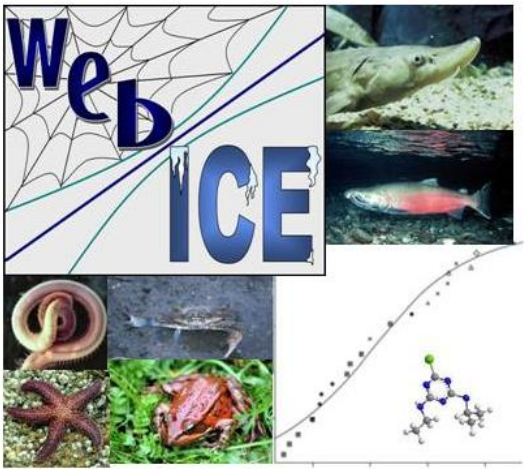
ICE Aquatic Toxicity Database Documentation



Sandy Raimondo, Crystal R. Jackson, and Mace G. Barron

April 10, 2013

U.S. Environmental Protection Agency
Office of Research and Development
National Health and Environmental Effects Research Laboratory
Gulf Ecology Division
Gulf Breeze, Fl 32561

ICE Aquatic Toxicity Database Quality Assurance Report

Table of Contents

1 Introduction 3
2 Data Sources 3
2.1 ECOTOX 3
2.2 Ambient Water Quality Criteria (AWQC) 4
2.3 Office of Pesticide Program Ecotoxicity Database 4
2.4 OPPT Premanufacture Notification (PMN) 4
2.5 High Production Volume (HPV) 5
2.6 Mayer and Ellersieck 1986 5
2.7 ORD 5
2.8 Open Literature 6
3 Master Database QC and Acceptance Criteria 6
3.1 Chemicals 7
3.1.1 Active Ingredient and Mixtures 7
3.1.2 Chemical names and CAS QA/QC 7
3.2 Organism 8
3.3 Test Conditions 8
3.4 Toxicity Values 9
3.4.1 Concentrations and Units 9
3.4.2 Data normalization 9
4 Standardization for ICE Models 10
4.1 Life stage 10
4.2 Freshwater (FW) or Saltwater (SW) Water Type 11
4.3 Temperatures 11
4.4 Dissolved Oxygen 11
4.5 Check for outliers 11
5 Quality Assurance and Control 12
6 Data fields 12
7 References 12
Appendix A 14
Appendix A-1. Total number of records collected and retained by source for database version 3.1 14
Appendix A-2. Process for preparing Ecotox downloads for inclusion into the database. 15
Appendix A-3. List of AWQC documents and publication years entered into the database 18
Appendix A-4. Cover sheet for open literature sources 19
Appendix A-5. Bibliography of references in database obtained from open literature. 20
Appendix A-6. Acceptable Chemical Grades with purities > 90% from Ecotox 23
Appendix A-7. List of elements and their associated compounds 24
Appendix A-8. Age classifications used to designate life stage in the database. 26
Appendix A-9. Temperature ranges used to standardize species in the model data subset. 31
Appendix A-10. List of data fields in master database 35
Appendix B. Algae ICE Module; Beta Technical Basis of the Development of Algae ICE Models for Web-ICE 36

1 Introduction

This document describes the compilation, review, standardization, and quality assurance/quality control (QA/QC) of the ICE Aquatic Toxicity Database (herein, database) developed and maintained by the US EPA Gulf Ecology Division. The database is composed of acute toxicity records for aquatic animal species and is used in the development of toxicological models that include, but may not be limited to, Interspecies Correlation Estimation (ICE) models (Raimondo et al., 2010), Species Sensitivity Distributions (SSDs) (Barron et al. 2012), and Quantitative Structure-Activity Relationship (QSAR) models. ICE models are least squares regressions of the relative sensitivity between the taxa of interest and that of a surrogate species (e.g., standard test species). Validated ICE models are available on the US Environmental Protection Agency (US EPA) internet application, Web-based Interspecies Correlation Estimation (Web-ICE) (http://www.epa.gov/ceampubl/fchain/webice/index.html). SSDs are cumulative probability distributions of toxicity values for multiple species that may be used to derive a hazard level for ecological risk assessment based on a specified percentile of the distribution. QSARs are regression models describing the relationship between chemical structures and biological activity and can be used to predict activity of new chemicals.

A separate database is maintained for algae toxicity data, the documentation for which is listed in Appendix B.

The document is organized by section, including: the project organization (Section 2), data sources used in developing the ICE database (3), the quality acceptance criteria applied to the master database (4), data normalization (5), additional standardization applied to data used in ICE models (6), quality assurance and control procedures (7), database organization (8), and technical appendices.

2 Data Sources

The database is composed entirely of secondary data (data previously collected for a different intended use). This section describes each data source in detail, its acquisition, and format. Data sources include both electronic and hard-copy formats. Hard-copy sources are entered into separate excel files identified by source(s) and original hardcopies are retained by the database manager or placed in the project study file. Those received electronically are saved as original, unaltered files and housed on a GED network drive. All data sources go through an extensive review process to ensure that each record meets acceptance criteria. A summary of the number of records from each data source are in Appendix A-1, which will be updated with each version of the database.

2.1 ECOTOX

The ECOTOXicology database (http://cfpub.epa.gov/ecotox/), developed by the USEPA/ORD/NHEERL Mid Continent Ecology Division, provides chemical toxicity information for aquatic organisms, terrestrial plants, and wildlife. It consists of toxicity data predominately from peer-reviewed literature, although there are some EPA records within the database as well. To obtain records for the database, ECOTOX is queried for acute, aquatic, animal records, which are downloaded in excel format. The procedure for preparing ECOTOX downloads for inclusion into the database is provided in Appendix A-2.

2.2 Ambient Water Quality Criteria (AWQC)

EPA is required by the Clean Water Act (Section 304(a)(1)) to develop criteria for water quality that accurately reflects the latest scientific knowledge. These criteria are based on data and scientific judgment on pollutant concentrations and environmental or human health effects. EPA's compilation of national recommended Ambient Water Quality Criteria (AWCQ) are published and publically available sources of toxicity data for fresh and saltwater organisms that maybe exposed to surface water pollutants. Data was compiled from 69 AWQC documents published from 1987 -2009 (Appendix A-3). Minimum data provided from the document's Table 1 are chemical name, species tested, water type, test and concentration type (e.g. static, measured), and toxicities (EC/LC50). Additional information provided by some documents include active ingredient, age, hardness, pH and corrected toxicity values for metals. Toxicity data are entered if records meet database acceptance criteria.

2.3 Office of Pesticide Program Ecotoxicity Database

The Office of Pesticide Program's Environmental Fate and Effects Division (EFED) Ecotoxicity database contains published and registrant submitted toxicity data for pesticides. Their database was acquired for this project in January 2007 and contained acute and chronic toxicity records for both aquatic and wildlife organisms. Data fields include chemical information, active ingredient, use category, taxa, test organism, test organism age, test conditions, toxicity values, and acceptance category (i.e. acceptable, supplemental). Water quality parameters are not provided, however each study is evaluated by EFED for conformance to OPPTS guidelines. Studies that contain major deviations from guidelines that affected the scientific integrity of the study are classified as unacceptable. Supplemental studies are those that are generally well conducted and employed Good Laboratory Practice, but the study did not meet all requirements listed for satisfaction of the FIFRA testing requirements (e.g. raw data not submitted). Core studies meet all FIFRA testing requirements, are well conducted, and all reported endpoints are validated by independent statistical analysis Only core and supplemental data are accepted into the database and receive an additional level of QA/QC outlined in Section 4.0.

2.4 OPPT Premanufacture Notification (PMN)

Premanufacture Notification (PMN) data that is submitted to EPA under the Toxic Substance Control Act (TOSCA) is Confidential Business Information (CBI). GED personnel with CBI

certifications obtain PMN toxicity data summaries in pdf format. Those data that meet the database acceptance criteria are entered into excel spreadsheets. Information includes chemical tested, species information and toxicities. In accordance with CBI procedures, the chemical identities are masked and data are not identifiable by chemical name and CAS number in files accessible by network connections. To censure data, a confidential identifier number (CIN) less than 100 (e.g., 1, 2, 3) is assigned to each CBI chemical in place of the chemical CAS, and a letter assigned in place of the chemical name. All chemicals with that same CAS number, regardless if they were CBI, are also assigned the same CIN in the database to allow development of ICE models while maintaining CBI requirements.

.

2.5 High Production Volume (HPV)

Under the High Production Volume (HPV) Challenge Program, companies make health and environmental effects data publicly available on chemicals produced or imported in the United States in quantities of 1 million pounds or more per year. HPV chemicals and associated information are publically available through the EPA (www.epa.gov/HPV/) as downloadable pdf documents for each chemical. HPV toxicity studies are encouraged to follow Good Laboratory Practice (GLP) and report test quality information for each chemical/species tested. Information obtained included chemical information and active ingredients, species information, toxicities, test information and water quality parameters. In addition, notes on test guidance were included (i.e. ASTM, OECD 203). Questionable data (i.e. missing information, species name errors) were not included into the database.

2.6 Mayer and Ellersieck 1986

The "Manual of Acute Toxicity: Interpretation and Data Base for 410 Chemicals and 66 Species of Freshwater Animals" is a compilation of records for freshwater aquatic organisms assembled to assess the influence of test conditions and physical, biological, and chemical properties on species sensitivity. Tests were conducted at the Columbia National Fisheries Research Laboratory (U.S. Department of Interior) from 1965-1984. The manual includes 4901 tests and provides information on chemicals tested, active ingredients, species and age information, test conditions, toxicities (EC/LC50), temperature, pH and hardness.

2.7 ORD

Mayer 1987. "A Handbook of Acute Toxicity Tests of Estuarine Organisms" includes toxicity tests conducted at the Gulf Ecology Division of the U.S. EPA Office of Research and Development (ORD) from 1961-1986. Data include chemical tested, active ingredient, species tested and age, test conditions, toxicities, temperature and salinity.

Mayer et al. 2008. This U.S. EPA report contains acute toxicity for 29 endangered and surrogates species using five chemicals. The report provided chemical and species information, toxicities, test conditions.

