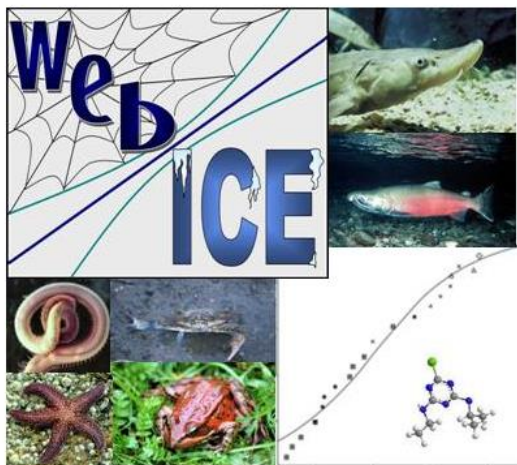


ICE Aquatic Toxicity Database Version 3.3 Documentation



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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.

The document is organized by section, including: 1) Introduction, 2) data sources used in developing the ICE database, 3) the quality acceptance criteria applied to the master database, 4) additional standardization applied to data used in ICE models, 5) quality assurance and control procedures, 6) data fields, 7) references, and technical appendices.

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

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 (AWQC) 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 1987-2013 (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 (OPP) 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. Additional acute mollusc data was acquired in April 2013. 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 Office of Chemical Safety and Pollution Prevention 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 (GLP), but the study did not meet all requirements listed for satisfaction of the OPP testing requirements (e.g. raw data not submitted). Core studies meet all OPP 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 3.0.

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 censor 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 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 surrogate 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). 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-4 provides a list of peer reviewed studies included in the database.

2.9 Procter & Gamble

Algal and zebrafish embryo toxicity data 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 development of the algal database is described in Appendix B. Zebrafish embryo toxicity data were compiled from public (ECOTOX and scientific literature), P&G-owned sources, and OECD (2012).

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 3.1- 3.4.

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 Grade	Active ingredient \geq 90% If Purity is "NR", test grade must be one listed in Appendix A-5
	Name	Synonyms conformed to ICE chemical name
Organism	Species	Fish, invertebrates, amphibians Name & taxonomy verified
	Life stage	Eggs excluded except for zebrafish embryos ²
Test Conditions	Test Media	Aquatic (no sediment, dietary, mixed dose or phototoxicity)
	Exposure type	Flow through (F), static (S), or static renewal (R)
	Exposure duration	Acute; 24 (fairy shrimp), 48 & 96 hrs
	Endpoint	EC50 or LC50
	Measurement	Mortality or immobility
Toxicity Value	Test Location	Laboratory
	Concentration	~, > or < excluded
	Units	$\mu\text{g/L}$, converted if needed
	Chemical Normalization ³	Pentachlorophenol to pH 6.5; Ammonia to TAN ⁴ , FW to pH 7, FW inverts to 20°C; Specific metals ⁵ to hardness 50 mg/L
	Element Conversions ⁶	Ag, Al, Cu, Cd, Co, Cr(III), Cr(VI), Hg, NH ₄ , Ni, Pb, Zn

¹ Included metal and other chemical salts, and specific congener mixtures² Zebrafish embryo toxicity tests conducted using methods similar to OECD (2013) fish embryo toxicity test (FET).³FW only, normalized according to AWQC⁴ Total Ammonia Nitrogen⁵ Ag, Cu, Cd, Cr(III), Pb, Ni, Zn⁶ 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 $\geq 90\%$. 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-5. 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 as PCB, Arochlors, and toxaphene. Any degradedates 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 public domain databases: the Allanwood Compendium of Pesticides (<http://www.alanwood.net/pesticides/>), Chemical Book (<http://www.chemicalbook.com>), or Sigma-Aldrich (<http://www.sigmaaldrich.com>). The CAS and name associated with each toxicity record are entered into the database as either the tested compound, as the element for Aluminum, Cadmium, Cobalt, Copper, Chromium (III), Chromium (VI), Lead, Mercury, Nickel, Silver, and Zinc, or as Pentachlorophenol or Ammonia for salts containing these chemicals. 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. ICE chemical names were curated using DSSTox (www.epa.gov/ncct/dsstox/). A single name and the confirmed chemical abstract services registry number (CAS-RN) from the source material were checked against DSSTox to validate their consistency. Names that were not contained within DSSTox's list of synonyms for a particular chemical were manually checked to validate the agreement between the chemical identifiers and confirm the chemical-data linkage with ICE.

