UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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OFFICE OF THE ADMINISTRATOR
SCIENCE ADVISORY BOARD

September 29, 1995

Honorable Carol M. Browner
Administrator
U.S. Environmental Protection Agency
401 M Street SW
Washington, DC 20460

Subject: Commentary on Bioaccumulation Modeling Issues

Dear Ms. Browner:

On April 28-29, 1994, a joint Bioaccumulation Subcommittee with representatives from the Ecological Processes and Effects Committee and the Drinking Water Committee of the Science Advisory Board met to engage in a consultation on approaches to estimating bioaccumulation potential of chemicals and to discuss various mass balance/food web models. At the meeting, Agency staff indicated that the ultimate goal of the Agency is to develop a uniform approach to bioaccumulation assessment for use in a number of regulatory efforts (e.g., development of aquatic life, human health, sediment, and wildlife criteria).

The validity and utility of any model are largely dependent on its underlying assumptions, the input parameters used, and the level of uncertainty acceptable in model outputs. Thus, rather than discussing pros/cons of any specific mass balance/food web (MB/FW) model, the Subcommittee prepared this commentary to provide more general advice on how and when the Agency should use MB/FW models to estimate bioaccumulation and what research is needed to improve model predictions.

Use of Mass Balance/Food Web Models to Predict Bioaccumulation

Bioconcentration factors (BCFs), based on laboratory studies of organisms exposed to water containing a chemical of concern, have been shown in some instances to underestimate bioaccumulation potential (specifically for hydrophobic compounds with log $K_{ow} \geq 4.5$ which are resistant to metabolism and degradation) since they do not account for biomagnification of chemicals in the food web as predators consume prey containing lipophilic compounds. Conversely, BCFs have been shown to overestimate bioaccumulation potential when a chemical is bound or tightly sorbed to sediment, i.e., not bioavailable. Thus, the development and application of models to predict bioaccumulation factors (BAFs) and biota-sediment accumulation factors (BSAFs), a measure of the uptake and accumulation by organisms of chemicals in sediments, are important in improving our ability to evaluate the fate of chemicals

in the environment. While available MB/FW models have a number of serious limitations (as noted below), they can be quite useful as tools for providing insights into environmental processes and interrelationships, for hypothesis testing, and for providing order-of-magnitude estimates of bioaccumulation potential for the classes of compounds for which they were developed.

Bioaccumulation in aquatic organisms is seen in several studies found in the open literature. Available information focuses on a few chemicals and trophic levels in an aquatic ecosystem. Compartmental models utilizing these data have been developed and have appeared in peer-reviewed publications. The Thomann and Gobas models are among the ones that represent this subject area. At the onset, therefore, it should be recognized that model development, enhancement, and validation efforts are ongoing in the ecological research arena. It should also be recognized that empirical information forms the basis of the Thomann and Gobas models. Conceptually, however, the models can be extended to include mechanistic knowledge of the processes involved in bioaccumulation. Given the state of scientific knowledge, it is natural to recommend that the Agency continue developing/improving modeling approaches for estimating (precisely and accurately) bioaccumulation of chemicals in aquatic organisms that are of regulatory interest. In making this recommendation, the Subcommittee observes that existing data and models are applicable for deriving an order-of-magnitude estimate of bioaccumulation for a class of chemicals with a log K_{ow} of 3.5 to 6.0 and for chemicals that do not degrade or transform. Scientists in the Subcommittee have two views on this recommendation: one that subscribes to the idea of conducting research and utilizing the information to enhance these other models to the extent that the scientific results allow; and the second that subscribes to the idea that extensive research to enhance these models would not prove useful for compounds other than those already studied and published in the literature. The following comments elaborate on the first view.

To improve the utility of BAFs and BSAFs for environmental regulation, including the calculation and application of water and sediment quality criteria, the Subcommittee highlighted several important limitations to currently available bioaccumulation models and made recommendations for how these limitations might be addressed.

a) MB/FW models such as the Thomann model, which have been developed for persistent, halogenated organic compounds, do not accurately predict bioaccumulation potential for chemicals that are significantly metabolized by food web organisms, degraded in the environment (including microbiological degradation), or not bioavailable. Similarly, because model development has been focused on a specific class of chemicals, the potential for adapting MB/FW models to other classes of chemicals--particularly those whose partitioning may be driven by mechanisms not represented by octanol/water partitioning--has not yet been addressed.

Recommendation 1: Significant uncertainties exist in the ability of MB/FW models (Thomann's and others) to predict accurately the extent of biomagnification or

bioaccumulation of many important chemical classes. Thus, validation of these models is necessary prior to their use. The Agency should conduct studies to determine whether reliable MB/FW models can be developed for other classes of chemical compounds and broaden validation of bioaccumulation models using data on compounds with different chemical properties and in different environmental settings (e.g., other than large lakes). These studies will require collection of additional field and laboratory data to test how well various classes of compounds can be modeled. Although Quantitative Structure-Activity Relationships (QSAR) may offer insights into the bioaccumulation potential of chemicals, these relationships should not be viewed as a substitute for such data.

b) The models contain many sources of uncertainty, and this uncertainty is often not adequately characterized.

Recommendation 2: The Agency should attempt to quantify the uncertainties in model outputs (i.e., place confidence limits on model predictions), including uncertainties resulting from the stochastic nature of natural systems and from' the natural variability among different types of aquatic ecosystems.