2.8 Open Literature

Data from published studies that are not currently in ECOTOX are acquired for taxa of interest (e.g. mussels, endangered species). Each published study is assigned a reference number and an evaluation sheet is used to determine study acceptability (Appendix A-4). Careful review of each source determines if the information meets acceptance criteria. The source must provide chemical tested, active ingredient, test species, age, test conditions, and toxicity. In addition temperature and dissolved oxygen or indication that an appropriate test guidelines was used (i.e. ASTM) must be provided. Appendix A-5 provides a list of peer reviewed studies included in the database.

3 Master Database QC and Acceptance Criteria

Data are only included in the database if they adhere to pre-determined acceptance criteria. These criteria evaluate test organisms (e.g., taxa, species confirmation), test chemicals (e.g. active ingredient), test duration and reported toxicity endpoint (e.g. mortality). The original source of data must clearly provide adequate information to assess these criteria for inclusion.

Data are subjected to two rounds of filtering; 1) first round filter for general criteria which determined data suitability for primary database, described in this Section and 2) second round filter for species-specific test conditions which determined data suitability for ICE model subset detailed in Section 5. It should be noted that some records included in hard copy data (e.g. Mayer and Ellersieck 1986) were not entered into electronic format if they did not meet some of the standardization criteria (e.g. active ingredient $\geq$ 90%) described below.

Standardization/quality criteria that are applied to all data sources in the first round of filtering are summarized in Table 1 and described in Sections 4.1- 4.4.

Table 1. Checklist of standardization criteria for inclusion into primary database.

Category	Data Information	Criteria
Chemical	Identity	Reported CAS, name or structure confirmed
		CAS corresponds to single compound or element
	Compound	Mixtures excluded except for chemical salts and specific congener mixtures[1]
	Purity	Active ingredient $\geq$ 90%
	Grade	If Purity is "NR", test grade must be one listed in Appendix A-6
	Name	Synonyms conformed to ICE chemical name

Category	Data Information	Criteria
Organism	Species	Fish, invertebrates, amphibians Name & taxonomy verified
	Life stage	Eggs excluded
Test Conditions	Test Media	Aquatic (FW/SW identified)
	Exposure type	F, S, SR (no sediment, dietary, mixed dose or phototoxicity)
	Exposure duration	Acute; 48 & 96 hrs
	Endpoint	EC50 or LC50
	Measurement	Mortality or immobility only
	Test Location	Laboratory only
Toxicity Value	Concentration	> or < excluded
	Units	ug/L, converted if needed
	Chemical Normalization[2]	PCP to pH 6.5 Ammonia to TAN[3] pH 8; Metals[4] to hardness 50 mg/L
	Element Normalization[5]	Ag, Al, Cu, Cd, Co, Cr(III), Cr(VI), Hg, NH4, Ni, Pb, Zn

[1] Included metal and other chemical salts, and specific congener mixtures (e.g., standard Aroclors, toxaphene)
[2] FW only, normalized according to AWQC
[3] Total Ammonia Nitrogen
[4] Ag, Cu, Cd, Cr(III), Pb, Ni, Zn
[5] Metals reported as salts were normalized to element

3.1 Chemicals

3.1.1 Active Ingredient and Mixtures

Inclusion of chemicals in the database required that the chemical tested have an active ingredient purity of ≥90%. This is determined from either the reported purity or the source/grade of the tested compound. Chemicals whose purity is not reported are accepted if the reported chemical grade is listed in Appendix A-6. If the chemical purity or grade is not reported or could not be determined through internet searches of commercial products, the record was not included. Mixtures are excluded, except for tests of single chemical salts and specific congener mixtures such PCB, Arochlors, and toxaphene. Any degredates and metabolites are also excluded unless they are identified as the tested compound (e.g., met identity and purity requirements). Formulations of chemicals are excluded unless they contained 90% or greater of the test compound as the active ingredient.

3.1.2 Chemical names and CAS QA/QC

Each toxicity record in the database required a Chemical Abstracts Service (CAS) registry number or a chemical name for the compound tested. A toxicity record is only included if the source provides sufficient information to identify the test compound (e.g., chemical name, formula, smiles string, CAS). CAS and chemical name congruency are checked and/or assigned using two public domain databases: the Allanwood Compendium of Pesticides (http://www.alanwood.net/pesticides/) and Chemical Book (http://www.chemicalbook.com). The CAS and name associated with each toxicity record are entered into the database as either the tested compound or as the element for specific metals (Appendix A-7). For records where CAS and chemical name are inconsistent or uncertain, additional internet sources, such as PubMed Compound (http://www.ncbi.nlm.nih.gov/pccompound), are consulted. The CAS or chemical name is either corrected or, in the case of uncertain chemical identity, the record removed.

Chemical name as reported in the original source is maintained in the database, as well as the assignment of an ICE chemical name for synonym control. A separate database is maintained for quality control (QC) of chemical name, synonyms and CAS numbers, as well as mode of action (MOA) and chemical class assignments. For complete description of MOA assignments see the Operating Procedure for developing the chemical information with the database (OP-GED/BPRB/MGB/2009-01-002/June 23, 2009). In brief, all chemicals are placed into one of 29 chemical class categories based on a review of chemical structure. Each chemical is run through ASTER (ASessment Tools for the Evaluation of Risk) to identify MOA based on the mode of acute toxicity in the fathead minnow and the structural fragments present in the chemical (Russom et al., 1997; EPA, 2007). Chemicals are assigned broad MOA (e.g. AChE inhibition) and specific MOA (e.g. OP-mediated AChE inhibition). Data fields in the chemical database included ICE chemical name, synonym(s), CAS, identification of mixtures, ASTER MOA assignment, broad and specific MOA assignments, and chemical class assignment.

3.2 Organism

The aquatic database contains only animal records and excludes the embryo and egg stages. Data sources must provide either common name and/or species names of the organisms tested. Verification of species, genus and family names is performed with the Integrated Taxonomic Information System (ITIS; www.itis.gov). If verification cannot be found in ITIS, other public domain internet websites are used (i.e. www.fishbase.com). Species names that cannot be verified are excluded. After verification, species are grouped into broader taxonomic categories (e.g., fish, crustacea). If only a common name is provided that is too general to determine species, genus and family (i.e. Ostracod, Amphipod) then the record is not included. Any organism that could only be verified at or is tested at taxonomic level of Order or higher was not included. Test organisms identified by only genus or family are accepted. Species synonyms are changed to reflect the most current nomenclature and common name.

3.3 Test Conditions

No sediment, dietary, mixed dose exposures**,** or photo-enhanced toxicity results are included in the database. The databases includes exposure types: static (S), flow through (F), static renewal (SR). Toxicity values reported as both measured (M) and nominal/unmeasured (N/U) are included. Acute toxicity results must be either immobilization (EC50) or mortality (EC/LC50). Test durations accepted were 48h and 96h tests.

Each species is designated as freshwater (FW) or saltwater (SW; estuarine or marine) based on the salinity of the test media and general knowledge of the species habitat requirements. If water type cannot be determined, records are designated as not reported (NR). Toxicity records classified as FW are stenohaline FW species or where reported test salinity is ≤ 1 ppt. Records classified as SW are SW species or where the salinity recorded is > 1 ppt.

3.4 Toxicity Values

3.4.1 Concentrations and Units

Open-ended toxicity values (i.e. > 100 mg/kg or <100 mg/kg) are excluded. All toxicity records are converted to µg/L (Table 2). If units could not be determined, the toxicity records are not included.

Table 2 Toxicity units and conversion factors

Unit	Alternate name	Conversion to ug/L
µg/L	PPB	= µg/L
mg/L	PPM	=mg/L * 1000
ng/L	PPT	= ng/L/ 1000
µmol/L	micromolar	= (µmol/L)*MW

3.4.2 Data normalization

The AWQC documents outline normalization procedures for pentachlorophenol (normalized to pH 6.5), ammonium compounds (converted to total ammonia nitrogen at pH 8) and specific metal salts (hardness of 50 mg/L CaC03; reporting as metal element). These normalizations are applied to records for these compounds prior to inclusion into the database according to the Operating Procedure for normalizing and reporting toxicity values for pentachlorophenol, and specific metal and ammonium compounds (OP-GED/BPRB/DNV/2009-03-002 October 1, 2009). Large metal salts (molecular weight >200) are not normalized because of uncertainty in the relationship between their toxicity, hardness, and dissociation, and are treated as separate compounds in the database.

4 Standardization for ICE Models

Data are further standardized for the development of ICE models to ensure models reflect species sensitivity and contained minimal extraneous variation. Toxicity records that meet these requirements are designed as a "Yes" in the "Meets model requirements" column. This section explains the additional standardization for data used to develop ICE models (herein, model data subset), summarized in Table 3.

Table 3. Standardization criteria for data included in ICE model development

Component	Information required	Acceptance requirements
Test organism	Life stage[1]	juvenile only: fish, amphibians, insects, mollusks[2], decapods all life stages: all other species
Test conditions	Test duration	48 hr: daphnids, midges, mosquitoes
		96 hr: all other species
	Temperature[3]	species specific (± 3C)
	Dissolved oxygen	Static: ≤48 hr 60-100%; >48 hr 40-100%. Static renewal or flow-through: 60-100%.
	Salinity	<1 ppt: FW species[4] 1-5ppt: *Cyprinodon bovinus* ≥15 ppt: SW species[5]

[1] if life stage not reported, determined through reported age/size; Appendix A-8
[2] glochidia excluded
[3] based on ASTM and equivalent test guidelines for test species; Appendix A-9
[4] Salmonid tests included are freshwater
[5] Striped bass (*Morone saxatilis*) tests are saltwater

4.1 Life stage

The life stage of each species is broadly defined as larvae, juvenile, or adult. Only the juvenile stages of fish, amphibians, mollusks, decapods and aquatic insects are used in the model data subset. For all other species, all life stages (except egg and embryo) are included. A specified life stage is recorded as reported in the original source. If a specific stage is not identified in the original source, life history and organism size are used to determine life stage (Appendix A-8). Fish larvae include hatchlings through full fin development. Juvenile fish are those with full fin development lacking sexual maturity, and adult fish are those that are sexually mature. In cases where only a weight is provided for a fish species, life stage is determined using length-weight regressions in the Fish Base Life History Tool (Froese and Pauly 2008). When length-weight regressions are not available or adequate information is not provided, age class is designated as

unknown. Records with an "unknown" life stage designation are only included in the model data subset for those species where all life stages are included, and where the egg and embryo stage can be ruled out.

