect bioaccumulation.

Dr. Gobas: I support the use of single value for Kow while a range of values are considered for biological and environmental variables. The reasons are:

a. Parameter estimation errors in parameters like fish weight and feeding preferences do not have a large effect on the model calculations, but errors in the selection of Kow do. For chemicals with high Kow, the literature presents a wide range of values, often varying by orders of magnitude. This variability does not represent an actual variability, like for example the weight of fish in a lake, which may range from 10 to 1000 g. The value of Kow at a specific temperature and pressure is fixed; there is no variability. The apparent variability in Kow represents measurement error. The error is minimized by using the values measured by the best techniques. This should be the strategy of choice rather than using a range of values.

b. The model includes many sources of uncertainty. Parameter error is only one of them. The effect of parameter error is easily assessed through sensitivity analysis and Monte Carlo simulation. It is therefore often assumed to express the model's uncertainty. However, a better and more comprehensive analysis of uncertainty includes the comparison of model predictions to actual data as it includes errors in model structure as well as parameter error as well as errors in empirical data. I recommend this approach rather than assessing the effect of the variability/uncertainty in each model parameter, such as the Kow, on the model outcome.

Dr. Jacobson: While the physical chemistry of a given chemical may be uniform, the literature indicates substantial variability in bioconcentration and bioaccumulation of the chemical in the environment. The methods of analysis should reflect this variation. Expected concentration in an average lake, stream, or wetland is meaningless in this context.

13. Are there data sources or references that you are aware of that we could use for information in either the aquatic food web chemical properties and the fish attribute databases?

Dr. Barnthouse: There are many sources of information concerning attributes of fish species that do not appear to have been consulted or fully utilized. With regard to defining the sizes of fish species, the NAWQA studies that were used to develop the body weight estimates (according to p. 11-19 of the data report) is far from being the only or the best source of such information. Carlander (1969, 1977, *Handbook of Freshwater Fishery Biology*, volumes 1 and 2, Iowa State University Press), synthesized a huge amount of information on size distributions and feeding preferences of relevant fish species. The FISHBASE database, which cited in Table 11-2 of the data report but doesn't appear to have been extensively used to derive parameter estimates, is also an excellent source of data. It it includes models (e.g., age-length and length-weight regressions) could be used to refine the food web module.

Dr. Gobas: The following data base is a good data base for physiological data on freshwater benthic invertebrate:

Morrison, H.A. 1995. Canadian Data Report of Fisheries and Aquatic Sciences No. 955. GLIFAS, Department of Fisheries & Oceans.

The following data bases are good data bases for physical-chemical properties:

Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volumes I, II, III, IV. 1992, 1993, 1995. Mackay, D., W.Y. Shiu and K.C. Ma. Lewis Publishers, Chelsea, Michigan, USA.

ChemFate. Howard, P.H. Syracuse Research Corporation. Lewis Publishers, Chelsea, Michigan, USA, ISBN 0-87371-785-6.

Environmental Fate Database (EFDB) : http://esc.syrres.com/~ESC/efdb.htm

Dr. Jacobson:

Barber, M. C., L. A. Suarez and R. R. Lassiter. 1991. Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario salmonids. *Canadian Journal of Fisheries and Aquatic Sciences* **48**: 318-337.

Becker, G. C. 1983. *Fishes of Wisconsin*. University of Wisconsin Press, Madison.

Cordle, F., R. Locke and J. Springer. 1982. Risk assessment in a federal regulatory agency: an assessment of risk associated with the human consumption of some species of fish contaminated with polychlorinated biphenyls (PCBs). *Environmental Health Perspectives* **45**: 171-182.

Davis, J. A. and C. E. Boyd. 1975. Concentrations of selected elements and ash in bluegill (Lepomis macrochirus) and certain other freshwater fish. *Transactions of the American Fisheries Society* **107**: 862-867.

Jackson, L. J. and D. E. Schindler. 1996. Field estimates of net trophic transfer of PCBs from prey fishes to Lake Michigan salmonids. *Environmental Science and Technology* **30**: 1861-1865.

Jenkins, R. E. and N. M. Burkhead. 1994. *Freshwater fishes of Virginia*. American Fisheries Society, Bethesda, Md.

Norstrom, R. J., A. E. McKinnon and A. S. W. deFreitas. 1976. A bioenergetics-based model for pollutant accumulation by fish. Simulation of PCB and methylmercury residue levels in Ottawa Rivery yellow perch (Perca flavescens). *Journal of the Fisheries Research Board of Canada* **33**: 248-267.

