ENVIRONMENTAL HAZARDS SUMMARY

OVERVIEW: Environmental hazards assessment is the process of identifying the adverse effects that a chemical may have on organisms in the environment. Currently, the CTSA process for environmental hazards assessment focusses on aquatic toxicity. Other environmental hazards could include mammalian toxicity, avian toxicity, and habitat alteration or destruction (e.g., altering the temperature of a stream by discharging cooling water).

This module collects data on measured or predicted toxicity of chemicals to aquatic organisms to characterize the potential aquatic toxicity hazard of chemical discharges to receiving waters. Toxic chemical discharges can also affect the quality of water that may be a source of drinking water and can be a detriment to the human food chain. Aquatic toxicity data are combined with estimated water concentrations from the Exposure Assessment module to assess the risk of chemical exposure to aquatic organisms in the Risk Characterization module.

GOALS:

- Assess the toxicity of chemicals to the aquatic environment.
- Guide the selection and use of chemicals that are less toxic to aquatic organisms.
- Determine the aquatic toxicity concern concentration (CC) of chemicals.
- Provide the CCs to the Risk Characterization module.

PEOPLE SKILLS: The following lists the types of skills or knowledge that are needed to complete this module.

- Expertise in aquatic toxicology, including knowledge of standard aquatic toxicity test methods, relative sensitivity of aquatic species to chemical contamination, mechanisms of toxic action, and relationships of the molecular structure of chemicals to toxic action.
- Knowledge of molecular structure and fate of chemicals in the aquatic environment.

Within a business or a DfE project team, the people who might supply these skills include an aquatic toxicologist, an environmental scientist, a chemist, and/or an environmental engineer. DfE project teams that do not have people with the necessary expertise to complete this module should seek outside assistance.

Note: The analysis presented in this module should only be undertaken by someone with expertise in environmental hazards (toxicity) assessment. Furthermore, peer-review of the completed environmental hazards summary is recommended.

DEFINITION OF TERMS:

Analog: A chemical compound structurally similar to another but differing often by a single element of the same valence and group of the periodic table as the element it replaces.

Aquatic Toxicity Concern Concentration (CC): The concentration of a chemical in the aquatic environment below which no significant risk to aquatic organisms is expected.

Aquatic Toxicity Profile: A compilation of the effective concentrations (EC), either measured or predicted, for a range of species.

Assessment Factor (AsF): Adjustment value used in the calculation of a CC that incorporates the uncertainty associated with: (1) toxicity data (e.g., laboratory test versus field test; measured versus estimated data); (2) acute exposures versus chronic exposures; and (3) species sensitivity.

Chronic Value: (See No Effect Concentration.)

Daphnid: Water flea; an aquatic invertebrate (*Daphnia* spp.) frequently used as the test organism in aquatic toxicity testing.

Effects Concentration (EC_{50}): The concentration of a chemical in water that causes 50 percent of the test organisms to show an adverse sublethal effect (such as growth inhibition) at the end of the specified exposure period. Typical units are mg/L.

Hydrolysis: A chemical transformation process in which a chemical reacts with water. In the process, a new carbon-oxygen bond is formed with oxygen derived from the water molecule, and a bond is cleaved within the chemical between carbon and some functional group.

Lethal Concentration (LC_{50}): The concentration of a chemical in water (or air) that causes death or complete immobilization in 50 percent of the test organisms at the end of the specified exposure period. LC_{50} values typically represent acute exposure periods, usually 48 or 96 hours but up to 14 days for fish. Typical units are mg/L (mg/m^3 or ppm for air).

Lowest-Observed Effect Concentration (LOEC): The lowest concentration at which there are statistically significant increases in adverse effects in the exposed population over its appropriate control group.

Maximum Allowable Toxicant Concentration (MATC): The range of measured values in the range from the no-observed effect concentration (NOEC) to the LOEC.

Measured Concentrations: Chemical concentrations measured in the aqueous test solution at specified intervals and at the end of an aquatic toxicity test period. EPA aquatic toxicity test methods in the Code of Federal Regulations require test results to be reported based on mean measured concentrations. Many tests results are based on nominal concentrations, however, to avoid the cost of chemical laboratory analysis.

No-Effect Concentration (NEC): The concentration of a chemical that results in no significant effects on the test organisms following a prescribed (usually chronic) exposure period. NEC is the geometric mean of the NOEC and the LOEC and is used to represent the threshold concentration. This value may alternatively be called the geometric mean of the maximum allowable toxicant concentration (GMATC), or the Chronic Value. Typical units are mg/L.

No-Observed Effect Concentration (NOEC): A concentration at which there are no statistically significant increases in adverse effects in the exposed population over its appropriate control group.