4.2 Freshwater (FW) or Saltwater (SW) Water Type

Only records designated as a FW water type or a SW water type with ≥15 ppt salinity are included in the ICE model subset, with the following specific exceptions. Only FW records for salmonid species are accepted to limit potential variability due to wide differences in test salinity for these euryhaline species. Only SW records for striped bass (*Morone saxatilis*) are accepted because of their juvenile life history characteristics. Only SW records for *Cyprinodon bovinus* with a salinity of 1 to 5 ppt were retained based on life history.

4.3 Temperatures

To limit variability associated with temperature, a 6 °C range (+/- 3°C) of temperatures optimal for each species was chosen based on standard test guidelines where provided, or life history where guidelines did not specify species-appropriate conditions. This range was chosen because (1) acceptable within-test temperature is typically +/-2 ° C and (2) it maximized data retention while maintaining a relatively narrow temperature range. Temperature ranges were generally consistent with ASTM and OPPTS recommend test ranges (Appendix A-9).

4.4 Dissolved Oxygen

Dissolved oxygen (DO) must be reported for inclusion into the model data subset. Where necessary, DO values are converted to % saturation to verify compliance with ASTM standards. Conversions to % saturation are calculated as:

$$\text{DO (\% saturation)} = \frac{\text{measured DO (mg/L)}}{\text{DO (mg/L at 100 \% saturation and 760 mm Hg)}} \times 100$$

Only records that met ASTM (2007) dissolved oxygen requirements are included in the model data subset:

- S tests ≤ 48h, 60-100%;
- S tests > 48 h, > 40% saturation;
- F or SR tests, > 60% saturation.

4.5 Check for outliers

When more than one toxicity value is available for a chemical and species using the standardization criteria for model development outlined in this section, the ratio of the maximum

and minimum values is calculated. Toxicity records with max/min ratios greater than 10 are examined for outliers and original sources of the data consulted. For example, if an outlier data record was obtained from ECOTOX, the original published research article that was entered into ECOTOX was obtained and checked. Outliers identified through this process to be questionable are removed. If an outlier cannot be determined, such as if only two records exist for a species and chemical and neither appear to be derived from poor quality studies, than all data records are retained, but excluded from model development within the model building algorithm.

5 Quality Assurance and Control

All records in the database are subjected to strict quality assurance and control in accordance to the Quality Assurance Project Plan (QAPP-GED/BPRB/JA/2012-01-001 January 17, 2012). Once all standardization is complete, duplicate records are identified and removed. Duplicate records are defined by having the same CAS, species, age and toxicity value.

6 Data fields

The data fields and associated code definitions included in the database are outlined in Appendix A-10.

7 References

Barron MG, Jackson CR, Awkerman JA. 2012. Evaluation of an *in silico* approach to developing aquatic toxicity species sensitivity distributions. Aquat Toxicol.

Froese, R. and D. Pauly. Editors. 2008.FishBase. World Wide Web electronic publication. http://www.fishbase.org/

Mayer, F.L.1987. Acute toxicity handbook of chemicals to estuarine oganisms. EPA/600/8-87/017. Gulf Breeze, Fl.

Mayer, F.L., D.R. Buckler, F.J. Dwyer, M.R. Ellersieck, L.C. Sappington, J.M. Besser, and C.M. Bridges. 2008. Endangered aquatic vertebrates: comparative and probabilistic based toxicology. EPA/600/R-08/045. Gulf Breeze, Fl.

Raimondo, S., C.R. Jackson, M.G. Barron. 2010. Influence of taxonomic relatedness and chemical mode of action in acute interspecies estimation models for aquatic species. Environmental Science and Technology. 44: 7711-7716.

Russom, C.L., S.P. Bradbury, S.J. Broderius, D.E. Hammermeister and R.A. Drummond. 1997. Predicting modes of toxic action from chemical structure: Acute toxicity in the fathead minnow (Pimephales promelas). Environ Toxicol Chem. 16: 948-967.

U.S. EPA (1986) Quality criteria for water. EPA 440/5-86-001. Washington, DC.

U.S. EPA. 2007. ECOTOX User Guide: ECOTOXicology Database System. Version 4.0. Available: http:/www.epa.gov/ecotox/

Appendix A

Appendix A-1. Total number of records collected and retained by source for database version 3.1.

Data Source	# records obtained	# records in database	Dates
AWQC	4453	4444	See Appendix A-3 for document and year
Mayer et al. 2008	87	87	2008
ECOTOX	285,799	9082	Last download March 2011
HPV	4706	465	Downloaded Feb 2008
Literature	586	209	1976-2008
Mayer 1987	375	367	1987
Mayer and Ellersieck 1986	2737	2730	1986
OPP	19382	2356	January 2007
OPPTS_PMN	111	61	December 2007
Total	318,236	19,801	

Appendix A-2. Process for preparing Ecotox downloads for inclusion into the database.

ECOTOX Columns	ICE Column	Concatenate or Delete Columns	Notes
Test Number	Dsource specific	Add ECO before #	Designates ECOTOX as original source in ICE database
CAS Number	cas reported	---	---
Chemical Name	chemical tested	---	---
Chemical Grade & Chemical Purity	AI	Concatenate: Purity (Grade)	Delete records with <90 Purity or Grades not in Appendix 6
Chemical Formulation	---	Deleted Column	---
Chemical Comment	---	---	---
Species Number	---	Deleted Column	---
Species Scientific Name	Species	---	---
Species Common Name	common name	---	---
Species, Kingdom, Phylum, Sub Phylum, Superclass, Class, Order	---	Deleted Columns	---
Species Family	Family	---	---
Species Genus	Genus	---	---
Organism Age, Age Units, Organism Lifestage, Organism Comment	age	Concatenate: Organism Age Units, Lifestage (Comment)	Delete records with codes EG, EM, BL
Endpoint	Dose Type	---	Delete EC50s for verts
Effect, Effect Measurement	---	Concatenate: Effect (Meas)	Only keep codes ITX(IMBL), ITX (MBLT), MOR (MORT), MOR (SURV). Use code list to idenitify other acceptable codes.
Exposure Type	Test Type	---	Only keep codes F, S, R

Chemical Analysis	Concentration Type	---	---
Exposure Duration Op (Days)	---	---	Delete Records with Operators (>,<,~)
Exposure Duration, Units	Test duration	Concatenate: Duration Unit	Only keep 2 or 4 d, 48 or 96 hr
Exposure Duration Min Op, Min, Max OP, Max	---	Deleted Column	---
Conc 1 Type, Ionic Fraction 1	---	Concatenate: Type, Fraction	Use for conversions
Conc 1 Op (ug/L)	---	---	Delete Records with Operators (>,<,~)
Conc 1 (ug/L)	---	---	Deleted NR
Conc 1 Min Op, Min 1, 1 Max OP, 1 Max	---	---	Deleted record with conc ranges (min and max)
Conc 2 Type, Ionic Fraction 2	---	Concatenate: Type, Fraction	Use for conversions
Conc 2 Op (ug/L)	---	---	Delete Records with Operators (>,<,~)
Conc 2 (ug/L)	---	---	Moved records with 2nd conc to another tab.
Conc 2 Min Op, Min 2, 2 Max OP, 2 Max	---	---	Deleted record with conc ranges (min and max)
Conc Units (ug/L)	---	---	Applies to both Conc 1 and 2. Moved those with non-ug/L units to another tab
Media Type	Water type	---	---
Test Location	---	Deleted Column once only lab records remained.	Only kept records with Lab test.
Temperature Mean Op, Mean, Min OP, Min, Max OP, Max, Units	Temp	Concatenate: OP Mean (OP Min-OP Max) Units	---

Hardness Mean Op, Mean, Min OP, Min, Max OP, Max, Units	Hardness	Concatenate: OP Mean (OP Min-OP Max) Units	---
pH Mean Op, Mean, Min OP, Min, Max OP, Max	pH	Concatenate: OP Mean (OP Min-OP Max)	---
Salinity Mean Op, Mean, Min OP, Min, Max Op, Max, Units	Salinity	Concatenate: OP Mean (OP Min-OP Max) Units	---
Dissolved Oxygen Mean Op, Mean, Min OP, Min, Max OP, Max, Units	Dissolved Oxygen	Concatenate: OP Mean (OP Min-OP Max) Units	---
General Comments	---	---	---
Author, Title, Source, Publication Year, Reference Number	---	Concatenate: Author. (Year) Title. Source. (ECOTOX Ref #)	---

Appendix A-3. List of AWQC documents and publication years entered into the database

Document Name	Year	Document Name	Year
AWQC updates	1999	Dichloroprpane/propenes	1980
2,4-dichlorophenol	1980	Dinitrotoluenes	1980
2,4-dimethylphenol	1980	Diphenylhydrazine	1980
2-chlorophenol	1980	Endosulfan	1980
Acenaphthene	1980	Endrin	1980
Acrolein	1980	Ethylbenzene	1980
Acrylonitrile	1980	Fluoranthene	1980
Aldrin/Dieldrin	1980	Haloethers	1980
Aluminum	1988	Halomethanes	1980
Ammonia	1989, 1999	Heptachlor	1980
Antimony	1980	Hexachlorobutadiene	1980
Arsenic	1984	Hexachlorocyclohexane	1980
Atrazine	2003 draft	Hexachlorocyclopentadiene	1980
Benzene	1980	Isophorone	1980
Benzidine	1980	Lead	2008 Draft
Beryllium	1980	Mercury	1984
Cadmium	2001	Naphthalene	1980
Carbon tetrachloride	1980	Nickel	1986
Chlordane	1980	Nitrobenzene	1980
Chloride	1988	Nitrophenols	1980
Chlorinated benzenes	1980	Nitrosamines	1980
Chlorinated ethanes	1980	Nonylphenol	2005
Chlorinated napthalenes	1980	Parathion	1986
Chlorinated phenols	1980	Pentachlorophenol	1986
Chlorine	1984	Phenol	1980
Chloroalkyl ethers	1980	Phthalate esters	1980
Chloroform	1980	Selenium	2004 Draft
Chlorpyrifos	1986	Silver	2007 update
Chromium	1984	Thallium	1980
Copper	1984	Toluene	1980
DDT	1980	Toxaphene	1986
Diazinon	2005	Tributyltin	2003
Dichlorobenzenes	1980	Trichloroethylene	1980
Dichloroethylenes	1980	Zinc	1987

Appendix A-4. Cover sheet for open literature sources

Citation: _____ **Ref number** _____

_____

Chemical:

CAS: _____ **Purity:** _____

ASTM guidelines: _____

Species: _____

_____

_____

Age: _____

Water Type:	Freshwater	Saltwater	
Test Type	Static	Flowthrough	Static Renewal
Concentration	Measured	Unmeasured (nominal)	NR
Study time	48h	96h	
Dosetype	LC50	EC50	
Toxicity (and units)			_____
Water Quality:	Temp _____	Hardness _____	
	pH _____	Salinity _____	

Notes: _____

_____

_____

Appendix A-5. Bibliography of references in database obtained from open literature.