A separate database is maintained for mode of action (MOA) assignments. For complete description of MOA assignments see the Mode of Action and QSAR Databases and Modeling Quality Assurance Project Plan (QAPP-GED/BPRB/MB/2014-01-001). In brief, chemicals are assigned a broad MOA (e.g. AChE inhibition) and a specific MOA (e.g. AChE inhibition -

Organophosphate). Data fields in the MOA chemical database included CAS, chemical name, broad and specific MOA assignments, chemical class assignment (for narcosis chemicals only), MOA source, and a notes column.

3.2 Organism

The aquatic database contains only animal records and excludes the egg stages except for zebrafish embryos. 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 (i.e. www.fishbase.com) or literature are used. Species names that cannot be verified are excluded. After verification, species are grouped into broader taxonomic categories (e.g., fish, crustaceans). If only a common name is provided that is too general to determine species, genus or 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 standardized 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), and static renewal (R). Toxicity values reported as both measured (M) and nominal/unmeasured (U) are included. Acute toxicity results must be either immobilization (EC50) or mortality (EC/LC50). Test durations accepted were 24h (fairy shrimp), 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. $> 100 \mu\text{g/L}$ or $< 100 \mu\text{g/L}$) and approximate values ($\sim 100 \mu\text{g/L}$) are excluded. All toxicity records are converted to $\mu\text{g/L}$ (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 a pH 7 for freshwater and 20°C for freshwater organisms) and specific metal salts (hardness of 50 mg/L CaCO₃; 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 ICE database chemical conversions and normalizations (OP-GED/BPRB/CRL/2015-01-001). Large metal salts and organometals are not normalized because of uncertainty in the relationship between their toxicity, hardness, and dissociation, and are treated as separate compounds in the database. These exceptions are further explained in the chemical normalization OP.

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 designated as a “True” 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, decapods juvenile and spat: molluscs ² immature aquatic lifestages: amphibians (includes embryo), insects all life stages: all other species no egg or embryo test for any species other than zebrafish embryos ³
Test conditions	Test duration	24-48 hr: fairy shrimp 48 hr: water fleas, midges, mosquitoes 96 hr: all other species
	Temperature ⁴	species specific (± 3 °C)
	Dissolved oxygen	Static: ≤ 48 hr 60-100%; >48 hr 40-100%. Static renewal or flow-through: 60-100%.
	Salinity	<1 ppt: FW species ⁵ ≥ 15 ppt: SW species ⁶

¹ if life stage not reported, determined through reported age/size; Appendix A-8

² glochidia excluded

³ Zebrafish embryo toxicity tests conducted using methods similar to OECD (2013) fish embryo toxicity test (FET).

⁴ based on ASTM and equivalent test guidelines for test species; Appendix A-9

⁵ Salmonid tests included are freshwater

⁶ Striped bass (*Morone saxatilis*) tests are saltwater

4.1 Life stage

The life stage of each species is broadly defined as embryo, larvae, juvenile, or adult. In the model data subset, only the juvenile stages of fish (with the exception of zebrafish embryos) and decapods; juvenile and spat of molluscs; and immature aquatic lifestages of amphibians and aquatic insects are used. For all other species, all life stages (except embryo) are included. Embryos are included as an immature lifestage for amphibians when the tadpole is considered an embryo. 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-6). 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. Zebrafish embryo

data were included where the tests were conducted using methods similar to OECD (2013) fish embryo toxicity test (FET). In model development, zebrafish embryo were kept separate from zebrafish juveniles such that separate models were developed for each life stage.

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

Only records designated as freshwater (FW) or saltwater (SW) 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.

4.3 Temperatures

To limit variability associated with temperature, a 6 °C range ($\pm 3^\circ\text{C}$) 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 $\pm 2^\circ\text{C}$ and (2) it maximized data retention while maintaining a relatively narrow temperature range. Temperature ranges were assigned for species where the reported temperatures exceeded a 6°C range. Temperature ranges were generally consistent with ASTM and OPPTS recommend test ranges (Appendix A-7). If temperature was reported in a record as a range (i.e., 19-22 °C), the average temperature was calculated to determine if temperature fell within the acceptable range. If the reported range was greater than 6 °C, then the record was excluded.

4.4 Dissolved Oxygen

Dissolved oxygen (DO) must be reported for inclusion into the model data subset or the record reported following standardized testing procedures which would meet the DO guidelines. If DO was reported as a range (i.e., 30-70%), then the average was used. 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 ≤ 48 h, 60-100%;
- S tests > 48 h, 40-100%;
- F or SR tests, 60-100%.

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.

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/MB/2015-01-001 July 2015). Once all standardization is complete, duplicate records are identified and removed. Duplicate records are defined by having the same source citation or authors, 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-8.

7 References

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8 Appendix A

Appendix A-1. Total number of records collected and retained by source for database version 3.3.

