WORKSHOP SUMMARY AND CONCLUSIONS

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Modeling the Fate of Chemicals In the Aquatic Environment

Edited by

Kenneth L. Dickson
Alan W. Maki
John Cairns, Jr.

ANN ARBOR SCIENCE
THE BUTTERWORTH GROUP

WORKSHOP SUMMARY AND CONCLUSIONS

C. M. Lee

Session Chairman

H. L. Bergman, W. P. Wood and J. H. Rodgers, Jr.

The potential of chemicals used in industrial and manufacturing processes, and consumer and agricultural products to create a hazard for human and environmental health has been given considerable attention in recent years. Indeed, legislation has been formulated and introduced to regulate the use of new chemicals [e.g., EEC Directive on the Discharge of Dangerous Substances (79/831/EEC) and the Toxic Substances Control Act (TSCA) of 1976]. Unfortunately, it is all too easy to ask searching questions about the impact of a chemical on the environment and a good deal less easy to provide the methodology and data that will give unequivocal answers. Much of the current approach to hazard assessment of chemicals is empirical and relies heavily on scientific judgment and the experience of the individual. This approach is not always easy to make compatible with the legal process. It is also true to say that the complexity of the questions asked and the expectations of the concerned community have in some cases outstripped the ability of science to provide the answers. Thus, considerable pressure remains to develop and refine the science of hazard assessment. For those who have had contact with it, mathematical modeling seems to hold a tantalizing prospect for objectively assimilating and manipulating the complex data generated during hazard assessment of a chemical. It also seems likely to enable us to move away from the present, rather simplistic, approach to take account of more complex processes and interactions in environmental compartments. The purpose of this workshop was, therefore, to examine this prospect against the following objectives:

1. to analyze the state-of-the-art of environmental fate modeling, considering both development and application;
2. to critically evaluate existing models for predicting environmental exposure concentrations of chemicals in various aquatic systems;
3. to critically examine the utility of various models as decision-making aids for their specific applications;
4. to position the role of environmental fate modeling for aquatic hazard assessment, considering both regulatory application and new product development; and
5. to develop recommendations for future research needs in environmental fate modeling.

CONTEXT

Previous workshops in this series [1-3] have presented a number of sequential assessment schemes whose general objective is to determine whether a chemical (1) is clearly acceptable for its proposed use, (2) is clearly unacceptable for its proposed use, or (3) needs further research before a decision can be made. These assessment schemes are generally based on a comparison of the exposure and effect concentrations of the chemical under review. The determination of its acceptability or otherwise is based on the size of the margin between two concentrations (Figure 1) [4]. Most schemes progress from simple to complex tests through a series of stages, each of which is followed by decision criteria. The intention inherent in this approach is to continually refine the estimates of exposure and effect concentrations until there is sufficient confidence to make a decision.

The exposure concentration of a chemical in the aquatic environment is determined by its use and disposal pattern and, subsequently, through its dispersion by a variety of physical and chemical transport mechanisms and its transformation through interactions with physical, chemical and biological entities in the open environment. In current hazard assessments, estimates of exposure concentrations are rarely based on more than a combination of production tonnage and dilution information. Dilution models alone, however, are notable to indicate potential problems associated with assimilation and transformation. In some schemes, biodegradation and hydrolysis information is used to indicate whether the actual concentration of the chemical in the environment is likely to be reduced substantially after its release [3]. Recent discussions in international groups such as the Organization for Economic and Cooperative Development (OECD) have recommended an increased data base for estimating the exposure concentration, including abiotic and biotic trans-