Adams WJ, Biddinger GR, Robillard KA, Gorsuch JW. 1995. A summary of the acute toxicity of 14 phthalate esters to respresentative aquatic organisms. *Environ Toxicol Chem* 14(9) 1569-1574.

Augspurger T, Keller AE, Black MC, Cope WG, Dwyer FJ. 2003.Water quality guidance for protection of freshwater mussels (Unionidae) from ammonia exposure. *Environ Toxicol Chem* 22 (11): 2569-2575.

Bentley RE, Dean JW, Ells SJ, Hollister TA, LeBlanc GA, Sauters S, Sleight BH. 1977. Laboratory evaluation of the toxicity of cyclotrimethylene trinitramine (RDX) to aquatic organisms. Final Report US Army Medical Research and development Command, Frederick Maryland Contract No: DAMD-17-74-C-4101.

Beyers DW, Keefe TJ, Carlson CA. 1994. Toxicity of carbaryl and malathion to two federally endangerd fishes, as estimated by regression and anova. *Environ Toxicol Chem* 13: 101-107.

Bills TD, Marking LL, Dawson VK, Rach JJ. 1988. Effects of Environmental factors on the toxicity of Chloramine-T to fish. United States Fish and Wildlife Service, Investigations in Fish Control 96.

Brecken-Folse JA, Mayer FL, Pedigo LE, Marking LL. 1994. Acute toxicity of 4-nitrophenol, 2,4-dinitrophenol, terbufos and trichlorfon to grass shrimp (*Palaemonetes* spp.) and sheepshead minnows (*Cyprinodon variegatus*) as affected by salinity and temperature. *Environ Toxicol Chem* 13: 67-77.

Bringolf RB, Cope WG, Eads CB, Lazaro PR, Barnhart MC, Shea D. 2007. Acute and chronic toxicity of technical-grade pesticides to glochidia and juveniles of freshwater mussels (Unionidae). *Environ Toxicol Chem* 26(10): 2086-2093.

Bringolf RB, Cope WG, Barnhart MC, Mosher S, Lazaro PR, Shea D. 2007. Acute and chronic toxicity of pesticide formulations (Atrazine, Chlorpyrifos, and Permethrin) to glochidia and juveniles of *Lampsilis siliquoidea*. *Environ Toxicol Chem* 26(10): 2101-2107.

Buhl KJ, Hamilton SJ. 1996. Toxicity of inorganic contaminants, individually and in environmental mixtures, to three endangered fishes (Colorado squawfish, bonytail, razorback sucker). *Arch. Environ. Contam. Toxicol*. 30: 84-92.

Burton DT, Turley SD, Peters GT. 1994. The acute and chronic toxicity of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) to the fathead minnow (Pimephales promelas). Chemosphere 29(3) 567-579.

Colombo I, de Wolf W, Thompson RS, Farrar DG, Hoke RA, L'Haridon J. 2008. Acute and chornic aquatic toxicity of ammonium perfluorooctanoate (APFO) to freshwater organisms. *Ecotox Environ Safety* 71: 749-756.

Cripe, GM. 2006. Contaminated sediment testing with the bivalve *Mulina lateralis*: culture refinement for organism availability. *Environ Toxicol Chem* 25(5): 1332-1336.

Daly HR, Campbell IC, Hart BT. 1990. Copper toxicity to *Paratya australiensis*: I. Influence of nitrilotriacetic acid and glycine. *Environ Toxicol Chem* 9: 997-1006.

Daly HR, Campbell IC, Hart BT. 1990. Copper toxicity to *Paratya australiensis*: II. Influence of bicarbonate and ionic strength. *Environ Toxicol Chem* 9: 1007-1011.

Dwyer FJ, Mayer FL, Sappington LC, Buckler DR, Bridges CM, Greer IE, Hardesty DK, Henke CE, Ingersoll CG, Kunz JL, Whites DW, Augspurger T, Mount DR, Hattala K, Neuderfer GN. 2005. Assessing contaminant sensitivity of endangered and threatened aquatic species: Part I. Acute toxicity of five chemicals. *Arch Environ Contam Toxicol* 48: 143-154.

Ferrari A, Anguiano OL, Soleno J, Venturino A, Pechen de D'Angelo AM. 2004. Different susceptibility of two aquatic vertebrates (*Oncorhynchus mykiss* and *Bufo arenarum*) to azinphos methyl and carbaryl. *Comp Biochem Physiol* Part C 139: 239-243.

Frias-Espericueta MG, Abad-Rosales S, Nevarez-Valazquez AC, Osuna-Lopez I, Paez-Osuna F, Lozano-Olvera R, Voltolina D. 2008. Histological effects of a combination of heavy metals on Pacific white shrimp *Litopenaeus vannamei* juveniles. *Aquatic Toxicology* 89: 152-157.

Giarratano E, Comoglio L, Amin O. 2007. Heavy metal toxicity in *Exosphaeroma gigas* (Crustacea, Isopoda) from the coastal zone of Beagle Channel. *Ecotox and Environ Safety* 68: 451-462.

Gillis PL, Mitchell RJ, Schwalb AN, McNichols KA, Mackie GL, Wood CM, Ackerman JD. 2008. Sensitivity of the glochidia (larvae) of freshwater mussels to copper: Assessing the effect of water hardness and dissolved organic carbon on the sensitivity of endangered species. *Aquatic Toxicology* 88: 137-145.

Hansen JA, Lipton J, Welsh PG. 2002. Relative sensitivity of bull trout (*Salvelinus confluentus*) and rainbow trout (*Oncorhynchus mykiss*) to acute copper toxicity. *Environ Toxicol Chem* 21(3):633-639.

Hedtke SF, West CW, Allen KN, Norberg-King TJ, Mount DI. 1986. Toxicity of pentachlorophenol to aquatic organisms under naturally varying and controlled environmental conditions. *Environ Toxicol Chem* 5: 531-542.

Little EE, Calfee RD. 2008. Toxicity of chlorine and copper to rainbow trout and to white sturgeon from the Kootenai River and Columbia River. Administrative Report for US Fish and Wildlife Service

Macken A, Giltrap M, Foley B, McGovern E, McHugh B, Davoren M. 2008. A model compound study: the ecotoxicological evaluation of five organic contaminants employing a battery of marine bioassays. *Environmental Pollution* 153: 627-637.

Mallatt J, Barron MG. 1988. High tolerance of lampreys to Kepone toxicity. *Arch. Environ. Contam. Toxicol.* 17: 73-80.

Mallatt J, Barron MG, McDonough C. 1986. Acute toxicity of methyl mercury to the larval lamprey, *Petromyzon marinus*. *Bull. Environ. Contam. Toxicol*. 37: 281-288.

Mancini ER, Steen A, Rausina GA, Wong DCL, Arnold WR, Gostomski GE, Davies T, Hockett JR, Stubblefield WA, Drottar KR, Springer TA, Errico P. 2002. MTBE Ambient water quality criteria development: A public/private partnership. Enviro. Sci. Technol. 36: 125-129.

Marking LL. 1970. Juglone (5-hydroxy-1,4-naphthoquinone) as a fish toxicant. *Trans Amer Fish Soc* 3: 510-514.

Marking LL, Bills TD. 1975. Toxicity of potassium permanganate to fish and its effectiveness for detoxifying antimycin. *Trans Am Fish Soc* 104(3): 579-583.

Marking LL, Hogan JW. 1967. Toxicity of Bayer 73 to Fish. United States Fish and Wildlife Service, Investigations in Fish Control 19:1-13.

Marking LL, Olson LE. 1975. Toxicity of the lampricide 3-Trifluoromethyl-4-nitrophenol (TFM) to nontarget fish in static tests. United States Fish and Wildlife Service, Investigations in Fish Control 60.

Marking LL, Bills TD, Chandler JH. 1977. Toxicity of furanance to fish, aquatic invertebrates, and frog eggs and larvae. United States Fish and Wildlife Service, Investigations in Fish Control 76.

Mauck WL, Olson LE, Marking LL. 1976. Toxicity of natural pyrethrins and five pyrethroids to fish. *Arch Environ Contamin Toxicol* 4:18-29.

Mummert AK, Neves RJ, Newcomb TJ, Cherry DS. 2003. Sensitivity of juvenile freshwater mussels (*Lampsilis fasciola, Villosa iris*) to total and un-ionized ammonia. *Environ Toxicol Chem* 22(11): 2545-2553.

Pesce SF, Cazenave J, Monferran MV, S Frede, DA Wunderlin. 2008. Integrated survey on toxic effects of lindane on neotropical fish: *Corydoras paleatus* and *Jenynsia multidentata*. *Environmental Pollution* 156: 775-783.

Randall RC, Ozretich RJ, Boese BL. 1983. Acute toxicity of butyl benzyl phthalate to the saltwater fish English sole, *Parophrys vetulus*. *Enviro. Sci. Technol*. 17(11): 670-672.

Rausina GA, Wong DCL, Arnold WR, Mancini ER, Steen AE. 2002. Toxicity of methyl tert-butyl ether to marine organisms: ambient water quality criteria calculation. *Chemosphere* 47: 525-534.

Richardson J. 1991. Acute toxicity of ammonia to juvenile inanga (*Galaxias maculatus*). New Zealand Journal of Marine and Freshwater Research 25: 327-330.

Rosen G, Lotufo GR. 2007. Toxicity of explosive compounds to the marine mussel, *Mytilus galloprovincialis* in aqueous exposures. *Ecotoxicology and Environmental Safety* 68: 228-236.