Nominal Concentrations: Chemical concentrations added to the aqueous test solution at the beginning of an aquatic toxicity test. Nominal concentrations can be higher than the actual concentration causing a toxic effect, particularly if the chemical is volatile or was added to the test solution at a concentration greater than its water solubility limit.

Octanol/Water Partition Coefficient (K_{ow}): The equilibrium ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system, typically expressed in log units (log K_{ow}). K_{ow} provides an indication of a chemical's water solubility, fat solubility (lipophilicity), its tendency to bioconcentrate in aquatic organisms, and to sorb to soil or sediment. It is often used in toxicity structure-activity relationships.

Structure-Activity Relationship (SAR): The relationship of the molecular structure and/or functional groups of a chemical with specific effects. SARs evaluate the molecular structure of a chemical and make qualitative or quantitative correlations of particular molecular structures and/or functional groups with specific effects.

Threshold Concentration: The concentration at which effects begin. (See No Effect Concentration.)

APPROACH/METHODOLOGY: The following presents a summary of the technical approach or methodology for conducting an environmental hazards assessment focussing on aquatic toxicity. Methodology details for Steps 3, 4, 5, and 6 follow this section.

Step 1: Obtain the CAS RN and synonyms, chemical structure, and pertinent chemical properties information for each chemical from the Chemical Properties module.

Step 2: Obtain environmental fate parameter values and reactivity data from the Environmental Fate Summary module. (For example, a chemical's K_{ow} is required to predict effect concentrations.) If a chemical is highly water-reactive (for example, hydrolysis half-life less than one hour) consider collecting toxicity data for the hydrolysis product(s).

Step 3: Construct an aquatic toxicity profile for each chemical. The most frequently used toxicity profile for aquatic organisms consists of the following:

- Fish acute toxicity value (usually a fish 96-hour LC_{50} value).
- Aquatic invertebrate acute toxicity value (usually a daphnid 48-hour LC_{50} value).
- Green algal toxicity value (usually an algal 96-hour EC_{50} value).
- Fish chronic value (usually a fish 28-day early life stage NEC).
- Aquatic invertebrate chronic toxicity value (usually a daphnid 21-day NEC).
- Algal chronic toxicity value (usually an algal 96-hour NEC value for biomass).

Step 4: Use data quality checks to evaluate the validity of the data obtained in Step 3. Data that appear invalid (e.g., based on nominal concentrations instead of measured concentrations; inconsistent with the physical/chemical properties of the chemical, etc.) should be replaced with data of better quality or predicted data.

Step 5: Calculate the CC for each chemical in water. Concentrations in water below the CC are assumed to present low (acceptable) risk to aquatic species.

Step 6: Rank chemicals for aquatic toxicity according to the lowest of their acute or chronic values. This ranking can be based on scoring the chemicals as High, Moderate, or Low concern for aquatic toxicity.

Step 7: Provide the CCs to the Risk Characterization module.

METHODOLOGY DETAILS: This section presents methodology details for completing Steps 3, 4, 5, and 6. If necessary, additional information on this and other steps can be found in previously published guidance (Table 5-15: Published Guidance on Aquatic Toxicity Assessment).

Details: Step 3, Constructing the Aquatic Toxicity Profile

The aquatic toxicity profile may consist of only valid measured data, only predicted values, or a combination of both. Depending on the availability of valid measured data or SARs to estimate data, the toxicity profile may contain a minimum of one acute or chronic value to the full compliment of three acute values and three chronic values. Examples from the Screen Reclamation CTSA (EPA, 1994c) are shown in Table 5-13.

TABLE 5-13: EXAMPLE AQUATIC TOXICITY PROFILES (in mg/L)								
Chemical	**Fish Acute**	**Daphnid Acute**	**Algal Acute**	**Fish Chronic**	**Daphnid Chronic**	**Algal Chronic**	**CC[a]**	**Chronic Eco[b] Hazard Rank**
Acetone	> 1000	> 1000	> 1000	490	100	76	7.6	Low
Sodium hypochlorite	< 1.7	< 2.0	< 2.0	< 0.17	< 0.2	< 0.2	< 0.02	Moderate
Solvent naphtha light aliphatic C^5 - C^{10}	0.64	0.86	0.23	0.05	0.05	0.11	0.005	High

a) CC is derived by dividing the lowest chronic value (in mg/L) by 10.
b) See Details: Step 6 for guidelines on ranking chemicals for aquatic toxicity.