Data Source	Approx. # records obtained	# records in database	Dates
AWQC	5080	4232	See Appendix A-3 for document and year
Mayer et al. 2008	87	87	2008
ECOTOX	299500	11022	Last download 2014
HPV	4700	430	Downloaded Feb 2008
Literature	1090	670	1976-2014
Mayer 1987	375	307	1987
Mayer and Ellersieck 1986	2740	2703	1986
OPP	19400	2081	January 2007
OPPTS_PMN	110	61	December 2007
P&G	303	303	December 2015
Total	333378	21896	

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

ECOTOX Columns	ICE Column	Concatenate or Delete Columns	Notes
Result Number (unique identifier; previously called AQUIRE or Test Number prior to March 2012)	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 identify 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

ECOTOX Columns	ICE Column	Concatenate or Delete Columns	Notes
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 (µg/L)	---	---	Delete Records with Operators (>,<,&sim)
Conc 1 (µg/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 (µg/L)	---	---	Delete Records with Operators (>,<,&sim)
Conc 2 (µg/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 (µg/L)	---	---	Applies to both Conc 1 and 2. Moved those with non-µg/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
AWQC updates	1995
2,4-dichlorophenol	1980
2,4-dimethylphenol	1980
2-chlorophenol	1980
Acenaphthene	1980
Acrolein	1980
Acrylonitrile	1980
Aldrin/Dieldrin	1980
Aluminum	1988
Ammonia	2013
Antimony	1980
Arsenic	1984
Atrazine (draft)	2003
Benzene	1980
Benzidine	1980
Beryllium	1980
Cadmium	2001
Carbon tetrachloride	1980
Chlordane	1980
Chloride	1988
Chlorinated benzenes	1980
Chlorinated ethanes	1980
Chlorinated naphthalenes	1980
Chlorinated phenols	1980
Chlorine	1984
Chloroalkyl ethers	1980
Chloroform	1980
Chlorpyrifos	1986
Chromium	1984
Copper	1984
DDT	1980
Diazinon	2005
Dichlorobenzenes	1980
Dichloroethylenes	1980

Document Name	Year
Dichloropropane/propenes	1980
Dinitrotoluenes	1980
Diphenylhydrazine	1980
Endosulfan	1980
Endrin	1980
Ethylbenzene	1980
Fluoranthene	1980
Haloethers	1980
Halomethanes	1980
Heptachlor	1980
Hexachlorobutadiene	1980
Hexachlorocyclohexane	1980
Hexachlorocyclopentadiene	1980
Isophorone	1980
Lead (draft)	2008
Mercury	1984
Naphthalene	1980
Nickel	1986
Nitrobenzene	1980
Nitrophenols	1980
Nitrosamines	1980
Nonylphenol	2005
Parathion	1986
Pentachlorophenol	1986
Phenol	1980
Phthalate esters	1980
Selenium (draft)	2004
Silver (update)	2007
Thallium	1980
Toluene	1980
Toxaphene	1986
Trichloroethylene	1980
Zinc	1987

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Appendix A-5. Acceptable Chemical Grades with purities \geq 90% from Ecotox

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

Appendix A-6. Age classifications used to designate life stage in the database.

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
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
	<i>Polyodon spathula</i>							>565		>3644	Mims and Knaub 1993, Froese and Pauly 2008
Anguillidae	<i>Anguilla sp.</i>	< 70		< 0.5	70-400		0.5-100	> 400		> 100	Hardy 1978a, Froese and Pauly 2008
	<i>Anguilla anguilla</i>	<80		<.65	80-500		.65-236.47	>500		236.47	Froese and Pauly 2008
Atherinopsidae	<i>Menidia sp.</i>	< 10	<7-10 d	< 0.1	10-75	7- 60 d	0.1-2.5	> 75	>50-60 d	> 2.5	Martin and Drewry 1978, Froese and Pauly 2008, personal communication Scott Kellman, Aquatic Biosystems, Ft Collins, CO 2015
	<i>Menidia beryllina</i>	<10			10-50			>50			Wurtsbaugh and Li 1985, Froese and Pauly 2008
	<i>Menidia menidia</i>	5			<9.3			>9.3			Froese and Pauly 2008, Conover et al. 2005
	<i>Menidia peninsulae</i>	3.89			32.5			>42.5			Middaugh and Hemmer 1987
Melanotaeniidae	<i>Melanotaenia nigrans</i>	<21			21-70			>70			Crowley and Ivanstoffs 1982
	<i>Melanotaenia splendida</i>							>129			Crowley and Ivanstoffs 1982
Pseudomugilidae	<i>Pseudomugil signifer</i>							>28			Froese and Pauly 2008
Adrianichthyidae	<i>Oryzias latipes</i>		<2 w			>2-6 w			>5 w		Personal communication Rodney Johnson, EPA, MED, 2015
Anostomidae	<i>Leporinus obtusidens</i>				<21.6		<189.54	>21.6		>189.54	Froese and Pauly 2008
Clupeidae		< 30		< 0.2	30-180		0.2-100	> 180		> 100	Jones et al. 1978, Froese and Pauly 2008
Catostomidae	<i>Catostomus sp.</i>	< 17		< 0.1	17-200		0.1-100	> 200		> 100	Jones et al. 1978, Froese and Pauly 2008

