TO: Distribution

TGG: JGL: EGJ: AC: AJO: RF

XF: None

FROM: T. G. Grumbles
DATE: September 18, 1991

VISTA

Interoffice Communication

SUBJ: ENVIRONMENTAL HAZARD COMMUNICATION REGULATION

Attached is information regarding an EPA effort to develop an "Environmental Hazard Communication" regulation. This effort would result in information distribution similar to OSHA's standard and potentially labeling.

CMA/SOCMA have been working hard with EPA and agreed to consider a pilot study on a draft standard. The draft (attached) was so bad, CMA has refused to participate unless modifications are made.

The attached info is for your review and no action is needed at this time.

Tom dlj

T. G. Grumbles

dlj
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Attachment

Distribution: Dave Penney, Allen Nielsen-Austin

EPA/CMA/SOCMA

ENVIRONMENTAL HAZARD COMMUNICATION

PILOT STUDY

EPA/CMA/SOCMA

ENVIRONMENTAL HAZARD COMMUNICATION

PILOT STUDY PROJECT PACKAGE

Contents:

The Pilot Study Project Package consists of two separate documents.

Environmental Hazard Communication Pilot Study

Describes the pilot study and presents questions to participants for use in assessing the conduct and results of the project.

* Purpose
* Guidelines for Performing the EHC Pilot Study
* Proprietary Chemical Identities
* Schedule
* Guidance for Presenting the Results of the Analysis
* Additional Information Relevant to EPA's Evaluation

CMA Hazard Communication Exercise Cost Worksheet

Pilot Study Guidance Document

Describes the specific tasks to be performed in the pilot study project, identifies the information that must be supplied, and offers guidance on data sources and information evaluation.

Part One: Data Evaluation

Section One	-	General Study Guidelines
Section Two	-	Environmental Toxicity Evaluation
Section Three	-	Environmental Fate Evaluation
Section Four	-	Possible Data Sources
Section Five	-	Test Descriptions and Evaluation Guidelines

Part Two: Material Safety Data Sheets and Labelling

Section One	-	Required Information
Section Two	-	Hazard Description Language
Section Three	-	Optional Labelling Descriptions

Environmental Hazard Communication Pilot Study

Purpose

In developing a possible approach to an Environmental Hazard Communication (EHC) program, EPA would like to work cooperatively with the Chemical Manufacturers Association (CMA) and the Synthetic Organic Chemical Manufacturers Association (SOCMA) as several of their member companies perform a pilot study on selected chemicals.

During the establishment of any program, EPA is interested in ensuring that it is based upon sound principles, is useful, and that it can be properly complied with. With regard to the EHC program, the Agency is at a stage where we are very flexible. For example, EPA will be exploring potential harmonization with European community initiatives. Beyond these considerations, there is a more specific intent for this exercise. The Agency perceives the goals of this effort as four-fold:

1) To ascertain what constitutes clear guidance for companies asked to generate environmental hazard communication;

2) To ensure that the provisions to be included in a proposed rule would result in concise hazard communication;

3) To permit a preliminary evaluation as to whether the provided guidance promotes the meaningful communication of valid information concerning significant environmental hazards; and

4) To assess the qualitative and quantitative costs of implementing a proposed rule.

Guidelines for Performing the EHC Pilot Study

The Agency values the comment of the regulated community and appreciates the time and effort that CMA/SOCMA and their member companies will be devoting to this exercise. To help speed the process and enhance the effectiveness of this analysis, EPA wishes to offer suggestions for performing the exercise.

1) Limit participation to no more than eight companies.

2) Perform the analysis on approximately 25-40 chemicals (three to five per company, depending on size and resources).

3) Choose a variety of chemical companies to perform the analysis, including:

   a) commodity chemical producers;

   b) specialty chemical manufacturers; and

   c) petrochemical firms.

4) Choose companies of different sizes (including small businesses, if possible).

5) Select a variety of chemicals to evaluate, including:

   a) several imported chemicals (to assess how data provided in the OECD base set is addressed); and

   b) both "hard" cases (chemicals with extensive and conflicting environmental effects/fate data) and "easy" cases (chemicals with limited and/or clearly defined data).

   Companies may select any chemical on the TSCA Inventory for this pilot study (including product formulations they manufacture). However, the chemicals selected should not include site-limited or closed-system chemicals.

6) Select chemicals representing a range of production volumes (e.g., >100,000 lbs; 10,000-100,000 lbs; <10,000 lbs).

7) Assign different manufacturers to analyze the same chemical (without consultation between the companies).

Using these guidelines should help maintain this exercise at a manageable level of scope and effort, while providing a reasonable representation of the chemicals and companies to be regulated.

Proprietary Chemical Identities

The Agency recognizes that many MSDSs withhold the chemical identity as proprietary information and the proposed EHC rule is not anticipated to modify this protection. In order to properly evaluate the results of this study, however, EPA needs to be notified of the precise chemical identity for each data sheet prepared in this exercise. Since it may be useful to explore how effectively EHC operates under proprietary constraints, companies wishing to prepare MSDSs where the chemical identity is not disclosed (and who wish to maintain this confidentiality from other member companies or CMA/SOCMA) may do so on a limited basis (these chemicals may not be suitable for the comparative analysis

between companies) and separately submit the chemical identity as Confidential Business Information (CBI), in writing, directly to Agency staff following standard TSCA CBI procedures. Any MSDSs submitted without the chemical identity should be coded to allow matching with the CBI disclosure by EPA. If participating companies are unwilling to reveal this information, they should consider selecting other chemicals for analysis.

Schedule

EPA is proposing the following schedule for this exercise. Agency staff will also research and evaluate environmental effects/fate data, and prepare environmental hazard communication data sheets for several of the chemicals selected for this exercise.

Week 1: EPA furnishes the Pilot Study Package (including the project description and guidance document) to CMA/SOCMA

Week 4: CMA/SOCMA provides EPA with a list of participating companies and chemicals proposed for analysis

Week 6: Meeting with CMA/SOCMA and participating companies, at which EPA discusses the project guidance

Week 12: CMA/SOCMA and member companies complete their analyses and deliver results to EPA

Guidance for Presenting the Results of the Analysis

The Pilot Study Guidance Document defines a number of major areas that must be addressed in providing environmental hazard communication. In addition to providing a copy of the required environmental hazard communication, it would be most helpful in the Agency's development of this program if you would provide general observations concerning these areas and indicating the following:

1) whether the language used in the guidance document provided clear instructions;

2) whether there are ambiguities in the guidance document that require clarification;

3) alternative language you would suggest to clarify any problem areas;

4) the extent to which you have supplemented the required data with information not specifically requested by the guidance document;

5) the time and level of analysis required to complete each major area;

6) the costs of obtaining and evaluating information, and preparing the environmental hazard communication data sheet (excluding any costs of developing the existing MSDS), i.e.,

   - What types of personnel were involved (professional levels and disciplines) and what were their responsibilities?

   - What kind of managerial and legal review did you conduct?

   - How many labor hours were required by each person for each task and what was the fully-loaded hourly rate for each level of staff?

   - What other (non-labor) costs were incurred, including computer database charges, supplies and reproduction?

   [A two-page Cost Worksheet has been attached to aid you in supplying the latter two pieces of information. Its use is optional, but will serve to provide the Agency with cost data that is consistent both in type and format.];

7) any trade secret concerns encountered in preparing the data sheet, and whether these differ from those found in current MSDSs or present any additional problems; and

8) whether the program would create any conflicts with other existing or anticipated hazard communication programs.

Listed under each major area are questions which may help to stimulate your thoughts in performing the analysis.

Search for Environmental Effects/Fate Data

- What references and databases were searched?
- To what extent did you use unpublished, company data?
- Does the language of the guidance document adequately and clearly describe how extensive a literature search you must conduct to obtain available and important environmental effects/fate data?
- Do the instructions specify a search of appropriate depth? If not, is the level of inquiry too great or too little?