Recommendation .3: The Agency should define the desired or acceptable range of uncertainty in the prediction and minimum criteria for use of MB/FW models for different applications of the methodology. For example, greater uncertainty would be tolerable in screening tests intended to identify chemicals for further testing than for models used in the promulgation of major regulations such as the Great Lakes Water Quality Initiative.

Recommendation 4: The Agency should focus field and laboratory data collection toward reducing uncertainties in existing bioaccumulation models. Research in this area can be prioritized by conducting sensitivity and uncertainty analyses to identify those processes to which model output is most sensitive.

c) Model outputs or predictions are only as good as the data upon which they are based.

Recommendation 5: To improve the quality of the data available for modeling efforts, the Agency should clarify quality assurance requirements for collection of field data as well as for screening of existing data.

Recommendation 6: The Agency should develop or identify standard analytical methods, particularly for measuring bioavailable fractions of organic chemicals in water, sediment, and biota, and for estimating rates of metabolism.

Recommendation 7: Only robust extant field data of acceptable quality, i.e., data elements with acceptable precision, as defined by the Agency, should be used for model validation. Acceptable variances for data elements are determined by conducting

sensitivity tests on the input parameters for a prospective model. If extant data are of unacceptable quality, then additional field data should be collected with the Data Quality Objectives set to yield acceptable precision for each data element. Subsequently, the predicted biomagnification or bioaccumulation of pollutants should be compared to field measurements to assess the bias of the model.

Recommendation 8: Because of the significant analytical difficulties associated with measuring the concentration of super-hydrophobic compounds in water, bioaccumulation modeling results for these compounds are highly uncertain. Until better approaches are developed for estimating water concentrations for compounds with log K_{ow} greater than about 6, decisionmakers must be particularly aware of the increased scientific uncertainties associated with attempts to model super-hydrophobic compounds and especially wary of the use of such results to support policy and regulatory decisions.

Recommendation 9: Since the process of model development and validation is iterative, MB/FW models used by the Agency to predict bioaccumulation should be updated at regular intervals using the best currently available empirical data.

Integration of Mechanistic and Empirical Models

The Subcommittee agrees with the Agency that both mechanistic and empirical modeling approaches are needed to improve bioaccumulation predictions. Although models of natural systems can never truly be verified or validated completely, high quality field data can be used to calibrate and confirm model predictions. In turn, model predictions should identify uncertainties in the field data and provide insight on what to measure, and when and where to sample.

For regulatory applications requiring the highest degree of accuracy or precision, BAFs or BSAFs should be based on field data and tested to determine the relation between the measured value and the specific driving variables known to affect the value (e.g., temperature, pH, nutritional factors). This procedure will allow extrapolation within reason to sites within the range of the tested variables. This approach is preferable to using inadequately validated models (mechanistic or empirical) and will ultimately result in a database that can provide for a good empirical model.

Following appropriate validation studies, including field data, model application can then be made on the basis of K_{ow}'s with adjustment for effects of biomagnification, metabolism, and other factors such as microbial alterations. However, the uncertainty associated with these predictions may not be acceptable for all applications. The Subcommittee agrees with the Agency that when site-specific BAFs or BSAFs cannot be measured but a high degree of accuracy and precision is desired, site-specific bioaccumulation models may be required to account for differences in bioavailability and sorption dynamics, food web structure, selectivity of predators with multiple prey choices, and other factors that affect a chemical's behavior in a given ecosystem. Mechanistic models also can be used for screening new chemicals by applying

them for a range of prototypical environments (e.g., stream, river, estuary, large temperate lake, shallow warm water fishery, system dominated by a benthic food web) to evaluate the bioaccumulation potential of the same chemical in different possible ecosystems.

Research to Improve Model Predictions

The Subcommittee supports the research priorities identified by the Agency, including the need to:

a) better characterize exposures of benthic organisms resulting from ingestion of sediments and sediment-bound chemicals;

b) determine the effect of food web structure on BAFs or BSAFs for generic ecosystems as a function of chemical class and K_{ow};

c) adapt food web models to incorporate residue-based analyses for ecological risk assessments; and

d) develop methods to incorporate BAFs and BSAFs into complex chemical mixture assessment procedures.

In addition, the Subcommittee urges the Agency to assess the effect on model predictions of environmental factors influencing bioavailability of chemicals (e.g., microbiological degradation, dissolved organic matter, matrix effects, water chemistry, sediment characteristics, presence/absence of light).

In summary, while the Subcommittee agrees that mass balance/food web models such as the Thomann model hold promise for predicting bioaccumulation of certain types of chemicals, we urge the Agency to further field test the models for additional classes of compounds and for additional environmental settings and assess the uncertainties in model predictions prior to their wide-spread application in a regulatory context. Ongoing peer review should be an integral part of this process. Finally, the use of models, no matter how refined, should be augmented by appropriately designed laboratory and field experiments and monitoring.

The Subcommittee appreciated the opportunity to meet with Agency staff to discuss approaches to estimating bioaccumulation, including the application of models such as that of Thomann and Gobas. We hope our comments and recommendations are helpful to the Agency and we look forward to your response.

Sincerely,

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Executive Committee

Dr. Mark A. Harwell, Chair
Ecological Processes and
Effects Committee

Dr. Verne Ray,
Drinking Water Committee

Dr. Anne McElroy, Co-Chair
Bioaccumulation Subcommittee

Attachments

U.S. Environmental Protection Agency

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[1]Dr. Reitz did not support all of the recommendations in the final report and resigned as co-chair of the Subcommittee.

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