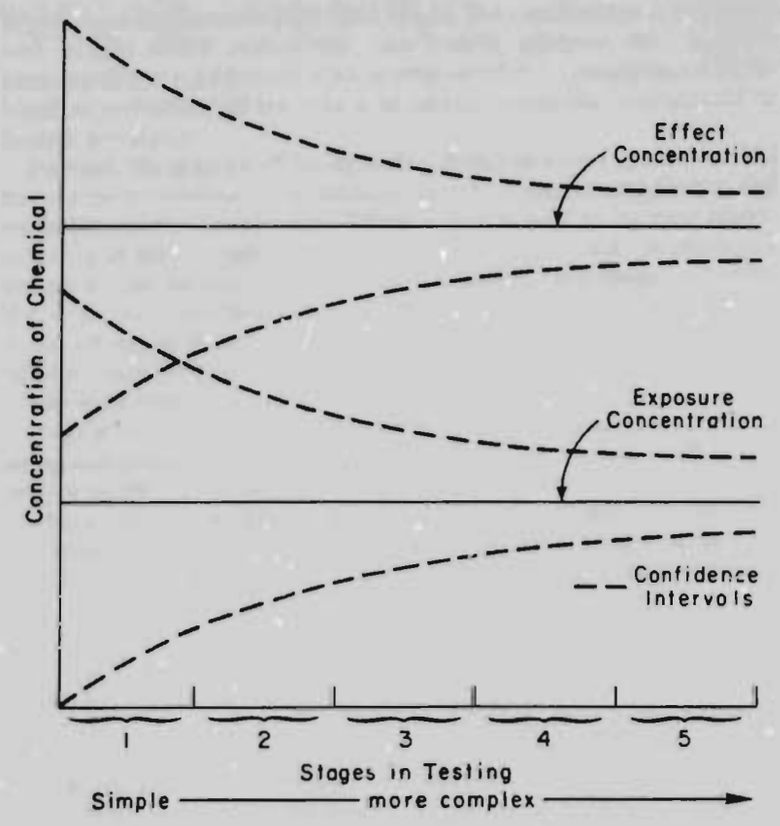

Figure 1. The principle of hazard evaluation (after Cairns et al. [1]).

formation and accumulation processes, and have extended the empirical schemes for utilizing and combining these data to refine estimates [5].

The current approach to determine effect concentrations of a chemical on the aquatic and terrestrial community involves gross simplification. It is clearly impossible to determine the effect of a chemical on every individual species; therefore, surrogates are chosen to represent important functional groups in the ecosystem. Extreme accuracy and precision in estimating the effect concentration are therefore not possible, and the confidence interval surrounding the estimate is large and usually measured in orders of magnitude.

The aim in this approach is always to assign a chemical to one of the above categories with the minimum expenditure of time, cost and effort.

When these assessments have been made, the conclusions are coupled with human safety assessments, cost/benefit analyses, etc., and the question of risk is addressed. Risk is considered to be the statistical likelihood or probability of the hazard being realized in the environment or human population.

Probably the greatest difficulty and challenge in assessing the potential hazard of a chemical is to account for the inherent complexity and variability in the environment. There is also a need to increase understanding of the relevance and utility of laboratory results in predicting events in the environment. In current hazard assessment schemes, decision criteria are based largely on empirical observation, and the data bases are created from tests that often are only the best option in the face of major compromises, which are usually enforced by practical, cost or effort considerations.

Estimating concentrations of chemicals in the aquatic environment using mathematical models will also demand compromises, which will be greater as the case departs from being site-specific to having widespread discharge. So long as this is recognized, it need not detract from the value of hazard assessment schemes. One objective of a hazard assessment scheme must be to select those chemicals that need a detailed examination. Another is to develop schemes that will lead to a correct judgment in the majority of cases. The problem is currently dealt with by making the decision criteria more or less conservative as the case demands. It is desirable to reduce the need for this conservatism to reduce the potential for failing safe chemicals. Environmental fate modeling may contribute to an improved estimate of the distribution of the chemical in environmental compartments. It may also qualitatively improve estimates of exposure concentrations, by taking account of a broader spectrum of physicochemical reactions and interactions, and quantitatively, by making more accurate integration of complex data and providing some associated confidence limits.

Despite the acknowledged limitations of current schemes, the recognition of an ordered approach and the delineation of the basic principles of hazard assessment achieved in earlier workshops [1-3] must be regarded as a quantum step forward. The task that now faces scientists in the field is to review and improve methods for estimating exposure and effect concentrations. As noted above, decisions on acceptability are made primarily on the basis of the margin between exposure and effect concentrations. It seems likely, on the basis of current methods and level of understanding, that the best chance of increasing the apparent safety margin is through a downward revision of the exposure concentration.

Nature and Scope of Contaminant Fate Models

There is a role for environmental fate models in the hazard evaluation process, in the initial and in the more detailed phases. Workshop participants were able to identify and have evaluated models that range from the very simple to the very complex, in terms of model architecture, data requirements and ease of application. No one model, however, has applicability to all stages of the assessment process, nor should a model built for one purpose be used for a different application without consulting the model developer. Workshop participants concluded that developers and users of fate models are distinct groups and should consult in advance to ensure that the model is designed to defined uses and to answer specific questions.

Some uses of environmental fate models discussed included the identification of potential problems requiring additional laboratory testing prior to introduction of a chemical into commerce, hazard assessment of specific uses of a substance, decisions on whether site-specific releases of a chemical will exceed environmental criteria or standards, decisions on the need to take remedial action to mitigate some perceived risk, and the evaluation of specific environmental processes.