Evaluation of Data Obtained in Search

- What type and quantity of data was obtained on the environmental effects/fate of the chemical?
- Could the data be expressed quantitatively or was it qualitative?

- Were there problems in interpreting the validity of the data?
- Was it difficult to draw conclusions concerning the most sensitive endpoint for an effect?
- Was it necessary or useful to use professional judgment or structure activity relationships (SAR) in the evaluation?

Classification of Environmental Hazard According to the EHC Pilot Study Guidance Document

- Was it difficult to draw conclusions about the relative environmental hazard of the chemical?
- Does the language used in the guidance document clearly define whether environmental hazard communication is required?

Preparation of Data Sheet

- For chemicals with extensive data, what difficulties are there in condensing the information in order to avoid a lengthy or confusing data sheet?

Provision of Applicable Regulatory Information on Data Sheet

- Can this information be presented to the customer in a clear fashion, avoiding possible confusion?

Provision of Use/Handling/Disposal Information

- Did you provide guidance on handling or use of the chemical in addition to the prescribed disposal language?
- Would you use available data and/or professional judgment to describe other factors that may mitigate environmental effects concerns? How often might this type of additional guidance be given and what type of language might be used? To what extent will this additional information be likely to conflict with the prescribed language or to confuse the recipient of the hazard communication?

Labeling

- If EPA requires environmental hazard labeling, how prescriptive should the requirement be (e.g., required language, symbols, etc.)?
- How would you modify an existing label (enlarged size, additional colors, additional label)?
- If possible, please supply EPA with a copy of the existing label?

Additional Information Relevant to EPA's Evaluation

The following optional information for each of the selected chemicals would be very helpful to EPA's evaluation of the results. Should you have this information available and be willing to share it with our reviewers, please provide it directly to EPA. The first item is especially important, as it

would assist the Agency in assessing a possible low volume exemption.

1) What is the approximate production volume of the chemical (indicate the range in which it falls, e.g., >100,000 lbs; 10,000-100,000 lbs; <10,000 lbs)? When was the chemical introduced into the marketplace?

2) Do you manufacture the chemical in the U.S., or is it imported?

3) Is the chemical marketed in a country that requires environmental effects or hazard communication? If so, where?

4) Is the chemical subject to Federal or State regulations that require the development of environmental effects information (specific TSCA §4, §5, or §8 regulations; FIFRA; other)?

5) If there was an existing MSDS for the selected chemical, was it mandatory under the OSHA Hazard Communication Standard? (Please provide a copy.)

ENVIRONMENTAL HAZARD COMMUNICATION PILOT STUDY
COST WORKSHEET

As part of the development of the Environmental Hazard Communication (EHC) Program, EPA will consider the cost of the program to industry. The following questions request information on the costs of various aspects of the pilot study. All questions refer only to the incremental costs you would expect to incur in conducting such a program during its first year. In other words, do not include any costs that you already incur to develop MSDSs, conduct literature searches, design and conduct training programs, etc. In reporting labor costs, include benefits and overhead.

SECTION ONE -- ONE-TIME COSTS
Please estimate all one-time costs associated with the EHC program.

	1) Program Familiarization Costs		2) Other one-time costs (Please Specify)_____	
LABOR COSTS	**HOURS**	**TOTAL DOLLARS***	**HOURS**	**TOTAL DOLLARS***
Managerial/Legal	_____	_____	_____	_____
Professional	_____	_____	_____	_____
Clerical	_____	_____	_____	_____
Other Labor (Specify)_____	_____	_____	_____	_____
NON-LABOR COSTS				
Computer Charges		_____		_____
Supply Costs**		_____		_____
Photocopying**		_____		_____
Other Non-Labor Costs (Specify)_____		_____		_____
TOTAL COSTS (should equal sum of above)		_____		_____

*Labor costs should include benefits and overhead.
** If not included in the overhead on labor.

3) What is the size of your company in terms of total sales?

Is it... $0 to $39 million ____ $40 to $100 million ____ Greater than $100 million ____

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Company Name _____ Chemical Name _____

Annual Chemical Production Volume _____ (thous. lbs.)

SECTION TWO -- CHEMICAL-SPECIFIC MSDS COSTS

Please answer these questions for EACH chemical to whose MSDS you added environmental hazard information. Photocopy as many copies of Section Two as you need so that you can report on each chemical. Any cost that cannot be assigned to a specific chemical, such as a computer access charge if you conducted a search for all chemicals at once or the managerial time expended to oversee the entire process, should be divided equally among all chemicals involved.

	1) Literature Search and Professional Evaluation including computer/library searches, review of data to determine hazards and identify relevant handling/ disposal information.		2) Summarize and present data for Environmental Hazard Section of an MSDS, including fate and effects, handling/disposal methods, and other applicable regulations.		3) Other costs not covered by questions 1 and 2 (specify) _____	
	HOURS	TOTAL DOLLARS*	HOURS	TOTAL DOLLARS*	HOURS	TOTAL DOLLARS*
LABOR COSTS						
Managerial/Legal						
Professional						
Clerical						
Other Labor (Specify) _____						
NON-LABOR COSTS						
Computer Charges						
Supply Costs**						
Photocopying**						
Other Non-Labor Costs (Specify) _____						
TOTAL COSTS						

* Labor costs should include benefits and overhead.

** If not included in the overhead on labor.

4) The costs estimated in Section Two may decrease in subsequent years as these activities are routinized. Assuming no salary increases, by what percent would you expect these initial costs to fall once this process has become routine? _____ %

5) Do you have any additional cost information/comments that would be relevant to EPA's estimation of the cost of this program? (Attach additional sheets if necessary.)

_____

_____

_____

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ENVIRONMENTAL HAZARD COMMUNICATION: PILOT STUDY GUIDANCE DOCUMENT

Part One: Data Evaluation

Section One - General Study Guidelines

For each chemical in this exercise, participants must evaluate the environmental toxicity data elements specified in Section Two below to determine if the chemical is environmentally hazardous. For each chemical determined to be environmentally hazardous on the basis of its environmental toxicity, the environmental fate data elements specified in Section Three must be evaluated. Suggested sources for this information are listed in Section Four. Test descriptions and guidelines for evaluating these data elements may be found in Section Five.

If any of the chemicals selected for this exercise is a mixture, the evaluation procedures depend upon the available information. If the mixture has been tested as a whole to determine whether the mixture is environmentally hazardous, the data generated by such testing should be used to determine whether the mixture is environmentally hazardous.

If the mixture has not been tested as a whole to determine whether the mixture is environmentally hazardous, the mixture should be presumed to present the same environmental hazards as are presented by each of the individual chemical substances that comprise one percent (by weight or volume) or greater of the mixture. In identifying the environmental hazards of such mixtures, manufacturers of mixtures may either rely upon data provided by the manufacturer(s) of the individual chemical substances which comprise the mixtures or locate data from other sources.

If data indicate that a chemical substance present in the mixture in concentrations of less than one percent could be released in concentrations which could present an environmental hazard in those concentrations, the environmental hazards presented by the mixture should be presumed to include the environmental hazards presented by that chemical substance.

For both individual chemicals and mixtures, if data indicate that the chemical or mixture breaks down into environmentally hazardous products when released into the environment, the chemical should be presumed to present the same environmental hazards as are presented by those breakdown products, and the breakdown products should be specifically identified, if possible.

Persons evaluating chemicals as part of this exercise must describe, in writing, (1) the sources consulted in order to locate the required toxicity data, and fate data where necessary; and (2) the results of all chemical evaluations performed. All

environmental toxicity parameters identified in Section Two should be reported as measured values. Estimated values may be used for the environmental fate parameters listed in Section Three, but where such estimated values are used, they must be specifically identified as estimates, and the methods used to derive them must be described. The use of estimated values, while permitted, is not required.