Post, J. R., R. Vandenbos and D. J. McQueen. 1996. Uptake rates of food-chain and waterborne mercury by fish: field measurements, a mechanistic model, and an assessment of uncertainties. *Canadian Journal of Fisheries and Aquatic Sciences* **53**: 395-407.

Rasmussen, J. B., R. J. Rowan, D. R. S. Lean and J. H. Carey. 1990. Food chain structure in Ontario lakes determines PCB levels in lake trout (Salvelinus namaycush) and other pelagic fish. *Canadian Journal of Fisheries and Aquatic Sciences* **47**: 2030-2038.

Rowan, D. J. and J. B. Rasmussen. 1992. Whydon't Great Lakes fish reflect environmental concentrations or organic contaminants? - An analysis of between-lake variability in the ecological partitioning of PCBs and DDT. *Journal of Great Lakes Research* **18**: 724-741.

Scott, W. B. and E. J. Crossman. 1973. *Freshwater fishes of Canada*. Fisheries Research Board of Canada, Ottawa.Bulletin 184.

14. Currently for chemicals for which BAFs are not available, a default value of one is assumed. For certain chemicals, this assumption is stated to be simply a placeholder and will be identified in the characterization of results as such. Can you recommend alternatives to this approach that would be scientifically defensible?

Dr. Barnthouse: Assuming a default value of 1 when data are unavailable is inconsistent with the goals of the 3MRA model. A model that is to be used to provide an exit from a regulatory process must be appropriately conservative. Assuming a BAF of 1 effectively eliminates the food web pathway as a source of exposure to ecological and human receptors. In theory, it would be preferable to assign each such chemical to a class based on structure-activity relationships, and to assign a BAF based on measured

BAFs for other chemicals within the same class. I realize that, in practice, many chemicals cannot be classified in this way. In such cases, either no assessment should be performed or a much more conservative default value should be used.

Dr. Gobas: Instead of using 1.0, the least risk averse, I suggest that the BAF model is applied using a Kow. This will deal with most organic substances, even organometallic complexes. For most metals, BAF values exist. Hence, there is no problem. This method is more defensible than simply using 1.0. It is based on structure-activity relationships (SAR), the value 1.0 is not. The Kow based SAR is very good for BAF estimations in aquatic ecosystems. The only major drawback is metabolic transfromation, which is not a function of Kow. However, for lower log Kow substances, lets say less than 4, metabolic transformation has to be quite high to have an effect on the biota concentration. This means that the BAF predictions are only incorrect if the rate of metabolism is very high. For higher Kow substances, small rates of metabolic transfromation can have a significant effect on the BAF. Certain organisms may lack the required enzymes, hence the assumption of a zero metabolic transformation rate is defensible especially in absence of empirical data to the contrary.

Another method is to use surrogate substances. For example, lets assume no BAF is available for a particular ester. Then, use available data for the BAF of other esters to create correlations (e.g. with Kow, molecular weight, total surface area or molar volume) from which the BAF can be estimated through interpolation. The rationale for this approach is that families of compounds share certain chemical characteristics that, in absence of better information, can be used to estimate the BAF.

Dr. Jacobson: Use the model to answer the question: how much greater than 1 would the BAF have to be such that the assessment results exceed the decision criteria? Estimate the probability that the BAF is equal to or exceeds this value based on a statistical model relating physical-chemical properties of similar chemicals and BAF.

Additional Comments and References

Dr. Gobas:

Burkhard, L.P. 1998. Comparison of two models for predicting bioaccumulation of hydrophobic organic chemicals in a Great Lakes food web. Environ. Toxicol. Chem. 17, 383-393.

Campfens, J. and D. Mackay. 1997. Fugacity-based model of PCB bioaccumulation in complex aquatic food webs. Environ. Sci. Technol. 31, 577-583.

DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, P.R. Paquin. 1991. Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem. 10: 1541-1586.

Gobas, F.A.P.C. and H.A. Morrison. 1999. Bioconcentration & Bioaccumulation in the Aquatic Environment. In "Handbook of Property Estimation methods for chemicals: Environmental and Health Sciences" (Boethling R. and Mackay, D. eds.), CRC Press. ISBN 1-56670-456-1, p. 139-232.

Gobas, F.A.P.C., J.P. Pasternak. K. Lien and R.K. Duncan. 1998. Development & Field-Validation of a multi-media exposure assessment model for waste load allocation in aquatic ecosystems: application to TCDD and TCDF in the Fraser River Watershed. Environ. Sci. Technol. 32: 2442-2449.