Shaw JR, Wood CM, Birge WJ, Hogstrand C. 1998. Toxicity of silver to the marine teleost (*Oligocottus maculosus*) effects of salinity and ammonia. *Environ Toxicol Chem* 17(4): 594-600.

Sousa A, Genio L, Mendo S, Barrosoi C. 2005. Comparison of the acute toxicity of tributlytin and copper to veliger larvae of *Nassarius reticulatus* (L.). *Appl. Organometal. Chem*. 19: 324-328.

Stratus Consulting, Inc. 1999. Sensitivity of bull trout (*Salvelinus confluentus*) to cadmium and zinc in water characteristic of the Coeur D'Alene River Basin: acute toxicity report. Final Report to U.S. EPA Region 10. 55 pp.

Varo I, Amat F, Navarro JC. 2008. Acute toxicity of dichlorvos to Aphanius iberus (Cuvier & Valenciennes, 1846) and its anti-cholinesterase effects on this species. *Aquatic Toxicology* 88: 53-61.

Valenti TW, Cherry DS, Neves RJ, Schmerfeld J. 2005. Acute and chromic toxicity of mercury to early life stages of the rainbow mussel, *Villosa iris* (Bivalvia: Unionidae). *Environ Toxicol Chem* 24(5): 1242-1246.

Wan MT, Buday C, Schroeder G, Kuo J, Pasternak J. 2006. Toxicity to *Daphnia magna, Hyalella azteca, Oncorhynchus kisutch, Oncorhynchus mykiss, Oncorhynchus tshawytscha*, and *Rana catesbeiana* of Atrazine, Metolachlor, Simazine, and their formulated products. *Bull Environ Contam Toxicol* 76: 52-58

Wan MT, Kuo J, Buday C, Schroeder G, Van Aggelen G, Pasternak J. 2005. Toxicity of α-, β-, (α + β)-Endosulfan and their formulated and degradation products to *Daphnia magna, Hyalella azteca, Oncorhynchus mykiss, Oncorhynchus kisutch*, and biological implications in streams. *Environ Toxicol Chem* 24(5): 1146-1154.

Wang N, Erickson RJ, Ingersoll CG, Ivey CD, Brunson EL, Augspurger T, Barnhart MC. 2008. Influence of pH on the acute toxicity of ammonia to juvenile freshwater mussel (Fatmucket, Lampsislis siliquoidea) *Environ Toxicol Chem* 27(5): 1141-1146.

Wang N, Ingersoll CG, Hardesty DK, Ivey CD, Kunz JL, May TW, Dwyer FJ, Roberts AD, Augspurger T, Kane CM, Neves RJ, Barnhart MC. 2007. Acute toxicity of copper, ammonia, and chlorine to glochidia and juveniles of freshwater mussels (Unionidae). *Environ Toxicol Chem* 26(10): 2036-2047.

Wang N, Augspurger T, Barnhart.MC, Bidwell JR, Cope WG, Dwyer FJ, Geis S, Greer IE, Ingersoll CG, Kane CM, May TW, Neves RJ, Newton TJ, Roberts AD, Whites DW. 2007. Intra- and interlaboratory variability in acute toxicity tests with glochidia and juveniles of freshwater mussels (Unionidae). *Environ Toxicol Chem* 26(10): 2029-2035.

Wang,N., Ingersoll,C.I., Ivey,C.D., Hardesty,D.K., May,T.W., Augspurger,T., Roberts,A.D., van Genderen,E., and Barnhart,M.C., 2010, Sensitivity of early life stages of freshwater mussels (Unionidae) to acute and chronic toxicity of lead, cadmium, and zinc in water, *Environ Toxicol Chem*, 29(9): 2053-2063,

Ware GW (ed). 1999. *Reviews of Environmental Contamination and Toxicology* Springer-Verlag, New York, NY.

Yin D, Hu S, Jin H, Yu L. 2003. Deriving freshwater quality criteria for 2,4,6-trichlorophenol for protection of aquatic life in China. Chemosphere 52: 67-73.

Appendix A-6. Acceptable Chemical Grades with purities ≥ 90% from Ecotox

Code	Definition
A	Analytical Grade
A or R	Analytical or Reagent Grade
A or S	Analytical or Spectrophotometric Grade
A or GU	Analytical or Guaranteed Grade
AASG	Atomic Absorbtion Spectometry Grade
ACS	American Chemical Society Grade
AL	Analysis Grade
AN	Analar Grade
AN or R	Analar or Reagant Grade
AR	A.R. Grade (Analytical Reagant Grade)
CH	Chromatographic Grade
CL	Clinical Grade
CT	Certified Grade
DG	Distilled in Glass Grade
EL	Electrophoresis Grade
GC	Gas Chromatography Grade
GU	Guaranteed Grade
GUR	Guaranteed Reagant Grade
HG	Histological Grade
HPLC	High Performance Liquid Chromatography Grade
L	Laboratory Grade
ME	Monsanto Electrical Grade
MK	Merck Grade
NAF	National Formulary Grade
NP	Normapur Grade
PAN	Pestanal Grade
PFG	Purified Grade
PG	Pure Grade
PH	Pharmaceutical Grade
PRG	Pesticide Residue Grade
PST	Pesticide Grade
R	Reagant Grade
RE	Reasearch Grade
RE or A	Research or Analytical Grade
RFG	Reference Grade
RS	Residue Grade
S	Spectrophotometric Grade
SC	Scintillation Grade
SO	Solvent Grade
SPC	Spectrochemical Grade

Code	Definition
T or P	Technical or Purified Grade
T or PU	Technical Grade or Pure
TAR	Technical or Analytical or Reagant Grade
TIS	Tissue Culture Grade
ULV	ULV Grade
UP	Ultrapure Grade
USP	United States Pharmacopeia Grade
UV	UV Grade
UV	UV Grade
UV	UV Grade

Appendix A-7. List of elements and their associated compounds

Compound	Compound CAS	Element	Element Cas
Aluminum chloride	7446700	Aluminum	7429905
Aluminum sulfate	10043013		
DiAmmonium hydrogen phosphate	7783280	Ammonia[1]	7664417
Ammonium bicarbonate	1066337		
Ammonium Acetate	631618		
Ammonium Carbonate	506876		
Ammonium Hydroxide	1336216		
Ammonium chloride	12125029		
Ammonium nitrate	6484522		
Ammonium sulfate	7783202		
Cadmium chloride	10108642	Cadmium	7440439
Cadmium nitrate	10325947		
Cadmium sulfate	10124364		
Cobalt chlroide	7646799	Cobalt	7440484
Copper I chloride	7758896	Copper	7440508
Copper II chloride	7447394		
Copper II nitrate	3251238		
Copper sulfate	7758987		
Copper sulfate pentahydrate	7758998		
Chromic nitrate	13548384	Chromium III	16065831
Chromium chloride	10025737		
Chromium oxide	1308389		
Chromium potassium sulfate	10141001		
Potassium dichromate	7778509	Chromium VI	18540299
Potassium chromate	7789006		
chromic acid	1333820		
Sodium chromate	7775113		
Sodium dichromate	10588019		

Compound	Compound CAS	Element	Element Cas
Lead Acetate	301042	Lead	7439921
Lead chloride	7758954		
Lead nitrate	10099748		
Mercuric acetate		Mercury	7439976
Mercuric chloride	7487947		
Mercuric nitrate	10045940		
Mercurous nitrate	10415755		
Mercuric thiocyanate			
Nickel chloride	7718549	Nickel	7440020
Nickel nitrate	13138459		
Nickel sulfate	7786814		
Silver nitrate	7761888	Silver	7440224
Zinc chloride	7646857	Zinc	7440666
Zinc nitrate	7779886		
Zinc sulfate	7733020		

[1] Toxicity reported as total ammonium nitrogen at pH 8 (see Section 4.2.3).

Appendix A-8. Age classifications used to designate life stage in the database.

Order	Family	Species	Larvae[a] Lengths (mm)	Larvae[a] weights (g)	Juvenile[b] Lengths (mm)	Juvenile[b] weights (g)	Adult Lengths (mm)	Adult weights (g)	Source
Acipenseriformes	Acipenseridae		< 30	< 0.2	30-700	0.2-900	> 700	> 900	Jones et al 1978, Bath and O'Connor 1981, Hastings et al. 1987, Froese and Pauly 2008
Anguilliformes	Anguillidae	*Anguilla* sp.	< 70	< 0.5	70-400	0.5-100	> 400	> 100	Hardy 1978a, Froese and Pauly 2008
Atheriniformes	Atherinopsidae Atherinidae		< 15	< 0.1	15-75	0.1-2.5	> 75	> 2.5	Martin and Drewry 1978, Froese and Pauly 2008
Clupeiformes	Clupeidae		< 30	< 0.2	30-180	0.2-100	> 180	> 100	Jones et al 1978, Froese and Pauly 2008
Cypriniformes	Catostomidae	*Catostomus* sp.	< 17	< 0.1	17-200	0.1-100	> 200	> 100	Jones et al 1978, Froese and Pauly 2008
	Cyprinidae	*Campostoma anomalum*	< 20	< 0.1	20-100	0.1-2	> 100	> 2	Buynak and Mohr 1980, Froese and Pauly 2008
		Carassius sp.	< 12	< 0.1	12-300	0.1-500	> 300	> 500	Jones et al 1978, Froese and Pauly 2008
		Cirrhinus mrigala	< 20	< 0.1	20-525	0.1-500	> 525	> 500	Alikunhi 1956, Chakrabarty and Murty 1972, Froese and Pauly 2008
		Cyprinus carpio	< 19	< 0.1	19-250	0.1-200	> 250	> 200	Jones et al 1978, Scott and Crossman 1979, Froese and Pauly 2008
		Gibelion catla	< 20	< 0.1	20-440	0.1-500	> 440	> 500	Alikunhi 1956, Chakrabarty and Murty 1972, Froese and Pauly 2008
		Gila elegans	< 9	n/a	9-260	n/a	> 260	n/a	Kaeding et al 1983, Marsh 2004, Froese and Pauly 2008
		Labeo sp.	< 20	< 0.2	20-100	0.2-20	> 100	> 20	Alikunhi 1956, Chakrabarty and Murty 1972, Cambray, J.A. 1985, Weyl and Booth 1999, Tedesco and Hugueny 2006, Froese and Pauly 2008
		Notropis sp.	< 15	< 0.1	15-40	0.1-0.5	> 40	> 0.5	Saksena, V.P. 1962, Ross 2001, Froese and Pauly 2008
		Pimephalas sp.	< 10	< 0.1	10-50	0.1-1.4	> 50	> 1.4	Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008
`		*Ptychocheilus lucius*	< 25	n/a	25-200	n/a	> 200	n/a	Vanicek and Kramer 1969, Tyus and Haines 1991, Froese and Pauly 2008
Cyprinodontiformes	Aplocheilidae	*Rivulus marmoratus*	< 12	n/a	12-40	n/a	> 40	n/a	Grageda et al 2004; Froese and Pauly 2008
	Cyprinodontidae	*Cyprinodon* sp.	< 12	< 0.1	12-30	0.1-0.5	> 30	> 0.5	Hardy 1978a, G.Cripe pers. Comm. USEPA-EPA Gulf Breeze, Fl