Section Two - Environmental Toxicity Evaluation

The following environmental toxicity data elements must be evaluated:

(i) Data elements for the freshwater aquatic environment:
- (A) Fish acute toxicity value.
- (B) Invertebrate acute toxicity value.
- (C) Green algal toxicity value (e.g., 96-hour EC_{50}).
- (D) Bacterial toxicity value (e.g., 3-hour EC_{50}).
- (E) Fish chronic value.
- (F) Invertebrate chronic value.
- (G) Green algal chronic value.

(ii) Data elements for the saltwater or marine environment:
- (A) Fish acute toxicity value.
- (B) Invertebrate acute toxicity value.
- (C) Green algal toxicity value (e.g., 96-hour EC_{50}).
- (D) Fish chronic value.
- (E) Invertebrate chronic value.
- (F) Green algal chronic value.

(iii) Data elements for the terrestrial environment:
- (A) Vascular plant toxicity value (e.g., early seedling growth EC_{50}).
- (B) Invertebrate acute toxicity value.
- (C) Avian acute oral LD_{50} value.
- (D) Avian chronic value.

If any environmental toxicity data element for a chemical falls within a "moderate" or higher rank, as described below, that chemical will be considered an environmentally hazardous chemical for which this study requires an environmental MSDS. Data that is based on at least one study conducted in accordance with established scientific principles and that indicates the presence of an environmental hazard (a "moderate" or higher ranking) is sufficient to establish an environmental hazard.

(i) Acute toxicity hazard concerns for aquatic organisms exposed to a chemical in water:

HIGH CONCERN: $EC_{50} \leq 1.0$ mg/L
MODERATE CONCERN: $EC_{50} > 1.0$ mg/L and ≤ 100.0 mg/L
LOW CONCERN: $EC_{50} > 100.0$ mg/L

(ii) Acute toxicity hazard concerns for benthic organisms or animals which are exposed through contaminated sediments:

HIGH CONCERN: $EC_{50} \leq 1.0$ mg/kg dry weight sediment
MODERATE CONCERN: $EC_{50} > 1.0$ mg/kg and ≤ 100.0 mg/kg
LOW CONCERN: $EC_{50} > 100.0$ mg/kg

(iii) Acute toxicity hazard concerns for terrestrial wildlife species via an oral dose:

HIGH CONCERN: $LD_{50} \leq 50.0$ mg/kg
MODERATE CONCERN: $LD_{50} > 50.0$ mg/kg and ≤ 500.0 mg/kg
LOW CONCERN: $LD_{50} > 500.0$ mg/kg

(iv) Acute toxicity hazard concerns for terrestrial wildlife species via diet or food:

HIGH CONCERN: $LD_{50} \leq 500.0$ mg/kg dry weight food
MODERATE CONCERN: $LD_{50} > 500.0$ mg/kg and ≤ 1000.0 mg/kg
LOW CONCERN: $LD_{50} > 1000.0$ mg/kg

(v) Acute toxicity hazard concerns for plants and soil organisms exposed through soil concentrations:

HIGH CONCERN: $EC_{50} \leq 1.0$ mg/kg dry weight soil
MODERATE CONCERN: $EC_{50} > 1.0$ mg/kg and ≤ 100.0 mg/kg
LOW CONCERN: $EC_{50} > 100.0$ mg/kg

(vi) Chronic toxicity hazard concerns for aquatic species exposed to a chemical in water:

HIGH CONCERN: chronic value ≤ 0.100 mg/L
MODERATE CONCERN: chronic value > 0.100 mg/L and ≤ 10.0 mg/L
LOW CONCERN: chronic value > 10.0 mg/L

(vii) Chronic toxicity hazard concerns for benthic organisms or animals that are exposed through contaminated sediments:

HIGH CONCERN: chronic value ≤ 0.1 mg/kg dry weight sediment
MODERATE CONCERN: chronic value > 0.1 mg/kg and ≤ 10.0 mg/kg
LOW CONCERN: chronic value > 10.0 mg/kg

(viii) Chronic toxicity hazard concerns for terrestrial wildlife species via diet or food:

HIGH CONCERN: chronic value ≤ 50.0 mg/kg dry weight food
MODERATE CONCERN: chronic value > 50.0 mg/kg and ≤ 100.0 mg/kg
LOW CONCERN: chronic value > 100.0 mg/kg

(ix) Chronic toxicity hazard concerns for plants and soil organisms exposed through soil concentrations:

HIGH CONCERN: chronic value ≤ 0.1 mg/kg dry weight soil
MODERATE CONCERN: chronic value > 0.1 mg/kg and ≤ 10.0 mg/kg
LOW CONCERN: chronic value > 10.0 mg/kg.

Section Three - Environmental Fate Evaluation

For each chemical determined to be environmentally hazardous, the following environmental fate data elements must be identified:

(i) The octanol/water partition coefficient.
(ii) Water solubility.
(iii) Boiling point.
(iv) Vapor pressure.
(v) Henry's Law constant.
(vi) Sorption/desorption to soils and sediments.
(vii) Melting temperature.
(viii) Fish bioconcentration factor.
(ix) Terrestrial invertebrate bioconcentration factor.

These environmental fate data should be used to evaluate the following fate factors, using the indicated ranking systems.

(i) Bioconcentration potential. (A) Bioconcentration potential when only the octanol/water partition coefficient (K_{ow}) is available:

HIGH POTENTIAL: Log $K_{ow} \geq 4.3$ and ≤ 8.0
MODERATE POTENTIAL: Log $K_{ow} \geq 3.5$ and < 4.3
LOW POTENTIAL: Log $K_{ow} < 3.5$

(B) Bioconcentration potential when the bioconcentration factor (BCF) is available for aquatic organisms and the BCF is based on exposure from a chemical being present in water:

HIGH POTENTIAL: BCF $\geq$ 1000
MODERATE POTENTIAL: BCF $\geq$ 250 and $<$ 1000
LOW POTENTIAL: BCF $<$ 250

(ii) Water Solubility.

VERY SOLUBLE	> 10,000 ppm
SOLUBLE	> 1,000 ppm to 10,000 ppm
MODERATELY SOLUBLE	> 100 ppm to 1,000 ppm
SLIGHTLY SOLUBLE	> 0.1 ppm to 100 ppm
INSOLUBLE	< 0.1 ppm

(iii) Soil Organic Carbon Partition Coefficient (Log K_{oc}).

VERY STRONG SORPTION	$\geq$ 4.5
STRONG SORPTION	$\geq$ 3.5, but $<$ 4.5
MODERATE SORPTION	$\geq$ 2.5, but $<$ 3.5
LOW SORPTION	$\geq$ 1.5, but $<$ 2.5
NEGLIGIBLE SORPTION	$<$ 1.5

(iv) Biodegradation.

RAPID	≥ 60% degradation over a test period of ≤ 7 days
MODERATE	≥ 30% degradation over a test period of ≤ 28 days
SLOW	< 30% degradation over a test period of ≤ 28 days
VERY SLOW	< 30% degradation over a test period of > 28 days

(v) Volatility (Henry's Law constant, in atm-m^3/mole).

VERY VOLATILE	$> 10^{-1}$
VOLATILE	$< 10^{-1}$, but $\geq 10^{-3}$
MODERATELY VOLATILE	$< 10^{-3}$, but $\geq 10^{-5}$
SLIGHTLY VOLATILE	$< 10^{-5}$, but $\geq 10^{-7}$
NONVOLATILE	$< 10^{-7}$

Section Four: Possible Data Sources

This section is meant to provide guidance on the literature and computerized data sources that may be used to meet the requirements of this exercise. The latest editions should always be used. These sources are not exhaustive. EPA encourages the use and identification of additional sources available to pilot study participants. By providing this information, EPA is not endorsing the data sources nor offering a judgment on the relative merits of any particular data source.

(a) Environmental toxicity data sources:

(1) General Literature

Handbook of Environmental Data on Organic Chemicals
Verschueren, Karel, 1983, Van Nostrand Reinhold Co., New York, NY. Contains chemical/physical properties, air pollution factors, water pollution factors, and biological effects.