Maclean, L.G. 1999. The role of sediment diagenesis in promoting chemical disequilibrium for organic contaminants in aquatic systems. Master Thesis. Resource & Environmental Management, Simon Fraser University.

Meylan, W.M., P.H. Howard, R.S. Boethling, D. Aronson, H. Printup and S. Gouchie. 1999. Improved Method for Estimating Bioconcentration/Bioaccumulation Factor from Octanol/Water Partition Coefficient. Environ. Toxicol. Chem. 18: 664-672.

Morrison, H.A., F.A.P.C. Gobas, R. Lazar, D.M. Whittle and G.D. Haffner. 1996. Development and Verification of a Steady-State Model of the Bioaccumulation of Organic Contaminants in Benthic Invertebrates. . Environ. Sci. Technol. 30, 3377-3384.

Morrison, H.A., F.A.P.C. Gobas, R. Lazar, D.M. Whittle and G.D. Haffner. 1997. Development and Verification of a Food-Chain Bioccumulation Model for Western Lake Erie . Environ. Sci. Technol. 31: 3267-3273.

Skoglund, R.S.; Swackhammer, D.L.; Environ. Sci. Technol. 1999, 1516.

Thomann R.V. and Connolly, J.P. 1984. Model of PCB in the Lake Michigan lake trout food chain. Environ. Sci. Technol. 18, 65-71.

Thomann, R.V. 1989. Bioaccumulation model of organic chemical distribution in aquatic food chains. Environ. Sci. Technol. 23, 699-707.

Thomann, R.V., Connolly J.P. and Parkerton T. 1991. Modeling accumulation of organic chemicals in aquatic food-webs. In "Chemical Dynamics in Fresh Water Ecosystems" (Gobas and McCorquodale eds), Lewis Publishers; this volume.

Thomann, R.V., J.P. Connolly, T.F. Parkerton. 1992. An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. Environ. Toxicol. Chem. 11: 615-629.

Dr. Jacobson: Page 2-3, 1st bullet. This would be a worthwhile addition to the functionality of the model.

Page 2-3, 2nd bullet. Validation in systems other than coldwater lakes (actually the Great Lakes) is needed.

Page 3-4, 1st full paragraph. Especially in the context of metals, I encourage the agency to examine the implications of an assumption of annual average concentration (current model assumption) versus time-varying concentration on uptake and BCF.

Page 3-14, last sentence of first paragraph. Information on the study sites would be helpful.

Page 3-14, 4th full paragraph (fish). Largemouth bass should be considered a piscivorous fish (TL4) of warmwater ponds.

Page 3-16, Section 3.1.6 (Dietary preferences). Variation among waterbodies should be carried through the analysis rather than averaged out at the outset through inappropriate resampling of the diet composition data set. The model description is inadequate to evaluate the model with respect to this point.

Page 3-17, Text Box 3-1. Fish and prey ***types***. Also, algorithm for selection of P_{ij} is problematic (see Response #11 above).

Page 3-18, 1st paragraph. Averaging of tissue concentrations is unnecessary and inappropriate, and counter to the OFT argument made in a preceding section of the report. While prey choice may be variable over the long-term and over space, within a water body and over the life span of a cohort of fish, diet specialization may occur.

Pages 3-18 to 3-28. Notation using superscripts for indexes is confusing. ***i*** is simply the biota type index.

Page 3-21, 2nd full paragraph. "...the dietary preferences in the Ecological Exposure module do not distinguish among the different biota types". On what basis are dietary preferences manifested in the Ecological Exposure module?

Page 3-27, 1st full paragraph. Individuals have preferences and greater angling success for particular species and sizes of fish. As a result, individuals are exposed to higher or lower concentrations than expected based on the TL3 average. Consider looking at individual biota types within TL3.

Page 4-1, Section 4.0. This section (consisting of one figure with caption) needs to be substantially expanded, to include details of implementation of the models, especially the Monte Carlo methods.

Page 11-9, 4th paragraph (variability) and Page 11-12, Section 11.3.2.1.1 (fish body weight). A measure of central tendency does not reflect variability.

Pages 11-37 to 11-41, Table 11B-3. Body weights for several classes of T3 fish are listed as 0.00. At least 1 significant digit should be shown.

Pages 11-42 to 11-57, Tables 11B-4 to 11B-19. Delete rows pertaining to primary producers. Label rows as predators and columns as prey. Clean up column numbers.