Chemical Mixtures: Chemical mixtures, such as petroleum products (e.g., mineral spirits or solvent naphtha), do not lend themselves to the standard assessment process using SARs. The chemical constituents and the percentage of each in a mixture can vary. The toxicity of mixtures can be determined by estimating the toxicity of each individual constituent and then evaluating the potential toxicity of the product through a weighted average. If the concentration of each constituent in the mixture is not known, one approach is to assume that each component is present in an equal percentage in the product and the geometric mean of the range of like toxicity values provides the best estimate of the toxicity. The geometric mean of *n* positive numbers is $(a \times b \times c...)^{1/n}$. If the concentration of the constituents is known, then the sum of the weight fractions of each constituent multiplied by its toxicity provides an estimate of the toxicity of the product.

Discrete (Single) Organic Chemicals: The toxicity profile for single organic chemicals can be constructed using effective concentrations based on toxicity test data (measured) or estimated toxicity values based on SARs.

Inorganic Chemicals: The toxicity of inorganic chemicals typically cannot be as accurately estimated using SARs as for organic chemicals. The toxicity profile for inorganic chemicals should therefore be constructed using effective concentrations based on measured toxicity test data if possible. If no data are available, actual data from the nearest analog can be used.

To construct the toxicity profile:

(1) Collect valid measured data from peer-reviewed on-line data bases such as Hazardous Substance Data Bank (HSDB) or from peer-reviewed open literature sources.

(2) When valid measured data are not available, use SAR estimates if available for the chemical class. The use, application, development, and validation of SARs have been presented in a number of publications (see section on previously published guidance). Computer models that calculate toxicity values based on SARs are also

available (see section on analytical models). The following data hierarchy is preferred for SAR estimates (from lowest to highest):

a) Valid measured data from the nearest analog.
b) Predicted value based on valid measured data from two analogs that bracket the chemical of concern.
c) Predicted value based on regression equation developed from valid measured data for a similar class of compounds.

Details: Step 4, Evaluating Data Quality

The following are examples of data quality checks. An exhaustive data quality evaluation requires expert judgment and experience.

(1) Determine if the effective concentrations are based on mean measured concentrations or nominal concentrations. Data based on mean measured concentrations are preferred, especially for volatile compounds.

(2) Determine if a chemical's physical/chemical properties are consistent with one another and with the chemical's effective concentrations. For example, a chemical with a low K_{ow} value would be expected to have a high water solubility limit. A chemical's LC_{50} value should be less than or equal to its water solubility limit unless it is a self-dispersing compound such as a surfactant. Measured concentrations that significantly exceed the water solubility limit of a compound suggest that the test laboratory may have artificially enhanced the water solubility to a level that cannot be realized in the environment.

(3) Compare the test methods against the chemical's physical/chemical properties. For example, highly water reactive chemicals (as measured by the hydrolysis half-life) should be tested in a flow-through system instead of a static system where pure stock material is added directly to the system. With the static system the test organism may only be exposed to the hydrolysis products.

Details: Step 5, Calculating the CCs

The CC for each chemical in water is calculated using the general equation:

CC = acute or chronic toxicity value ÷ AsF

AsFs are dependent on the amount and type of toxicity data contained in a toxicity profile and reflect the amount of uncertainty about the potential effects associated with a toxicity value. In general, the more complete the hazard profile and the greater the quality of the toxicity data, the smaller the factor used.

One of the following specific equations is used, depending on the availability of data:

a) If the toxicity profile only contains one or two acute toxicity values (no chronic values):

CC = lowest acute value ÷ 1000

b) If the toxicity profile contains three acute values (no chronic values):

CC = lowest acute value ÷ 100

c) If the toxicity profile contains one chronic value:

CC = chronic value ÷ 10, if the value is for the most sensitive species.

Otherwise:

CC = acute value for the most sensitive species ÷ 100

d) If the toxicity profile contains three chronic values:

CC = lowest chronic value ÷ 10

e) If the toxicity profile contains a measured chronic value from a field study:

CC = measured chronic value ÷ 1

Examples from the Screen Reclamation CTSA (EPA, 1994c) are shown in Table 5-13.