The Acute Oral Toxicity, Repellency, and Hazard Potential of 998 Chemicals to One or More Species of Wild and Domestic Birds
Schafer, Jr., E.W., Bowles, Jr. W.A., and Hurlbut J., 1983, Archives of Environmental Contamination and Toxicology 12:355-382.

The Acute Oral Toxicity and Repellency of 933 Chemicals to House and Deer Mice
Schaefer, Jr., E.W., and Bowles, Jr., W.A., 1985, Archives of Environmental Contamination and Toxicology 14:111-129.

Manual of Acute Toxicity: Interpretation and Data Base for 410 Chemicals and 66 Species of Freshwater Animals
Mayer, Jr., F.L., and Ellersieck, M.R., 1986, Washington, DC: Fish and Wildlife Service, U.S. Department of the Interior, Resources Publication 160.

Handbook of Toxicity of Pesticides to Wildlife
Hudson, R.H., Tucker, R.K., and Haegele, M.A., 1984, Washington, DC: Fish and Wildlife Service, U.S. Department of the Interior, Resource Publication No. 153.

Toxicity of Power Plant Chemicals to Aquatic Life
Becker, C.D. and Thatcher, T.O., 1973, U.S. Atomic Energy Commission, WASH-1249, UC-11.

Toxicities of Selected Substances to Freshwater Biota
Hohreiter, D.W., 1980, Argonne, IL: Argonne National Laboratory, ANL/ES-94, Available from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161.

Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas)
Brooke, L.T., Call, D.J., Geiger, D.L., and Northcott, C.E. (editors), 1984, Vol. 1, Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas)
Geiger, D.L., Northcott, C.E., Call, D.J., and Brooke, L.T. (editors), 1985, Vol. 2, Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas)
Geiger, D.L., Poirier, S.H., Brooke, L.T., and Call, D.J. (editors), 1986, Vol. 3, Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas)
Geiger, D.L., Call, D.J., and Brooke, L.T. (editors), 1988, Vol. 4, Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas)
Geiger, D.L., Brooke, L.T., and Call, D.J. (editors), 1990, Vol. 5, Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior.

Fish Toxicity Screening Data. Part 1: Lethal Effects of 964 Chemicals Upon Steelhead Trout and Bridgelip Sucker, and Part 2: Lethal Effects of 2,014 Chemicals Upon Sockeye Salmon, Steelhead Trout and Threespine Stickleback
MacPhee, C. and Cheng, F.F. 1974 and reprinted 1989, Washington, DC: U.S. Environmental Protection Agency, EPA-560/6-89-0001, Available from the National Technical Information Service (NTIS), U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161, PB89-156715.

Part 1: The Toxicity of 3400 Chemicals to Fish, and Part 2: The Toxicity of 1085 Chemicals to Fish
Wood, E.M. (Part 1), 1953 and reprinted 1987, and Hollis, E.H. and Lennon, R.E. (Part 2), 1954 and reprinted 1987, Washington, DC: U.S. Environmental Protection Agency, EPA-560/6-87-002, Available from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161, PB87-200275.

(2) Ambient Water Quality Criteria

Information on the aquatic toxicity of over a hundred chemicals has been published by the U.S. Environmental Protection Agency, Office of Water Regulations and Standards. Individual criteria documents may be obtained from the National Technical Information Service (NTIS), U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161

(3) Computerized Data Bases

The NIH-EPA Chemical Information System (CIS), maintained by the Computer Sciences Corporation (CSC) in Falls Church, Virginia, contains three environmental toxicity data bases: AQUIRE, TERRE-TOX, and PHYTOTOX. The data bases include detailed descriptions of the studies used to generate the data.

The Aquatic Information Retrieval System (AQUIRE) contains published aquatic toxicity data (e.g., effective concentrations) and bioconcentration factors for aquatic species, communities and ecosystems.

TERRE-TOX contains published toxicity data for vertebrate and invertebrate terrestrial animals, such as wild mammals, bees, earthworms and laboratory animals. See Meyers and Schiller (1986; Meyers, S.M. and Schiller, S.M. TERRE-TOX: A data base for effects of anthropogenic substances on terrestrial animals. Journal of Chemical information and Computer Sciences. 26:33-36) for a more detailed description of this data base.

PHYTOTOX contains published toxicity data for terrestrial vascular plants. See Royce et al. (1984; Royce, C.L., Fletcher, J.S., and Risser, P.G. PHYTOTOX: A database dealing with the effects of organic chemicals on terrestrial vascular plants. Journal of Chemical Information and Computer Sciences. 24:7-10) for a more detailed description of this data base.

(b) Environmental fate data sources:

(1) General Literature

CRC Handbook of Chemistry and Physics
CRC Press, 1990, Chemical Rubber Company, Boca Raton, FL.

The Merck Index
Merck and Company, 1989, Rahway, NJ.

Handbook of Environmental Data on Organic Chemicals
Verschueren, K., 1983, Van Nostrand Reinhold Company, New York, NY.

Handbook of Chemical Property Estimation Methods
Lyman, W., 1982, McGraw-Hill Book Company, New York, NY.

Lange's Handbook of Chemistry
Lange, N.A., 1985, McGraw-Hill Book Company, New York, NY.

The Condensed Chemical Dictionary
Hawley, G.G., (Ed.), 1981, Van Nostrand Reinhold Company, New York, NY.

(2) Computerized Data Bases

The Environmental Fate Data Base (EFDB) created and maintained by Syracuse Research Corporation, Merrill Lane, Syracuse, NY 13210-4080 (telephone 315-426-3200) contains measured and estimated physical-chemical properties as well as environmental fate data. The data base also provides literature references for sources of environmental fate and physical-chemical properties data.

The Medchem data base (Medicinal Chemistry Project, Pomona College, Claremont, CA) contains measured octanol water partition coefficients. The database is available through Daylight Chemical Information Systems 18500 Von Karman Ave., Suite 450, Irvine, CA 92715 (telephone 714-476-0451).

The Arizona Data Base contains measured water solubilities, melting points, boiling points and references. The data base, developed at the University of Arizona, Tucson, is available on floppy disk for personal computers. Contact Dr. Samuel Yalkowski, College of Pharmacy, University of Arizona, Tucson, AZ 85721 (telephone 602-626-1289) for more information.

The Soil Transport and Fate Data Base developed for EPA's Office of Research and Development by Utah State University contains data on the transport and transformation of chemicals in soils. The current version is undergoing revision and will soon be available through Utah State University Division of Environmental Engineering, Logan, UT 84322.

Section Five: Test Descriptions and Evaluation Guidelines

The environmental fate and toxicity profiles of a chemical consist of data elements which characterize the fate and effects of a chemical in the environment. Although EPA recognizes that most industrial chemicals will have little or no information available for them, the total amount of information potentially available for some chemicals could be quite extensive.

The environmental fate profile for a chemical would consist of all of the fate and transport parameters needed to characterize a chemical's transport, partitioning, transformations, and disappearance in the environment. A chemical's environment may include surface water, sediments, soil, the atmosphere, groundwater, and the biota which live in each of these compartments.

The environmental toxicity profile for a chemical would consist of all of the adverse effects of that chemical upon organisms in the environment, as identified in these guidelines, and upon the populations, communities, and ecosystems to which those organisms belong. Each data element in these profiles consists of (1) the type of the fate attribute or effect, (2) a time period, and (3) a value, for example, effects expressed in milligrams per liter or half-lives in days.

While some companies may want to add as much information as possible to their MSDS because of some unique toxic properties of the chemical and/or of its broad application and environmental exposure, EPA, for this study, requires only a subset of the total possible amount of information to be included in MSDSs submitted during this exercise. That subset is identified in Sections Two and Three of this document. This section includes information on both mandatory and optional data elements.