At previous Pellston workshops, two kinds of models have been described and discussed with respect to their use in predicting the fate of chemicals in the environment: (1) physical (microcosms) models and (2) mathematical (rate) models. This book has emphasized mathematical environmental fate models. Those who are interested in physical models should consult the literature [3,6,7].

Environmental fate models are used to predict the behavior and expected exposure concentration of a chemical in the environment through use of some mathematical construct. Such models can be as simple as a logical relationship or single algebraic equation, or they can be so complex as to require solution with a computer. They may use either theoretical or empirical data and can be based on either equilibrium (steady-state) or dynamic (nonsteady-state) conditions. Because models are so diverse in their structure, the terminology applied to them can be somewhat confusing (e.g., theoretical vs empirical, equilibrium vs dynamic, stochastic vs parametric ... see also other papers in this volume by Yeh, by Lassiter, and by Di Toro et al.). To minimize confusion, we suggest adoption of the following classification of mathematical contaminant fate models (after Di Toro et al. [8]):

1. partitioning models, e.g., the Mackay-Neely unit world model [9];

2. simplified fate model, e.g., Stanford Research International (SRI), Exposure Analysis Modeling System (EXAMS), Chemical Manufacturing Association—HydroQual Inc. (CMA-HydroQual) and the Mackay Level III;
3. detailed dynamic fate model, e.g., Sediment Radionuclide Transport Model (SERATRA), Hydrologic Simulation Program—FORTRAN (HSPF) and the Unified Transport Model (UTM).

Within these three broad categories of approaches, most current models are developed for a specific environment or effluent type. The case studies session at this workshop considered runoff, groundwater, river, lake estuary and effluent models. All of these model classes or model types are needed, and each is normally used for a different purpose. For instance, partitioning models can be used to estimate quickly where a chemical will tend to go in the various environmental compartments if allowed to proceed to equilibrium. This helps direct further fate modeling and effects testing. A simplified fate model for movement of a chemical in a river can be used to estimate environmental concentration at various points downstream.

Despite the apparent differences among modeling strategies and model types, there is a remarkable similarity among available models with regard to the component processes of parameters that are incorporated. Examination of currently available ground- and surface-water models reveals that a base set of processes incorporating physical, chemical and biological phenomena appear to be common to all. The partitioning processes, such as sediment sorption/desorption, are relatively rapid and reach equilibrium with the aqueous chemical concentration in a short period of time. On the other hand, the kinetic (e.g., biotransformation and photolysis) and transport processes are time- and event-driven, and require more complex algorithms and data sets for successful application.

Implicit in all of these models is the assumption that the processes are decomposable (or can be dissected) and then recomposable. The models also assume that the chemical subject has no influence on the constituent processes. To date, most of the modeled processes have incorporated episodic or excursions that appear to be of considerable importance in nature in controlling the ultimate disposition of a chemical.

Models as a Tool in the Hazard Assessment Process

Environmental fate models can contribute to the consistency of the hazard assessment process and provide a framework for decision-

making. Workshop participants discussed the similarities and differences in the existing models and the implications for their use. In general, all of the models discussed are quite similar in the environmental processes dealt with, but all processes are not equally well understood. Because of this, even though there are differences in the degree of detail by which these processes are described from one model to another, it is not yet clear how these differences will affect the correctness of the final conclusion. More distinct differences, however, exist among the models in terms of their spatial and temporal scales and the way in which transport is handled. The applicability of a specific model is often determined by its respective spatial and temporal scales.

Validation studies conducted to date indicate that the model predictions are consistent with observations; however, only a limited number of chemical classes and environments have been tested. Further work is continuing to test model components individually and in complex mixtures for an increasing range of chemical classes and under a range of environmental conditions. Sensitivity analyses of models' outputs to uncertainties in inputs are essential to any validation study, and increasing effort is being directed at establishing realistic ranges for many of the environmental data inputs required by the models. These ranges of environmental data inputs are to be compiled into data bases to facilitate the use of these models in hazard assessments. Only in this way can a representative range of environments and associated predicted concentrations be developed as part of the hazard assessment.

Mathematical models were considered to offer a number of particular advantages to the hazard assessment process. These major advantages are discussed within a decision-making context.

Organize Thinking and Decision Framework

To arrive at an environmental exposure concentration (EEC) for a chemical, one must consider more than simple dilution of an input in most cases. For this prediction, it is logical to consider the relevant processes that may dissipate the chemical in a given system. Models tend to provide a step-by-step decision framework from which an estimate of exposure concentration can be calculated. A model user may become aware of a process or processes that are important but would not have been considered without the use of a model.