Details: Step 6, Ranking Chemicals for Aquatic Toxicity

Chemicals can be ranked for aquatic toxicity according to the following criteria:

a) For chronic values:

≤ 0.1 mg/L .....High
> 0.1 to ≤ 10 mg/L .....Moderate
> 10 mg/L .....Low

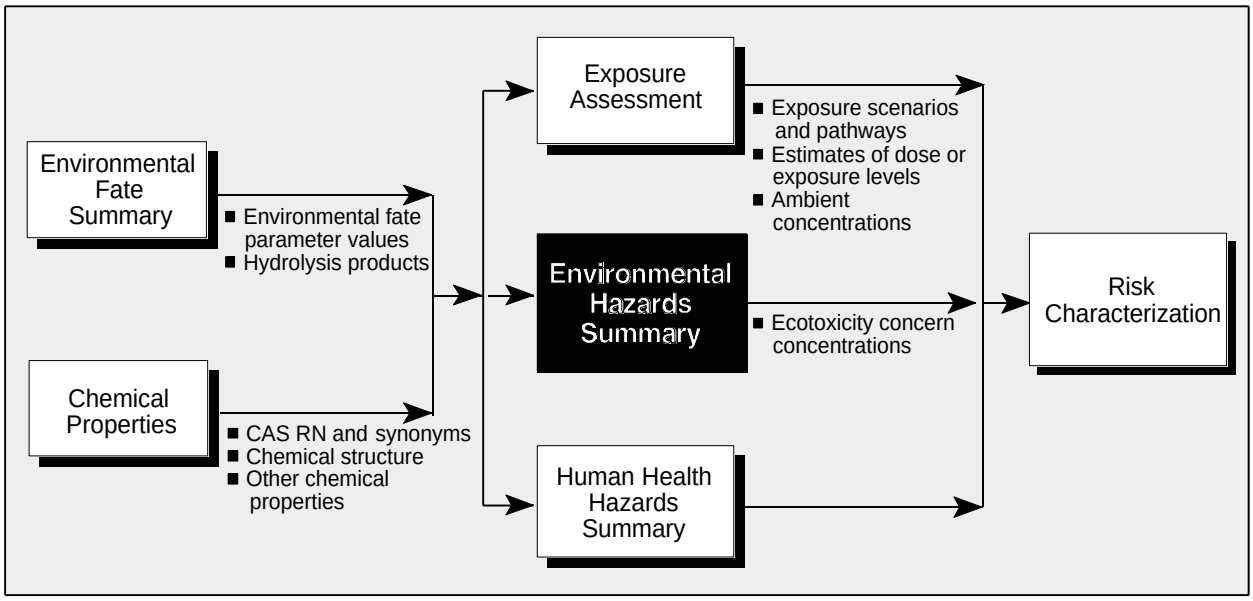
b) For acute values:

≤ 1 mg/L .....High
> 1 to ≤ 100 mg/L .....Moderate
> 100 mg/L .....Low

Chronic toxicity ranking takes precedent over the acute ranking. This relative ranking of toxicity can be used to guide the selection and use of chemicals that are less hazardous to aquatic organisms. Examples from the Screen Reclamation CTSA (EPA, 1994c) are shown in Table 5-13.

FLOW OF INFORMATION: This module can be used alone as a final data point to guide the selection and use of chemicals that are less toxic to aquatic organisms. In a CTSA, this module receives data from the Environmental Fate Summary and Chemical Properties modules and transfers data to the Risk Characterization module. Example information flows are shown in Figure 5-6.

FIGURE 5-6: ENVIRONMENTAL HAZARDS SUMMARY MODULE: EXAMPLE INFORMATION FLOWS



ANALYTICAL MODELS: Table 5-14 presents references for SAR models that can be used to predict aquatic toxicity values. Since different SAR models may provide different or conflicting results, one model should be used consistently throughout a particular CTSA project.

TABLE 5-14: ANALYTICAL MODELS USED IN AQUATIC TOXICITY ASSESSMENT

Reference	Type of Model
Clements, R.G. and J.V. Nabholz. 1994. *ECOSAR: A Computer Program for Estimating the Ecotoxicity of Industrial Chemicals Based on Structure-Activity Relationships; User's Guide.*	PC format analytical model developed within the constraints of the regulatory program office of Office of Pollution Prevention and Toxics (OPPT). Uses SARs to predict acute and chronic ecotoxicity concentrations for daphnid, fish and algae. EPA uses this system exclusively for evaluating new and existing chemicals.

TABLE 5-14: ANALYTICAL MODELS USED IN AQUATIC TOXICITY ASSESSMENT	
Reference	**Type of Model**
Hunter, R.S. and F.D. Culver. 1992. *MicroQSAR Version 2.0: A Structure-Activity Based Chemical Modeling and Information System*.	Personal computer-based system of models. Uses quantitative SARs to estimate chemical properties and aquatic toxicity values.
QSAR: A Structure-Activity Based Chemical Modeling and Information System. 1986.	Available on-line and in PC format. Uses quantitative SARs to estimate chemical properties, environmental fate parameters, aquatic LC_{50} in 7 common test organisms, and NEC in fathead minnow.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.