The most reliable data available should be reported for each data element. However, reporting the lowest toxicity (i.e., the toxicity for the most sensitive species), or the most conservative value found, takes precedence over reliability. For example, assume that acute toxicity values are found for four species: fathead minnow, bluegill sunfish, rainbow trout, and carp. The toxicity data for the fathead minnow is the more reliable, but the rainbow trout has the lowest toxicity value. At a minimum, the rainbow trout toxicity value should be reported. Information on potency takes precedence over test data reliability for two reasons. First, the objective of this exercise is the communication of hazard information; therefore, information for the greatest hazards should be reported. Second, potency information is more quantitative, and test data reliability determinations are less quantitative and more subjective.

If multiple information is found for the same data element and all of the data are of equal reliability, then all of the information can be listed, or the geometric mean of the values may be reported. For example, if four acute toxicity values (i.e., 96-hour LC_{50} values) are found for rainbow trout for the same substance and they are of equal reliability, then the MSDS could list all of the values, the range of the values, or the geometric mean of the values.

The values reported on the MSDS must be for the substance identified as the subject of the MSDS. For example, substance G has high water solubility and is toxic to rainbow trout (RT) at 140.0 mg/L as a 24-hour LC_{50}, based on 100 percent active ingredients (AI). Substance G is marketed as a product formulation (XYZ) containing 15 percent substance G, 15 percent surfactant S, and 70 percent water. The toxicity of the formulated product to RT is 8.3 mg/L as a 24-hour LC_{50}. The toxicity of the surfactant S based on 100 percent AI is 2.1 mg/L as a 24-hour LC_{50} to RT. If a manufacturer prepared an MSDS for the pure substance G, the acute toxicity value of 140.0 mg/L should be reported. Likewise, if an MSDS is prepared for the product, XYZ, then the acute toxicity value of 8.3 mg/L should be reported. However, if the manufacturer wishes to market a 30 percent aqueous dispersion of substance G (i.e., 30 percent substance G and 70 percent water), the acute toxicity value of the formulated product XYZ should <u>not</u> be reported because of the substantial influence of the surfactant S. The manufacturer should either report the acute value for substance G as 100 percent AI and clearly indicate that it is based on 100 percent AI, or adjust the acute toxicity value based on 100 percent AI (i.e., 140.0 mg/L) to reflect the dilution by water, i.e., 470.0 mg/L [which was calculated by dividing the acute toxicity value of 140.0 mg/L, based on 100 percent AI, by 0.30, which is the purity of the new formulated aqueous dispersion].

<u>Description of environmental toxicity data elements</u>

(i) Fish acute toxicity value. The fish acute value can be reported as either an EC_{50} or an LC_{50} value. Acute toxicity values range from a few hours, e.g., a 3-hour LC_{50}, to 14 days. The 96-hour value is preferred. The 24-hour EC_{50} value is also valuable to know because it can be compared to the 96-hour EC_{50}. This comparison can give an assessor a indicator of the size of the acute to chronic ratio (ACR). The ratio between the 24-hour EC_{50} and the 96-hour EC_{50} (i.e., the 24-hour EC_{50} divided by the 96-hour EC_{50}) is called the chronicity indicator (ChI). If this ratio is less than 2, then the ACR is probably less than ten; and if the ratio is greater than 2, then the ACR has a higher probability of being greater than 10. The greater the ratio the larger the ACR.

(ii) Invertebrate acute toxicity value. The invertebrate (planktonic crustaceans) acute value can be as either an EC_{50} or an LC_{50} value. Acute toxicity values range from a few hours to several days. The 48-hour value is generally measured for freshwater species, for example, daphnids and ceriodaphnids, and the 96-hour value is generally measured for saltwater species, for example, mysids and penaeids. The 24-hour EC_{50} value is also valuable to know because it can be used to estimate the ChI. For freshwater species the 24-hour EC_{50} is compared to the 48-hour EC_{50}, and for saltwater species the 24-hour EC_{50} is compared to the 96-hour EC_{50}.

(iii) Benthic invertebrate acute toxicity value. Benthic invertebrates include crustaceans, insects, and detritivores. The acute value is reported as either an EC_{50} or an LC_{50} value. Acute toxicity values range from a few hours to several days. Acute toxicity tests may be done with and without sediments. When sediments are included, exposure concentrations and effective concentrations are generally reported as milligrams per kilogram, i.e., milligrams of test substance per kilogram of dry weight of sediment.

(iv) Green algal toxicity value. The green algal toxicity value is reported as the EC_{50} value since sublethal effects on population growth are measured. The algal toxicity test is generally reported as a 72-hour or 96-hour value. In fact, the algal toxicity test is a multigenerational test, and, therefore, is a chronic toxicity test with respect to green algae. The 96-hour no-effect-concentration (NEC) should also be reported with the 96-hour EC_{50}. The 96-hour NEC is equivalent to the chronic value (ChV) or the geometric mean of the maximum allowable toxicant concentration (GMATC). The 96-hour NEC can be calculated by determining the no-observed-effect-concentration (NOEC) and the lowest-observed-effect-concentration (LOEC). The range of concentrations between the NOEC and the LOEC is the MATC. It is inappropriate to compute the ChI ratio for this test since it is considered a chronic toxicity test with respect to algae.

(v) Bacterial toxicity value. The bacterial toxicity value is reported as an EC_{50} value since sublethal effects on population metabolism, for example, inhibition of oxygen consumption, or population growth, are measured. The bacterial toxicity test is generally reported as a 3-hour to 96-hour value. As with the algal toxicity test, this test is a multigenerational test, and, therefore, is a chronic toxicity test with respect to bacteria.

(vi) Vascular plant (macrophyte) toxicity test. The vascular plant toxicity test is reported as an EC_{50} value since sublethal effects, such as growth, are measured. This test may

last from several hours to 30 days depending upon the objective of the study. If the exposure period is hours to several days and this exposure period is a short portion of the complete life cycle of the plant, then the results of the test should be reported as an acute toxicity test. However, if the exposure period is close to 30 days and is a significant portion of the life cycle of the macrophyte, then the results of the test should be reported as a chronic toxicity test and the ChV should be determined if possible.

(vii) Fish chronic value. The fish chronic value is generally reported as a chronic NEC or MATC based on sublethal effects, but it can be based on lethality. Chronic EC_{50} and LC_{50} values are also reported occasionally. Fish chronic toxicity tests include multigenerational tests, i.e., two generations; whole life cycle tests; and partial life cycle tests, for example, early life stage toxicity tests. Fish chronic toxicity tests generally last from 28 days to 2 years. Shortened early life stage (ELS) toxicity tests lasting 7 to 8 days have recently been proposed as substitutes for the 28-day to 62-day ELS toxicity tests. In some cases the 8-day ELS toxicity test may be substituted for the longer ELS toxicity test. However, the shortened ELS test should not be used to test chemicals which (A) have low water solubility, (B) need to be metabolically activated, such as anilines, before their full toxic potential can be realized, (C) are strong teratogens, or (D) affect female fertility. Using a shortened test with these chemicals could significantly underestimate toxicity.

(viii) Invertebrate chronic value. The invertebrate chronic value is generally reported as a chronic NEC or MATC based on sublethal effects, but it can be based on lethality. Chronic EC_{50} and LC_{50} values are also reported occasionally. Invertebrate chronic toxicity tests include multigenerational tests, i.e., several generations; whole life cycle tests; and partial life cycle tests, for example, daphnid reproduction inhibition tests. Invertebrate chronic toxicity tests generally last from 14 days to several months. Shortened early life stage (ELS) toxicity tests lasting 7 days and using ceriodaphnids have recently been proposed as substitutes for the 14-day to 21-day daphnid reproduction inhibition tests. In some cases the 7-day ceriodaphnid reproduction inhibition test may be substituted for the longer daphnid toxicity test. However, it should not be used to test chemicals which (A) have low water solubility, (B) need to be metabolically activated, such as anilines, before their full toxic potential can be realized, (C) are strong teratogens, or (D) delay daphnid reproduction significantly. Using such a shortened test with these chemicals could significantly underestimate toxicity.