Order	Family	Species	Larvae[a] Lengths (mm)	Larvae[a] weights (g)	Juvenile[b] Lengths (mm)	Juvenile[b] weights (g)	Adult Lengths (mm)	Adult weights (g)	Source
	Fundulidae	*Fundulus* sp.	< 25	< 0.1	25-40	0.1-1	> 40	> 1	Hardy 1978a, Able and Fahay 1998, Froese and Pauly 2008
	Poeciliidae		< 10	< 0.1	10-25	0.1-0.25	> 25	> 0.25	Hardy 1978b, Froese and Pauly 2008
Esociformes	Esocidae	*Esox* sp.	< 20	< 0.1	20-200	0.1-55	> 200	> 55	Jones et al 1978, Scott and Chapman 1979, Froese and Pauly 2008
Gasterosteiformes	Gasterosteidae		< 15	n/a	15-45	n/a	> 45	n/a	Hardy 1978a, Able and Fahay 1998
Mugiliformes	Mugilidae		< 35	< 0.2	35-350	0.2-300	> 350	> 300	Martin and Drewry 1978, Froese and Pauly 2008
Perciformes	Anabantidae	*Anabas testudineus*	< 10	< 0.1	10-110	0.1-25	> 110	> 25	Mookerjee and Mazumdar 1946, Froese and Pauly 2008
	Centrarchidae	*Lepomis* sp.	< 13	< 0.1	13-125	0.1-25	> 125	> 25	Hardy 1978b, Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008
		Micropterus sp.	< 17	< 0.2	17-250	0.2-175	> 250	> 175	Hardy 1978b, Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008
		Pomoxis sp.	< 15	< 0.1	15-200	0.1-70	> 200	> 70	Hardy 1978b, Froese and Pauly 2008
	Cichlidae		< 20	< 0.3	20-80	0.3-30	> 80	> 30	Global invasive species database 2005, Froese and Pauly 2008, Hassan-Williams and Bonner 2008, M.Peterson pers.comm.
	Gobiidae	*Gobiosoma bosc*	< 7	n/a	7-30	n/a	> 30	n/a	Ruple 1984, Froese and Pauly 2008
	Moronidae	*Morone americana*	< 20	n/a	20-150	n/a	> 150	n/a	Hardy 1978b, Froese and Pauly 2008
		Morone saxatilis	< 36	n/a	36-400	n/a	> 400	n/a	Hardy 1978b, Froese and Pauly 2008
	Percidae	*Etheostoma* sp.	< 18	< 0.1	18-35	0.1-0.4	> 35	> 0.4	Johnson 1984, Fisher 1990, Froese and Pauly 2008
		Perca flavescens	< 20	< 0.1	20-125	0.1-20	> 125	> 20	Hardy 1978b, Froese and Pauly 2008
		Sander vitreus	< 20	< 0.1	20-250	0.1-177	> 250	> 177	Hardy 1978b, Froese and Pauly 2008
	Sciaenidae	*Leiostomus xanthurus*	< 15	< 0.1	15-200	0.1-90	> 200	> 90	Johnson 1978, Froese and Pauly 2008
	Sparidae	*Lagadon rhomboides*	< 15	< 0.1	15-120	0.1-60	> 120	> 60	Johnson 1978, Froese and Pauly 2008
Pleuronectiformes	Pleuronectidae	*Platichthys* sp.	< 7	< 0.1	7-200	0.1-80	> 200	> 80	Ahlstrom et al 1984, Froese and Pauly 2008
Salmoniformes	Salmonidae	*Oncorhynchus* sp.	< 25	< 0.2	25-200	0.2-100	> 200	> 100	Scott and Chapman 1979, Kendall and Behnke 1984, Ross 2001, Froese and Pauly 2008, Ueberschar and Froese 2008
		Salmo sp.	< 25	< 0.2	25-200	0.2-5.3	> 200	> 75	Kendall and Behnke 1984, Jonsson 1985, Gorodilov 1996, Marschall et al. 1998, Froese and Pauly 2008, Ueberschar and Froese 2008
		Salvelinus sp.	<20	< 0.2	20-200	0.2-100	> 200	> 100	Kendall and Behnke 1984, Froese and Pauly

									2008, Ueberschar and Froese 2008
Siluriformes	Bagridae		< 10	n/a	10-90	n/a	> 90	n/a	Rahman et al. 2004, Froese and Pauly 2008
	Heteropneustidae		< 12	n/a	12-120	n/a	> 120	n/a	Thakur et al. 1974, Froese and Pauly 2008
	Ictaluridae		< 20	< 0.1	20-250	0.1-100	> 250	> 100	Jones et al 1978, Scott and Crossman 1979; Froese and Pauly 2008
Tetraodontiformes	Monacanthidae	*Stephanolepis hispidus*	< 8 mm	< 0.1	8-75	0.1-9	> 75	> 9	Martin and Drewry 1978, Rogers et al 2001, Froese and Pauly 2008

[a] also included nauplii, zoea (Crustaceans); Yolk-sac fry, fry alevin, glass eel stage (Fishes); glochidia (Mollusca)

[b] also included immature, Young of year, black eel stage, fingerling, parr, yearling (Fishes); spat (Mollusca)

n/a - length weight regressions not available

Sources for Age Classifications

Able, K.W. and M. P. Fahay. 1998. The first year in the life of estuarine fishes in the Middle Atlantic Bight. Rutgers University Press New Brunswick, NJ.

Ahlstrom, E.H., K. Amaoka, D.A. Hensley, H.G. Moser, and B.Y. Sumida. 1984. Pleuoronectiformes: Development. In: Ontogeny and systematics of fishes. American Society of Ichthyologists and Herpetologists, La Jolla, California.

Alikunhi, K.H. 1956. Observations on the fecundity, larval development and early growth of *Labeo bata* (Hamilton). Indian J. Fishes 3(1): 216-229.

Bath, D.W., J.M. O'Connor. 1981. Development and Identification of larval Atlantic Sturgeon (*Acipenser oxyrhynchus*) and shortnose sturgeon (*A. brevirostrum*) from the Hudson River Estuary, New York. Copeia 1981 (3) 711-717.

Buynak, G.L. and H.W. Mohr. 1980. Larval development of stoneroller, cutlips minnow, and river chub with diagnostic keys, including four additional cyprinids. The Progressive Fish Culturist 42 (3) 127-135.

Cambray, J.A. 1985. Early ontogeny of Labeo capensis (Pisces: Cyprinidae). S. Afr. J. Zool. 20: 190-196.

Chakrabarty, R.D. and D.S. Murty. 1972. Life history of Indian major carps, Cirrhinus mrigala (Ham.), Catla catla (Ham.), and Labeo rohita (Ham.). J. Inldand Fish. Soc. India. Vol IV: 132-161.

Fisher, W.L. 1990. Life history and ecology of the orangefin darter *Etheostoma bellum* (Pisces: Percidae). American Midland Naturalist 123 (2) 268-281.

Froese, R. and D. Pauly. Editors. 2008.FishBase. World Wide Web electronic publication. www.fishbase.org, version (06/2008).

Global Invasive Species Database, 2005. Oreochromis mossambicus. Available from http://www.issg.org/database/species/ecology.asp?fr=1&si=131 [Accessed July 29, 2008].

Gorodilov, Y.N. 1996. Description of the early ontogeny of the Atlantic salmon, *Salmo salar*, with a novel system of interval (state) identification. Environmental Biology of Fishes 47: 109-127.

Grageda, M.V.C., Y. Sakakura, and A. Hagiwara. 2004. Early development of the self-fertilizing mangrove killifish *Rivulus marmoratus* reared in the laboratory. Ichthyological Research 51: 309-315.

Hardy, J.D. 1978a. Development of Fishes of the Mid-Atlantic Bight, an atlas of egg, larval and juvenile stages: Volume 2 Anguillidae through Syngnathidae. Biological Services Program FWS/OBS-78/12. US Department of the Interior, Fish and Wildlife Service, Solomons, Maryland.

Hardy, J.D. 1978b. Development of Fishes of the Mid-Atlantic Bight, an atlas of egg, larval and juvenile stages: Volume 3 Aphredoderidae through

Rachycentridae. Biological Services Program FWS/OBS-78/12. US Department of the Interior, Fish and Wildlife Service, Solomons, Maryland.

Hassan-Williams, C. and T. H. Bonner. Texas State University – San Marcos Biology Department/ Aquatic Station http://www.bio.txstate.edu/~tbonner/txfishes/oreochromis%20mossambicus.htm [Accessed July 29, 2008]

Hastings, R.W., J.C. O'Herron II, K. Schick, M.A. Lazzari. 1987. Occurrence and distribution of shortnose sturgeon, *Acipenser brevirostrum*, in the Upper Tidal Delaware River. Estuaries 10(4) 337-341.

Johnson, G.D. 1978. Development of Fishes of the Mid-Atlantic Bight, an atlas of egg, larval and juvenile stages: Volume 4 Carangidae through Ephippidae. Biological Services Program FWS/OBS-78/12. US Department of the Interior, Fish and Wildlife Service, Solomons, Maryland.

Johnson, G.D. 1984. Percoidei: Development and Relationships. In: Ontogeny and systematics of fishes. American Society of Ichthyologists and Herpetologists, La Jolla, California.