PUBLISHED GUIDANCE: Table 5-15 presents references for published guidance on environmental toxicity assessment and the use of SARs.

TABLE 5-15: PUBLISHED GUIDANCE ON AQUATIC TOXICITY ASSESSMENT	
Reference	**Type of Guidance**
Clements, R.G., Ed. 1988. *Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure Activity Relationships*.	Describes the use of SARs by EPA OPPT.
Clements, R.G., et. al. 1993a. "The Use and Application of QSARs in the Office of Toxic Substances for Ecological Hazard Assessment of New Chemicals."	Describes the use and application of QSARs for the hazard assessment of new chemicals.
Clements, R.G., et. al. 1993b. "The Use of Quantitative Structure-Activity Relationships (QSARs) as Screening Tools in Environmental Assessment."	Describes the development, validation, and application of SARs in EPA OPPT.
Clements, R.G., Ed. 1994. *Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure-Activity Relationships*.	Describes the use of SARs by EPA OPPT.
Lipnick, R.L. 1993. "Baseline Toxicity QSAR Models: A Means to Assess Mechanism of Toxicity for Aquatic Organisms and Mammals."	Describes the development, validation, and application of SARs in EPA OPPT.
Nabholz, J.V. 1991. "Environmental Hazard and Risk Assessment Under the United States Toxic Substances Control Act."	Detailed discussion of a comprehensive toxicity profile and risk assessment for existing chemicals.

TABLE 5-15: PUBLISHED GUIDANCE ON AQUATIC TOXICITY ASSESSMENT	
Reference	**Type of Guidance**
Nabholz, J.V., et. al. 1993a. "Environmental Risk Assessment of New Chemicals Under the Toxic Substances Control Act (TSCA) Section Five."	Describes the toxicity profile outlined in Step 3.
Nabholz, J.V., et. al. 1993b. "Validation of Structure-Activity Relationships Used by the U.S. EPA's Office of Pollution Prevention and Toxics for the Environmental Hazard Assessment of Industrial Chemicals."	Describes the development, validation, and application of SARs in EPA OPPT.
U.S. Environmental Protection Agency. 1984b. *Estimating Concern Levels for Concentrations of Chemical Substances in the Environment*.	Describes the use of AsFs to determine the CC for a chemical.
Zeeman, M.G. and James Gilford. 1993. "Ecological Hazard Evaluation and Risk Assessment Under EPA's Toxic Substances Control Act (TSCA): An Introduction."	Provides an overview of the process used in the environmental toxicity assessment of chemicals.
Zeeman, M.G., et. al. 1993. "The Development of SAR/QSAR for Use Under EPA's Toxic Substances Control Act (TSCA): An Introduction."	Describes the development, validation, and application of SARs in EPA OPPT.
Zeeman, M.G. 1995a. "EPA's Framework for Ecological Effects Assessment."	Provides an overview of the process used in the environmental toxicity assessment of chemicals.
Zeeman. M.G. 1995b. "Ecotoxicity Testing and Estimation Methods Developed Under Section 5 of the Toxic Substances Control Act (TSCA)."	Describes the development, validation, and application of SARs in EPA OPPT.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.

DATA SOURCES: Table 5-16 lists sources of aquatic toxicity data.

TABLE 5-16: SOURCES OF AQUATIC TOXICITY DATA	
Reference	**Type of Data**
Aquatic Information Retrieval (AQUIRE) Data Base. UNDATED.	Comprehensive data base of measured aquatic toxicity values derived from open literature. Some data not peer-reviewed. Data should be confirmed with original literature citation.

TABLE 5-16: SOURCES OF AQUATIC TOXICITY DATA

Reference	Type of Data
Brooke, L.T., et. al., Ed. 1984 - 1990. *Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas).*	Comprehensive source of measured fish toxicity values for a single species (fathead minnows), including fish LC_{50} data.
Call, D.J. and D.L. Geiger, Eds. 1992. *Sub-chronic Toxicities of Industrial and Agricultural Chemicals to Fathead Minnows (Pimephales promelas).*	Source of measured fish toxicity values for a single species (fathead minnows), including fish EC_{50} data.
HSDB®. Hazardous Substances Data Bank (HSDB). Updated Periodically.	Measured aquatic toxicity values derived from open literature. Peer-reviewed.
U.S. Atomic Energy Commission. 1973. *Toxicity of Power Plant Chemicals to Aquatic Life*.	Aquatic toxicity values for inorganic chemicals.
U.S. Environmental Protection Agency. UNDATEDe. *Ambient Water Quality Criteria Documents*.	Aquatic toxicity values for chemicals for which ambient water quality criteria have been developed. Useful for organic and inorganic compounds.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.