(ix) Benthic (oyster) acute value. The oyster acute toxicity test generally consists of measuring the ability of a chemical to reduce shell deposition or kill oyster larvae. While reduction of shell deposition is a sublethal effect reported as a EC_{50}, the effects to larvae may include death. Test length for the shell deposition test is 96 hours, while test length for the larval test may be hours to several days.

(x) Marine mammalian acute toxicity. Acute toxicity tests using marine mammals are rare, but may consist of an acute oral LD_{50} or a dietary toxicity test. Death is the primary effect, but observations concerning sublethal effects may also be made.

(xi) Marine mammalian chronic value. As with acute toxicity testing with marine mammals, chronic toxicity testing is rare. A manufacturer may find information correlating body burdens of a chemical with effects in wild populations.

(xii) Vascular plant (early seedling growth) toxicity. Toxicity testing for vascular plants can involve early seedling growth, seed germination and root elongation, or screening mature plants for sensitivity to herbicidal activity of new chemicals. Toxicity testing with the early growth stages of vascular plants is preferred. Toxic effects are generally sublethal and are reported as an EC_{50} value. Test periods are variable and generally depend upon species characteristics, for example, time to germination and growth rate. If a test is extended long enough relative to the plant's life cycle, chronic values may be obtained.

(xiii) Terrestrial invertebrate acute toxicity value. The terrestrial invertebrate most commonly tested is the earthworm. Tests can be done with natural or artificial soil and, simply, with filter paper. Tests may last from several days to 14 days. Death is the primary effect, but sublethal effects can be measured also. Effective concentrations are generally reported as milligrams of substance per kilogram of dry weight soil. Tests using filter paper report effective concentrations as milligrams of substance per square centimeter of filter paper, which is difficult to relate to a soil exposure concentration. For this reason, testing with soil is preferred.

(xiv) Soil microbial toxicity. Testing of soil microbes for sensitivity to chemicals has been done for many years and test methodology varies greatly. EPA has proposed two environmental test protocols for studying the effects of chemicals on the soil microbial community: Soil microbial community toxicity test (§797.3700, FR 52:36360-36363[1987]) and Soil-core microcosm test (§797.3775, FR 52:36363-26371[1986]). Tests with natural soil communities and natural soils are preferred over single species cultures in a growth medium. Most

tests are long enough, i.e., days, that these tests can be considered a chronic toxicity test for microbes and chronic values can be determined.

(xv) Avian and wild mammalian acute oral toxicity. Acute toxicity testing with birds and wild mammals involves a single oral dose, given as a gavage, followed by 14 days of observation. Death is the primary effect and LD_{50} values are reported based on an average body weight, specifically, milligrams of substance per kilogram of fresh weight. Testing of birds and wild mammals for acute oral toxicity is similar to the rat oral LD_{50} toxicity test used in human health effects testing.

(xvi) Avian dietary toxicity. Acute toxicity testing with birds involves exposure to contaminated food for 5 days followed by 3 or more days of observations for toxic effects. Death is the primary effect and LC_{50} values are reported based on an average concentration of the substance in food, specifically in milligrams or parts per million (ppm) of substance per kilogram of dry weight of food.

(xvii) Avian and wild mammalian chronic value. Chronic toxicity testing of birds and wild mammals for chronic toxicity generally involves measuring the inhibition of reproductive potential. Dosing generally involves continuous exposure to contaminated food, but could be through gavage. Effective concentrations are reported either as the average concentration of the substance in food (i.e., milligrams of substance per kilogram of dry weight food), or are based on an average body weight (i.e., milligrams of substance per kilogram of fresh body weight). Many of the effects measured are similar to effects measured in developmental toxicity testing using domesticated mammals for human health assessment.

Description of environmental fate data elements

(i) Octanol/water partition coefficient. The octanol/water partition coefficient (K_{ow}) is reported as the concentration of the chemical in each phase and the ratio of the chemical's concentration in the octanol to that in water. A log value is generally used. In the study of the environmental fate of organic chemicals, K_{ow} has been shown to be correlated to water solubility, soil/sediment adsorption, and bioconcentration. The measurement or estimation of K_{ow} can be considered to be the necessary first step in assessing the fate of chemicals.

(ii) Water solubility. Water solubility is reported at saturation at 25° C. Water solubility affects both the fate and transport of chemicals. Generally, highly soluble chemicals become quickly distributed by the hydrologic cycle, have low adsorption coefficients for soils and sediments, and tend to be

more easily degraded by microorganisms. In addition, chemical transformation processes such as hydrolysis and oxidation tend to occur more readily if a compound is water soluble.

(iii) Boiling temperature. Boiling temperature at atmospheric pressure, where possible, is reported. Reduced pressure boiling points should reported with the pressure at which the measurements were made. Where decomposition occurs prior to boiling it should be reported. The data may be used to characterize the physical state of the material, to evaluate the manner and extent that the chemical will be transported in the environment, and as a guide in the selection and design of other tests.

(iv) Vapor pressure, and (v) Henry's Law constant. The vapor pressure is reported at ambient temperature where possible. The temperature of measurements taken at other than ambient temperature is also reported. Vapor pressure values provide indications of the tendency of pure substances to vaporize in an unperturbed situation, and thus provide a method of ranking the relative volatilities of chemicals. Vapor pressure data combined with water solubility data permit the calculation of Henry's law constant, a parameter essential to the calculation of volatility from water.

(vi) Sediment and soil adsorption isotherm. The sediment and soil adsorption isotherm data are reported as the Freundlich isotherm values determined for K, n, 1/n, a soil partition coefficient or soil adsorption ratio (K_d), and a soil organic carbon partition coefficient (K_{oc}). A plot of x/m versus C_e is also provided. The adsorption of chemicals to soils and sediments is an important process that affects a chemical's distribution in the environment. Information on the adsorption potential is needed under certain circumstances to assess the transport of chemicals in the environment.

(vii) Melting temperature. The melting temperature is reported as the temperature range at which the sample decomposes before melting, decomposes on melting, oxidizes (or other reaction) in air on melting, softens over a range of temperatures, melts sharply, or was examined and did not melt. The data may be used to assess the potential for movement of materials in the environment, to determine the physical state of the substance under environmental conditions, to evaluate possible health and environmental effects, and to serve as input for chemical property estimation methods.

(viii) Fish bioconcentration factor. The fish bioconcentration factor is reported as the mean test substance concentration in the fish at steady state divided by the mean test substance concentration in solution at the same time over a

28-day test period. The data can be used for assessing the propensity of a chemical substance to bioconcentrate in freshwater fish.

(ix) Terrestrial invertebrate bioconcentration factor. The terrestrial invertebrate bioconcentration factor is reported as the mean test substance concentration in the animal at steady state divided by the mean test substance concentration in solution at the same time over a 28-day test period. The data can be used for assessing the propensity of a chemical substance to bioconcentrate in terrestrial invertebrates.

Test evaluation guidelines

These guidelines are provided to assist manufacturers and employers in evaluating the relative reliability of testing studies when multiple values are available for a specific test, or when conflicting data are found for a single data element. The MSDS should contain the best and most reliable information available for each fate and toxicity data element. Species sensitivity, however, takes precedence over data reliability.

Some test data reliability assessments appear in the Aquatic Information Retrieval (AQUIRE) data base (Table 1) maintained by the United States Environmental Research Laboratory at Duluth, Minnesota. The most reliable test data is defined as review code "1" by AQUIRE. The Office of Toxic Substances (OTS) has found that every test may offer some useful information. Therefore, if the only study available for a given data element falls into the lowest AQUIRE review code of "4", it must be used in the MSDS until a more reliable study is found.

Environmental data of sufficient quality to permit sound scientific judgments should be reported provided that they contain the necessary components of the environmental data elements as specified in this study. The data should be of suitable quality and completeness as specified by OPTS and OECD test guidelines. Data generated using the most appropriate test procedure for the particular chemical are the most useful. In evaluating the experimental design, the use of generally accepted methods, sufficient numbers of measurements for statistical reliability, and sufficient controls should be considered. Each study should be evaluated in terms of whether the study was conducted in conformance with the design, whether good laboratory practices were observed, and whether results were reproducible.