Defensible or Accountable Decisions

An accountable decision may not be a totally defensible decision, but it can demonstrate how all of the options were considered. This does not

mean that models can serve to replace well trained and experienced professionals, but models may greatly aid a newcomer to the profession.

Temporal Control of Decisions

Chemical fate models may reduce the variability in decisions that are made by an office (public or private) because of changes in personnel. The framework of complex models usually attempts to consider all relevant processes or parameters that may serve to reduce environmental concentrations of the chemical in question. The error in decisions introduced by the relative experience of a model user can never be eliminated, but it can be reduced. Ample and clear documentation by model developers is paramount and would go a long way toward reducing "model user's risk" (analogous to Type II statistical error). With using a model as a decision-making tool goes the responsibility for the user to feed back and develop any insights or suggestions that may arise through experiences concerning model construction or documentation. Models of chemical fate in multimedia environments may also be useful in experimental design when more information is required for decision-making. The critical points in space or time may be identified, and the resources for information-gathering can be distributed appropriately.

Information Reduction for Decision-Making

When faced with large numbers of inputs concerning both the chemical and receiving environment, a decision-maker or team of decision-makers may be hard-pressed to arrive at an agreeable simultaneous solution to multiple processes contributing to the reduction of the environmental concentration. Many of these decisions have further complications of limited time and resources. A model of chemical fate allows the examination of a variety of scenarios to assess the range of possibilities that are open to the distribution of a chemical after release and which will have a bearing on the ultimate decision on acceptability.

Quality Control or Assurance

Chemical fate models may have some utility in serving as a minimal quality control. Given a range of information about a particular chemical and candidate receiving environment, both experienced and inexperienced users ideally should arrive at the same decision. For the less-than-clear-cut decision, more information may be required (or more expertise may be brought to bear on the problem).

FUTURE RESEARCH NEEDS

Although there is a plethora of areas that require further research, the following were thought by the workshop participants to be the most crucial to advancement.

1. Sediment/chemical interactions: such processes and equilibrium phenomena as sediment-associated decay rates, sorption and sediment/water exchange need to be described.
2. Sediment transport dynamics: movement of a sorbed chemical with the bed load; sedimentation and resuspension are important factors.
3. Dynamics of mixtures as opposed to discrete compounds: does a mixture act as a discrete compound?
4. Biotransformation rates: are water column transformations adequately described by zero-, first- or second-order expression? What are the sediment-associated biodegradation rates?
5. Episodic events: models may require incorporation of episodic events that are important in both fate and effects of chemicals.
6. Validation and calibration: adequate field data are required for validation and calibration of chemical fate models.
7. Dynamic model development: there is a need for development of time- and spatially variable models in light of the limitations of the currently predominant equilibrium and steady-state models.
8. Need for harmonization of systematics and terminology: of seemingly small importance at first sight, but in a field where many people have no background in mathematical modeling this will be essential.
9. Importance of degradation products: degradation products may be of importance in the hazard evaluation process, but current models are keyed to primary degradation. This problem may be resolved via iteration using current models, but this should be clearly translated to the user.
10. Bioaccumulation: bioaccumulation may play a role in increasing the body burden of some chemicals in some organisms. More confidence in the predictability of this event could be gained through further research.
11. Coupling fate and effects models: although not a topic specifically covered by this workshop, it became clear that this will be essential in the future and that there is little current experience of the associated problems.

CONCLUSIONS

Hazard assessment of chemicals released to the aquatic environment is a function of exposure and effect concentration. Therefore, the ability to

predict environmental exposure concentrations is essential for hazard assessment.

There are two groups interested in models: producers/developers and users. Communication is essential between these two groups, and is presently lacking, so that producers do not always appreciate the needs and objectives of users, and users do not always understand the implications of model construction, especially concerning data manipulation. The comparability of laboratory-derived data on process mechanisms with actual mechanisms in the environment is not well understood. Furthermore, there is a lack of good field data to validate models and to serve as data bases for assessment purposes.

The utility of a model depends on its being matched to the objective, which must be clearly stated. The limited number of validation studies has demonstrated the feasibility of predictive models for hazard assessment. Furthermore, the validation and improvement of models of proven utility should receive higher priority than the development of conceptually new models.

There is no doubt that this workshop brought into the hazard assessment arena for the first time a new and important scientific discipline. As suggested at the beginning of this chapter, environmental data modeling holds out the tantalizing prospect of providing the means to take hazard assessment another major step forward. Initially, however, it is expected that environmental fate models will raise more problems than they solve. However, in the process of resolving these problems, we will inevitably come to a better understanding of the reactions and interactions that govern the fate of chemicals released to the environment.

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