Jones, P.W., F.D. Martin and J.D. Hardy. 1978. Development of Fishes of the Mid-Atlantic Bight, an atlas of egg, larval and juvenile stages**:** Volume 1 Acipenseridae through Ictaluridae. Biological Services Program FWS/OBS-78/12. US Department of the Interior, Fish and Wildlife Service, Solomons, Maryland.

Jonsson, B. 1985. Life history patterns of freshwater resident and sea-run migrant brown trout in Norway. Transactions of the American Fisheries Society 114: 182-194.

Kaeding, L.R. and M.A. Zimmerman. 1983. Life history and ecology of the humpback chub in the little Colorado and Colorado rivers of the Grand Canyon. Transactions of the American Fisheries Society 112: 577-594.

Kendall, A.W. and R.J. Behnke. 1984. Salmonidae: Development and Relationships. In: Ontogeny and systematics of fishes. American Society of Ichthyologists and Herpetologists, La Jolla, California.

Marschall, E.A., T.P. Quinn, D.A. Roff, J.A. Hutchings, N.B. Metcalfe, T.A. Bakke, R.L. Saunders, and N.L. Poff. 1998. A framework for understanding Atlantic salmon (*Salmo salar*) life history. Can. J. Fish. Aquat. Sci (55 Suppl 1): 48-58.

Martin, F.D. and G.E. Drewry. 1978, Development of Fishes of the Mid-Atlantic Bight, an atlas of egg, larval and juvenile stages: Volume 6 Stromateidae through Ogcocephalidae. Biological Services Program FWS/OBS-78/12. US Department of the Interior, Fish and Wildlife Service. Solomons, Maryland.

Marsh, P.C. 2004. Threatened fishes of the world: *Gila elegans* Baird and Girard 1853 (Cyprinidae). Environmental Biology of Fishes 70: 144.

Mookerjee, H.K., S.R. Mazumdar. 1946. On the life-history, breeding and rearing of Anabas testudineus (Bloch). J. Dept. Sci. Calcutta Univ. 2(1): 101-140.

Rahman, M.R., M.A. Rahman, M.N. Khan, and M.G. Hussain. 2004. Observation on the embryonic and larval development of Silurid catfish, Gulsha (*Mystus cavasius* Ham.). Pakistan Journal of Biological Sciences 7 (6): 1070-1075.

Rogers, J.S., J.A. Hare and D.G. Lindquist. 2001. Otolith record of age, growth, and ontogeny in larval and pelagic juvenile *Stephanolepis hispidus* (Pisces: Monacanthidae). Marine Biology 138: 945-953.

Ross, S.T. 2001 Inland Fishes of Mississippi. University Press of Mississippi, Jackson, MS.

Ruple, D. 1984. Gobiodidei: Development. In: Ontogeny and systematics of fishes. American Society of Ichthyologists and Herpetologists, La Jolla, California.

Saksena, V.P. 1962. The post-hatching stages of the red shiner, *Notropis lutrensis*. Copeia 1962 (3): 539-544.

Scott, W.B. and E.J. Crossman. 1979. Freshwater Fishes of Canada. Fisheries Research Board of Canada, Ottawa. Bulletin 184.

Tedesco, P. and B. Hugueny. 2006. Life history strategies affect climate based spatial synchrony in population dynamics of West African freshwater

fishes. Oikos 115: 117-127.

Thakur, N.K., R.N. Pal, and H.A. Khan. 1974. Embryonic and larval development of Heteropneustes fossilis (Bloch). J. Inldand Fish. Soc. India. VI: 33-44.

Tyus, H. and G.B. Haines. 1991. Distribution, habitat use, and growth of age-0 Colorado squawfish in the green river basin, Colorado and Utah. Transactions of the American Fisheries Society 120: 79-89.

Ueberschar, B and R. Froese. Editors. 2008. LarvalBase. World Wide Web electronic publication www.larvalbase.org, version (07/2008)

Vanicek, C.D. and R.H. Kramer. 1969. Life history of the Colorado squawfish, *Ptychocheilus lucius*, and the Colorado chub, *Gila robusta*, in the green river in Dinosaur National Monument, 1964-1966. Transactions of the American Fisheries Society 98(2): 193-208.

Weyl, O.L.F. and A.J. Booth. 1999. On the life history of a cyprinid fish, *Labeo cylindricus*. Environmental Biology of Fishes 55: 215-225.

Appendix A-9. Temperature ranges used to standardize species in the model data subset.

Species	ICE Temperature ACTUAL[8]	ICE Temp Acceptance Range	Species from Guidelines	ASTM[1]	OPP[2]	OPPTS 1996[3]	OECD 203[4]	EPA 1975[5]	EPA 1993[6]
Acipenser brevirostrum	17	14-20	x	x	x	x	x	x	x
Allorchestes compressa	19.7-21	17-23	x	x	x	x	x	x	x
Ameiurus melas	18-24	18-24	x	x	x	x	x	x	x
Americamysis bahia	25-29	24-29	*Americamysis bahia*	25-29	21-23	23-27	x	x	19-21, 24-26
Asellus aquaticus	13	10-16	x	x	x	x	x	x	x
Asterias forbesi	20	17-23	x	x	x	x	x	x	x
Atherix variegata	15	12-18	x	x	x	x	x	x	x
Bufo boreas	22	19-25	*Bufo* sp.	20-24	x	x	x	x	x
Caecidotea brevicauda	15-21	15-21	x	x	x	x	x	x	x
Caecidotea intermedia	20	17-23	x	x	x	x	x	x	x
Carassius auratus	17-21	17-23	*Carassius auratus*	15-24	x	x	x	20-24	x
Catostomus commersonii	3.6-22.5	10-16	x	x	x	x	x	x	x
Ceriodaphnia dubia	24.1-26.2	21-27	*Ceriodaphnia dubia*	23-27	x	x	x	x	19-21, 24-26
Channa marulius	26	23-29	x	x	x	x	x	x	x
Chironomus plumosus	20-22	19-25	*Chironomus* sp.	20-24	x	x	x	20-24	x
Chironomus tentans	20-22	19-25	*Chironomus* sp.	20-24	x	x	x	20-24	x
Claassenia sabulosa	15-16	12-18	x	x	x	x	x	x	x
Crangonyx pseudogracilis	8.6-13	8-14	x	x	x	x	x	x	x
Crassostrea virginica	X[7]	19-25	*Crassostrea virginica*	20-24	x	x	x	x	x
Cyprinodon bovinus	20	17-23	x	x	x	x	x	x	x
Cyprinodon variegatus	22	19-25	*Cyprinodon variegatus*	20-24	21-23	20-24	x	20-24	19-21, 24-26
Cyprinus carpio	18-22.5	18-24	*Cyprinus carpio*	x	x	20-24	20-24	x	x
Cypris subglobosa	20.4	17-23	x	x	x	x	x	x	x
Daphnia magna	18-23.8	18-24	*Daphnia magna*	18-22	x	18-22	x	15-19	19-21, 24-26
Daphnia pulex	19-21	16-22	*Daphnia pulex*	18-22	x	18-22	x	15-19	19-21, 24-26
Dugesia tigrina	20	18-24	*Dugesia tigrina*	20-24	x	x	x	x	x

Species	ICE Temperature ACTUAL[8]	ICE Temp Acceptance Range	Species from Guidelines	ASTM[1]	OPP[2]	OPPTS 1996[3]	OECD 203[4]	EPA 1975[5]	EPA 1993[6]
Erimonax monachus	17	15-21	x	x	x	x	x	x	x
Esox lucius	12-18	12-18	x	x	x	x	x	x	x
Etheostoma fonticola	22	19-25	x	x	x	x	x	x	x
Etheostoma lepidum	22	19-25	x	x	x	x	x	x	x
Farfantepenaeus duorarum	20	19-25	*Farfantepenaeus duorarum*	20-24	x	x	x	20-24	x
Gambusia affinis	15.5-19.9	14-20	x	x	x	x	x	x	x
Gammarus fasciatus	15-19	14-20	*Gammarus fasciatus*	15-19	x	17-19	x	15-19	x
Gammarus lacustris	15	14-20	*Gammarus lacustris*	15-19	x	17-19	x	15-19	x
Gammarus pseudolimnaeus	15-18.4	14-20	*Gammarus pseudolimnaeus*	15-19	x	17-19	x	15-19	x
Gasterosteus aculeatus	20	18-24	*Gasterosteus aculeatus*	15-19	x	10-14	x	20-24	x
Gila elegans	22-26	21-27	x	x	x	x	x	x	x
Hyalella azteca	18.2-25	18.5-24.5	x	x	x	x	x	x	x
Ictalurus punctatus	17.8-24	18-24	*Ictalurus punctatus*	15-24	x	20-24	x	20-24	x
Lagodon rhomboides	22-24	21-25	*Lagodon rhomboides*	20-24	x	x	x	20-24	x
Lepomis cyanellus	17-22	16.5-23.5	*Lepomis cyanellus*	15-24	x	x	x	x	x
Lepomis macrochirus	18-24	18-24	*Lepomis macrochirus*	15-24	x	20-24	21-25	20-24	x
Lepomis microlophus	18-24	18-24	x	x	x	x	x	x	x
Lumbriculus variegatus	20-25	19-25	x	x	x	x	x	x	x
Menidia beryllina	21-23	19-25	*Menidia* sp.	20-24	21-23	20-24	x	20-24	19-21, 24-26
Menidia menidia	21-23	19-25	*Menidia* sp.	20-24	21-23	20-24	x	20-24	19-21, 24-26
Metapenaeus dobsoni	27.5	24-30	x	x	x	x	x	x	x
Micropterus dolomieu	17-28	17-23	x	x	x	x	x	x	x
Micropterus salmoides	17-22	17-23	x	x	x	x	x	x	x
Morone saxatilis	12-25	15-21							
Neanthes virens	20	17-23	x	x	x	x	x	x	x
Notropis mekistocholas	17	14-20	x	x	x	x	x	x	x
Oncorhynchus clarkii	10-14.4	9-15	x	x	x	x	x	x	x
Oncorhynchus gilae	12	9-15	x	x	x	x	x	x	x
Oncorhynchus kisutch	12-13	9-15	*Oncorhynchus kisutch*	10-14	x	10-14	x	10-14	x
Oncorhynchus mykiss	10-14	9-15	*Oncorhynchus mykiss*	10-14	x	10-14	13-17	10-14	11-13
Oncorhynchus tshawytscha	10-12.2	9-15	x	x	x	x	x	x	x