Toxicity studies

Test methods

The following test methods are listed in the order of their reliability, ranked from best to worst with regard to technical

support: 1) flow-through method with measured concentrations; 2) static-renewal method with measured concentrations; 3) static method with measured concentrations; 4) flow-though method with nominal concentrations; 5) static-renewal method with nominal concentrations; and 6) static method with nominal concentrations. This ranking is applicable for most organic and inorganic chemicals which are stable and non-volatile and are tested for toxicity to water column organisms. Compounds which are volatile, not stable, or tested in sediments or soil may require further study to ensure the greatest amount of reliability.

Volatile chemicals, e.g., toluene and terpenes, must be tested using measured concentrations. Tests which use nominal concentrations should be reported as "less than or equal to" values.

Chemicals which hydrolyze are best characterized using the static-renewal (24 hour replacement) methods and nominal concentrations since the chemical is known to disappear over time. In addition, no aqueous stock solution should be prepared. The chemical should be added directly to the exposure chambers and the organisms added within 10 minutes. If possible, the toxicity of the hydrolysis product should be provided for comparative toxicity purposes and for hazard and risk assessment of chronic exposures. Testing the hydrolysis product requires that the chemical be prepared in an aqueous stock solution which has been allowed to age until all of the parent material has completely hydrolyzed, i.e., age the stock solution for at least six hydrolysis half-lives.

Tests with sediments or soils are usually done using static methods.

Tests with algae and bacteria are done with static methods.

Mitigation testing using humic acid is generally done with static methods and nominal concentrations.

Test length

The length of toxicity tests can be a critical factor in evaluating toxicity test studies, and certain length tests are preferred for differed organisms. The preferred test lengths for different organisms are as follows:

Fish acute toxicity tests of 14-day and 96-hour durations have equal preference and both should be reported if available; if only one value is reported, then the 96-hour test is preferred. The order of preference for other shorter exposures are 72-hour > 48-hour > 24-hour > shorter exposures.

Invertebrate (daphnid) acute toxicity tests of 48 hours are preferred over the 24-hour test. Daphnid acute toxicity tests of 72 hours and 96 hours are suspect because there is a high probability that the daphnids are starving. Marine invertebrate acute toxicity tests are generally done for 96 hours, and this is the preferred length of test. The order of preference for shorter exposures are 72-hour > 48-hour > 24-hour > shorter exposures.

Green algal toxicity tests of 96 hours are preferred over the 72-hour test. Toxicity values, i.e., EC_{50}, based on inhibition of biomass is preferred to those based on inhibition of growth rate. The order of preference for shorter exposures are 48-hour > 24-hour > shorter exposures.

Bacterial toxicity tests are generally 3 hours to 6 hours.

The longer the exposure period, the better the results when testing aquatic macrophyes (e.g., duckweed). Therefore, 30-day tests are preferred over 14-day tests, etc.

The order of preference for fish chronic toxicity tests from greatest preference to least preference are 1) whole life cycle; 2) partial life cycle to include adult exposure, spawning, and the early life stages through the juvenile life stage; 3) early life stage which includes zygotes less than 24 hours old through the juvenile life stage; and 4) partial life cycle tests of the juvenile through adult life stages, or just adult stages. Partial life cycle tests utilizing just one life stage, e.g., 30-day exposure of adults, are least preferred because these tests generally do not include the most sensitive life stages, which are generally from zygote through juvenile stages.

Invertebrate chronic values based on tests of 21-day exposures for daphnids are preferred; however, the OECD daphnid reproductive toxicity test is just 14 days. The 7-day toxicity test using ceriodaphnids should only be used with chemicals having water solubilities greater than 10 mg/L; the 7-day test should not be used with chemicals which exhibit any specific toxicity in addition to simple narcosis. Chemicals which are known to have a specific mode of toxic action (e.g., anilines) need time to be metabolically activated and/or need time for their full expression of toxicity. The 4-day chronic toxicity test with ceriodaphnids is least preferred because the exposure period is probably too short for all effects to be expressed.

Benthic toxicity tests using contaminated sediments should be as long as possible, preferably at least 30 days.

The early seedling growth test is partially dependent on the species being tested but should be at least 28 days or longer. The longest tests are generally preferred over shorter tests.

The earthworm toxicity test should be as long as possible.

The soil microbial community toxicity test should be as long as possible.

Limit tests

The results of limit tests, i.e., tests done with one concentration, such as 1000 mg/L, should be reported directly. For example, chemical A is tested with fish at 1000.0 mg 100 percent active ingredients (AI) per liter and all fish are killed within 24 hours. These results should be reported as a 24-hour LC_{100} = 1000.0 mg/L (100% AI). These results should not be reported as a 96-hour LC_{50} < 1000.0 mg/L (100% AI). Although this is true, it is very misleading about the toxicity actually observed in the limit test. Likewise, if no fish died within 96 hours, more information is communicated by reporting these results as a 96-hour NOEC = 1000.0 mg/L (100% AI) rather than as a 96-hour LC_{50} > 1000.0 mg/L (100% AI).

Cationic chemicals

The total organic carbon (TOC) concentration of dilution water should be reported whenever the results of testing cationic chemicals, i.e., inorganic or organic, are reported. Dissolved organic carbon (DOC) binds with cationic chemicals and makes them less bioavailable to aquatic organisms and, therefore, less toxic. Toxicity values can vary greatly depending on the amount of TOC in dilution water during toxicity testing. Toxicity values measured in clean dilution water (i.e., TOC < 2 mg/L) are preferred because these measurements more accurately reflect the intrinsic toxicity of the cationic chemical. If mitigation testing is done, i.e., toxicity testing with known amounts of DOC added to dilution water, so that the amount of toxicity mitigation can be correlated with the amount of DOC in water, then these results should also be reported along with the toxicity values measured in clean dilution water.

Acids

When reporting the toxicity results of acids, the pH should also be reported. For example, organic acid A is tested with fish and the 96-hour LC_{50} = 200.0 mg/L. The pH at the LC_{50} concentration should also be reported so that the reader can determine if death was caused by the hydrogen ion content of the dilution water, intrinsic toxicity from the organic acid, or a combination of both factors.

Chronic values for algae and bacteria

When reporting the EC_{50} values for inhibition of growth in microalgae and microbial species, the chronic values should also be reported.

Reporting chronic values

The preferred chronic value to be reported is the geometric mean of the MATC. If the MATC is not available, then the NOEC is preferred. If the NOEC is not available, then the EC_{10} should be reported.

Fate studies

Octanol/water partition coefficient

K_{ow} values measured using the generator column method are considered most reliable for chemicals with K_{ow} values greater than 10^3. For chemicals with K_{ow} values less than 10^3 but greater than 10, both the standard shake flask method and the generator column method are of adequate reliability. The shake flask method is considered reliable for K_{ow} less than or equal to 10.

Water Solubility

Water solubility methods using conventional aqueous saturation methods or the generator column method are preferred. The generator column method is considered most reliable for water solubilities of less than or equal to 1 ppm. The generator column or shake flask method can be used reliably for substances with water solubilities greater than 1 ppm but no greater than 1000 ppm. Results from the shake flask test are considered reliable for chemicals with water solubilities greater than 1000 mg/L (ppm).

Water solubilities measured at environmentally relevant temperatures are preferred over those measured at elevated temperatures. Water solubilities measured over an environmentally relevant pH range are preferred for ionizable compounds over single pH measurements.

Boiling Point

Any of the methods for the determination of boiling point referenced in the OTS/OECD test guidelines are considered of equal and adequate reliability.

Vapor Pressure

The isoteniscope procedure (ASTM 1978) is considered most reliable for pure liquids with vapor pressures from 0.1 to 100 kPa. The gas saturation (or transpiration) method is considered most reliable for vapor pressures of solids or liquids from 10^{-5} to 10^{3} kPa.

The gas saturation method is considered more reliable for impure chemicals than the isoteniscope method.

Soil/Sediment Adsorption Isotherm (AdI)

Soil/sediment adsorption isotherms conducted using specific analytical techniques and well characterized soils/sediments are considered the most reliable.

Melting Temperature

Any of the methods for the determination of melting temperature referenced in the OTS/OECD test guidelines are considered of equal and adequate reliability.

UV/Visible Absorbance Spectrum

Any of the methods for the determination of the UV/Visible absorbance spectrum referenced in the OTS/OECD test guidelines are considered of equal and adequate reliability.

Biodegradation

In general, biodegradation tests of 28 days or greater using radiolabelled test chemicals are considered most reliable. Tests using specific analytical techniques for parent compounds are also considered highly reliable. Tests using nonspecific analytical techniques are generally of lower reliability. Their reliability is ranked in descending order as follows: 1) CO_2 evolution, 2) loss of dissolved organic carbon, 3) O_2 uptake (BOD). This ranking is relative, however; 5-day BOD values, for example, may be highly reliable for a conservative judgment if data show positive results, i.e., good degradability.

Tests using intact environmental samples are ranked as more reliable than those using composite samples.

Wastewater treatment plant simulation tests which emulate full scale treatment plant operating parameters are considered more reliable than those which do not.

Bioconcentration

Fish and invertebrate bioconcentration/bioaccumulation tests should be long enough for the organisms to reach an equilibrium of chemical residues. If study length does not permit equilibrium to be attained, then the equilibrium should be predicted using statistical methods. Bioconcentration factors (BCF) based on studies where equilibrium is attained are considered more reliable.

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Table 1. Modified reliability codes for the Aquatic Information Retrieval (AQUIRE) toxicity data base, from Pilli et al. (1988).

The AQUIRE review code indicates the type and completeness of methods documentation accompanying the study data and the compliance of these methods with Agency toxicity test protocols. Review code assignments for tests are based on the criteria outlined in each of the following rating sections:

A. REVIEW CODE = 1 Meets all the following criteria:
(1) methodology section cites acceptable procedures and quality of data assured;
(2) satisfactory control;
(3) measured toxicant concentration;
(4) a solvent control if a solvent is used;
(5) for organic and nonmetallic inorganic chemicals, the test water temperature, pH, and dissolved oxygen are reported; and
(6) for metals, the test water temperature, pH, dissolved oxygen, and either alkalinity or hardness are reported (alkalinity or hardness data not required for saltwater tests).

B. REVIEW CODE = 2 Meets some criteria:
(1) control mortality not reported, or high but accounted for statistically;
(2) unmeasured toxicant concentration;
(3) test water chemistry variables not reported; and
(4) no solvent control when a solvent is used in the test.

C. REVIEW CODE = 3 Does not meet criteria:
(1) methods section shows weaknesses in experimental procedures, or insufficient methodology description to judge quality of experiments;
(2) control mortality unsatisfactory, e.g., greater than 10% and not accounted for statistically;
(3) a static test with unmeasured concentrations conducted in the presence of precipitate or some undissolved chemical or in an unacceptable container;
(4) the test was conducted with chlorinated tap water, distilled water or rain water; and
(5) residue effects do not meet criteria set for inclusion in AQUIRE.

D. REVIEW CODE = 4 Abstract or foreign paper:

Indicates data are available only in a limited format. Data only available in abstract form are coded from the abstract. The English abstract and/or table of data are used to review foreign papers.

Part Two: Material Safety Data Sheets and Labelling

Section One: Required Information

As part of this exercise, environmental hazard information is to be provided either in a new section on the material safety data sheet (MSDS) required by OSHA, or in a supplemental attachment to such an MSDS, for each chemical determined to be environmentally hazardous according to the criteria in Section Two of Part One. If an MSDS is not required by OSHA for a study chemical and that chemical meets the criteria for being an environmentally hazardous chemical, the participant should develop an environmental MSDS, which should be in English and include all the information required by the EPA in this study.

Environmental toxicity and fate information must be included on all MSDSs prepared for environmentally hazardous chemicals in the study. At least one value must be listed for each data element specified in Sections Two and Three of Part One of this project description. If multiple values exist for a single data element, the most environmentally conservative value should be listed. If no data are available for a required data element, the statement "No Available Data" should be listed for that element.

An environmental hazard description must be included in the MSDS for chemicals which exhibit a moderate or high hazard to organisms living in the natural environment, as identified in Section Two. Environmental hazard descriptions are required only for the greatest (i) aquatic hazard and (ii) terrestrial hazard categories identified for each chemical. Once the highest hazard has been characterized for each category, additional language describing lower degrees of hazard within that category is voluntary. For example, if a chemical exhibits a high hazard to freshwater aquatic organisms and a moderate hazard to saltwater aquatic organisms, the only description required is that of the high hazard. If a chemical is moderately hazardous to aquatic organisms and highly hazardous to terrestrial organisms, however, then hazard descriptions for both the aquatic hazard and the terrestrial hazard must be included in the MSDS.

The MSDS entry should include recommendations for using or disposing of the chemical in ways which correspond to the perceived environmental hazards of the chemical, and should identify actions to be taken to prevent and control accidental spills and other releases of the chemical that could present environmental hazards, with procedures for cleaning up such spills and releases. It should also include citations to applicable federal regulations concerning the disposal of the chemical, and a statement that there may also be state and local regulations applicable to disposal.

For this exercise, the MSDS should list the name, address and telephone number of the manufacturer or other responsible party preparing the MSDS, who can provide additional information on the chemical.

The MSDS must include the chemical identity used on the label, and the following information, as appropriate:

(i) If the chemical is a single substance, its chemical and common name(s).

(ii) If the chemical is a mixture which has been tested as a whole to determine whether it is environmentally hazardous, the chemical and common name(s) of the ingredients which contribute to its known environmental hazards, and the common name(s) of the mixture itself.

(iii) If the chemical is a mixture which has not been tested as a whole:

(A) The chemical and common name(s) of all ingredients which have been determined to be environmentally hazardous, and which comprise 1% or greater of the composition; and,

(B) The chemical and common name(s) of all ingredients which have been determined to be environmentally hazardous, and which comprise less than 1% of the mixture, if data indicate that the ingredient(s) could be released from the mixture in concentrations which could present an environmental hazard.

(iv) If the chemical or common name(s) are claimed confidential, a generic chemical name must be used.

Section Two: Hazard Description Language

At a minimum, the following language, or language which is qualitatively similar and expresses the same degree of caution, must be included in the MSDS for each chemical in the study presenting the described hazard.

High aquatic toxicity. If a chemical exhibits high toxicity toward any species of aquatic organisms, then language similar to the following language should be included in the MSDS: "This chemical is highly toxic to aquatic organisms. Do not release directly to natural waters."

Moderate aquatic toxicity. If a chemical exhibits moderate toxicity toward any species of aquatic organisms, then language similar to the following language should be included in the MSDS: "This chemical is moderately toxic to aquatic organisms. Aquatic organisms may be killed by this chemical if it is released directly to natural waters."

High terrestrial toxicity. If a chemical exhibits high toxicity toward any species of the terrestrial environment, then language similar to the following language should be included in the MSDS: "This chemical is highly toxic to terrestrial organisms. Do not release directly to the natural terrestrial environment."

Moderate terrestrial toxicity. If a chemical exhibits moderate toxicity toward any species of the terrestrial environment, then language similar to the following language should be included in the MSDS: "This chemical is moderately toxic to terrestrial organisms. Direct release to land may result in harm to terrestrial organisms."

Section Three: Optional Labelling Descriptions

Companies participating in the study are encouraged, but not required, to indicate what language may be included in labels on study chemicals found to be environmentally hazardous. In this connection, companies addressing labelling language are asked to indicate in what ways existing labels would be modified to include environmental hazard communication information.