Species	ICE Temperature ACTUAL[8]	ICE Temp Acceptance Range	Species from Guidelines	ASTM[1]	OPP[2]	OPPTS 1996[3]	OECD 203[4]	EPA 1975[5]	EPA 1993[6]
Orconectes nais	15-21	15-21	*Orconectes* sp.	15-24	x	x	x	20-24	x
Oreochromis mossambicus	24-29	24-29	x	x	x	x	x	x	x
Oryzias latipes	23-25	20-26	*Oryzias latipes*	x	x	x	21-25	x	x
Paratanytarsus dissimilis	20-23.8	19-25	x	x	x	x	x	x	x
Paratanytarsus parthenogeneticus	20-23	19-25	x	x	x	x	x	x	x
Perca flavescens	12-18	12-18	x	x	x	x	x	x	x
Pimephales promelas	22-27.4	21-27	*Pimephales promelas*	23-27	x	21-25	21-25	20-24	19-21, 24-26
Planorbella trivolvis	20	17-23	x	x	x	x	x	x	x
Poecilia reticulata	23-25	20-26	*Poecilia reticulata*	x	x	21-25	21-25	x	x
Poeciliopsis occidentalis	22	19-25	x	x	x	x	x	x	x
Pomoxis nigromaculatus	18	15-21	x	x	x	x	x	x	x
Pteronarcella badia	10-16	10-16	x	x	x	x	x	x	x
Pteronarcys californica	10	9-15	*Pteronarcys* sp.	10-14	x	x	x	10-14	x
Ptychocheilus lucius	22-26	21-27	x	x	x	x	x	x	x
Rana sphenocephala	20-22	19-25	*Rana sp.*	20-24	x	x	x	x	x
Salmo salar	12-17	11-17	*Salmo salar*	x	x	10-14	x	x	x
Salmo trutta	11.9-17	11-17	x	x	x	x	x	x	x
Salvelinus confluentus	7.6-12.1	7-13	x	x	x	x	x	x	x
Salvelinus fontinalis	12-12.2	9-15	*Salvelinus fontinalis*	10-14	x	10-14	x	10-14	11-13
Salvelinus namaycush	10-15	9-15	x	x	x	x	x	x	x
Sander vitreus	12-18	12-18	x	x	x	x	x	x	x
Simocephalus serrulatus	15-21	15-21	x	x	x	x	x	x	x
Xyrauchen texanus	22-26	21-27	x	x	x	x	x	x	x

References

1. ASTM. 2007. Standard guide for conducting acute toxicity tests on test materials with fishes, macroinvertebrates, and amphibians. E 729-96

2. Reider, D and A.C. Bryceland. 1986. Standard evaluation procedure acute toxicity test for estuarine and marine organisms. EPA 540/9-86-137.

3. Ecological Effects Test Guidelines. OPPTS 850.1075 Fish Acute Toxicity Test, Freshwater and Marine. EPA 712-C-96-118. April 1996

4.OECD. 1992. OECD guideline for testing of chemicals. 203.

5. US EPA. 1975. Methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. EPA 660/3-75-009.
6. US EPA. 1993. Methods for measuring the acute toxicity of effluents and receiving waters to freshwater and marine organisms. EPA 600/4-90/O27F
7. Data from OPP (see Section 3.3 above).
8. Temperature range may not encompass OPP datasource (see Section 3.3).

Appendix A-10. List of data fields in master database

Data Field	Description
ID	Unique Web-ICE record identification number
DSource specific	Specific data source (e.g. ECO12207 = Ecotox Acquire # 12207)
DSource category	General category of data (i.e. literature, ECOTOX, Mayer 1987)
Chemical tested	Chemical name as reported in original source
CAS reported	CAS reported by original source
ICE chemical	Standardized name
ICE CAS	CAS registry number
AI	Active ingredient or chemical grade of chemical tested
Water Type	Freshwater (FW); Saltwater (SW) or NR (not recorded)
Taxa	Broad taxa of test species
Common name	Common name of test species
Species	Species tested ("none" = genus only e.g. Daphnia sp.)
Genus	Genus name of test species
Family	Family name of test species
Age	Age as reported (size, weight, etc.)
Age class	ICE age class (L = larvae, J = juvenile, A = adult, U = Unknown)
Test duration	48h; 96h; NR (not recorded)
Dose Type	LC50; EC50; NR (not recorded)
Test Type	F (flow through); S (static); SR (static renewal); NR (not recorded)
Concentration Type	M (measured); U (nominal/unmeasured); NR (not recorded)
Temp	Test temperature as reported
SAL	Test salinity as reported
DO	Test dissolved oxygen as reported
pH	Test pH as reported
Hardness	Test hardness as reported
ICE toxicity (µg/L)	Toxicity used for ICE models after normalizations
Guidelines	Guidelines reported for test (i.e. ASTM). If field says confirmed then record was verified to meet ICE standardizations
Date entered	Date data entered
Meets Model REQ	Yes/No field - does record meet ICE model standardization requirements

Appendix B. Algae ICE Module; Beta Technical Basis of the Development of Algae ICE Models for Web-ICE

This technical basis was last updated April 10, 2013

Introduction

This document summarizes the data used in the Web-ICE v3.2.1 Algae Modules. The Algae Modules were developed under a Cooperative Research and Development Agreement between the Office of Research and Development of the U.S. EPA and the Procter and Gamble Company (P&G).

The Algae Modules allow estimation of toxicity in selected species or genera of freshwater or marine algae by inputting the known toxicity in another algal species. Both the Algae Modules and this technical basis document will be updated periodically as the database, interspecies algal models, or functionality is revised. Users are encouraged to report any issues to EPA via the Web-ICE contact page.

Overview of Algae Database and Model Development

The process of obtaining data and ICE model creation is provided below:

1. A compilation of public (ECOTOX and scientific literature), EPA (Office of Pesticide Programs Toxicity Database) and P&G-owned algal toxicity data were compiled into an ACCESS database. The database of acute toxicity data for freshwater or marine algae: EC50 or equivalent values for short-term algal growth in biomass or cell number.
2. Duplicate records were removed, as well as records containing open ended (greater than or less than) toxicity values. After initial processing, over 17,000 studies comprising over 500 species and nearly 1500 chemicals were included in the initial database.
3. A general quality review of each algal acute study was performed by assessing the source of the record for conformance to standard methods and guidelines, such as OECD, USEPA and ASTM.
4. The database was then restructured to include: (1) the 11 algal genera with sufficient toxicity records (EC50 or equivalent) to allow ICE model development, (2) only 72 or 96-hr acute toxicity data, (3) newly calculated toxicity values (i.e., over 80 EC50s were recalculated), (4) additional P&G studies, (5) harmonized algal taxonomic names, (6) test material names that were confirmed and coordinated, and (7) calculated geometric means and variance per taxon per chemical. This restructured database contained approximately 3500 EC50 records with 791 unique chemicals and 74 species of algae.
5. A preliminary assessment of the influence of type of EC50 (e.g., E_rC_{50} and E_bC_{50}) separately and combined was completed. An ErC50 was based on growth rate while an EbC50 was based on biomass. The same data is used to determine each endpoint but different statistical approaches are used. The biomass parameter generally provides a lower value compared with growth rate, but both types of EC50s were included based on correlation analysis.

6. An extensive quality assurance review of the records in the restructured database was completed following general USEPA Science Advisory Board recommendations (Table 1) The final database used in Web-ICE models consisted of 1647 unique studies with approximately 457 chemicals, and 69 Species of Green Algae, Blue-Green Algae and Diatoms.
7. The final database was used to generate 44 Genus-level models and 58 species level models that were cross-validated (Raimondo et al. 2007).
8. Only significant models ($p<0.05$) that had three or more chemicals were included in the Algae Module.

References

ASTM (American Society for Testing and Materials). 2011. Standard Guide for Conducting Static Toxicity Tests with Microalgae. ASTM E1218 - 04e1. ASTM International, West Conshohocken, PA, 2006, DOI: 10.1520/E1218-04E01, www.astm.org.

OECD (Organization for Economic Cooperation and Development). 1996. OECD Guidelines for the Testing of Chemicals. Freshwater Alga and Cyanobacteria, Growth Inhibition Test. Paris, France 26p.

Raimondo, S., Mineau, P., and Barron, M.G. 2007. Estimation of Chemical Toxicity to Wildlife Species Using Interspecies Correlation models. Env. Sci. Technol 41(16):5888-5894.

USEPA. 1996. Ecological Effects Test Guidelines OPPTS 850.5400, Algal Toxicity, Tiers I and II. EPA 712-C-96-164, 11p.

Table 1. Checklist of standardization criteria for inclusion into algal database used to create ICE models.

Category	Data Information	Criteria
Chemical	Identity	Reported CAS, name or structure confirmed [a] CAS corresponds to single compound or element
	Compound	Mixtures excluded except for metal and specific chemical salts
	Purity	Active ingredient $\geq$ 90% [b, c]
	Grade	If Purity is "NR", test grade conformed to Web-ICE requirements
	Name	Harmonized within the algal database
Organism	Species	Algae and diatoms Name & taxonomy verified
Test Conditions	Test Media	Aquatic (FW/SW identified)
	Exposure type	F, S, SR (no sediment, dietary, mixed dose or phototoxicity)
	Exposure duration	Acute; 72 & 96 hrs
	Endpoint	EC50 (
	Measurement	growth rate, biomass or cell density
	Test Location	Laboratory only
Toxicity Value	Concentration	> or < excluded
	Units	ug/L, converted if needed
	Chemical Normalization	Metals: no hardness correction [c]
	Element Normalization [d]	Ag, Al, Cu, Cd, Co, Cr(III), Cr(VI), Hg, Ni, Pb, Zn

[a] Some proprietary data encoded with false CAS number to avoid chemical identification

[b] Beta version includes chemicals with AI <90% if equivalent for all species tested with that chemical.

[c] Tests performed in standard test media [e.g., OECD 201: OECD Guideline for Freshwater Alga and Cyanobacteria, Growth Inhibition Test (2006); ASTM E1218-20: Standard Guide for Conducting Static Toxicity Tests with Microalgae (2009); EU Method C_3: Algal Inhibition Test]

[d] Metals reported as salts were normalized to element