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
Cyprinidae	<i>Abramis brama</i>							>387		>607	Froese and Pauly 2008
	<i>Bairdianus bendelisis</i>	<70			70-83			>83			Gairola et al. 1990, Froese and Pauly 2008
	<i>Campostoma anomalum</i>	< 20		< 0.1	20-100		0.1-2	> 100		> 2	Buynak and Mohr 1980b, Froese and Pauly 2008
	<i>Carassius sp.</i>	< 12		< 0.1	12-300		0.1-500	> 300		> 500	Jones et al. 1978, Froese and Pauly 2008
	<i>Cirrhinus mrigala</i>	< 20		< 0.1	20-525		0.1-500	> 525		> 500	Alikunhi 1956, Chakrabarty and Murty 1972, Froese and Pauly 2008
	<i>Cyprinus carpio</i>	< 19		< 0.1	19-250		0.1-200	> 250		> 200	Jones et al. 1978, Scott and Crossman 1979, Froese and Pauly 2008
	<i>Cyprinella spiloptera</i>							>38			Gotelli and Pyron 1991
	<i>Cyprinella whipplei</i>							>106			Gotelli and Pyron 1991
	<i>Gibelion catla</i>	< 20		< 0.1	20-440		0.1-500	> 440		> 500	Alikunhi 1956, Chakrabarty and Murty 1972, Froese and Pauly 2008
	<i>Gila elegans</i>	<28			28-260			> 260			Kaeding and Zimmerman 1983, Marsh 2004, Froese and Pauly 2008
	<i>Hybognathus amarus</i>	<9.2			9.2-18.8			>60	18 m		Magana 2007
	<i>Labeo sp.</i>	< 20		< 0.2	20-100		0.2-20	> 100		> 20	Alikunhi 1956, Chakrabarty and Murty 1972, Cambray 1985, Weyl and Booth 1999, Tedesco and Hugueny 2006, Froese and Pauly 2008
	<i>Notemigonus crysoleucas</i>	<14.7		0.09	14.7-64		.09-5.31	>64		>5.31	Buynak and Mohr 1980a, Froese and Pauly 2008
	<i>Notropis sp.</i>	< 15		< 0.1	15-40		0.1-0.5	> 40		> 0.5	Saksena 1962, Ross 2001, Froese and Pauly 2008
	<i>Phoxinus eos</i>	5.6-15			15-28			>28			Froese and Pauly 2008
	<i>Pimephales sp.</i>	< 10		< 0.1	10-50		0.1-1.4	> 50		> 1.4	Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
	<i>Pimephales promelas</i>	4-5.2		<.01	5.2-57	<4 m	.01-2	>57	>3-4 m	>2	Froese and Pauly 2008, personal communication Tim Dawson, EPA, MED, 2015
	<i>Pseudorasbora parva</i>							>20			Froese and Pauly 2015
	<i>Ptychocheilus lucius</i>	< 25			25-420	>25 d	>0.05 g	>420			Vanicek and Kramer 1969, Tyus and Haines 1991, Froese and Pauly 2008
	<i>Puntius conchonius</i>	<8			8-60			>60			Amenla and Dey 2013
	<i>Puntius sophore</i>							>50		>1.8	Hossain et al. 2012, Froese and Pauly 2008
	<i>Puntius ticto</i>	<14	<14 d	<.1	14-80	14-48 d	.1-15.1	>80	>48 d	15.1	Banik and Saha 2012, Froese and Pauly 2008
	<i>Rasbora daniconius</i>							>72		>3.3	Froese and Pauly 2008
	<i>Rhinichthys osculus</i>	<9		<.1	9-40		.1-4.6	>40		4.6	COSEWIC 2006, Froese and Pauly 2008
	<i>Scardinius erythrophthalmus</i>	<12		<0.01	12-81		.01-6.37	>81		>6.37	Wolnicki et al. 2009, Froese and Pauly 2008
	<i>Trigonostigma heteromorpha</i>	4+						>38			Froese and Pauly 2008
Aplocheilidae	<i>Rivulus marmoratus</i>	< 12			12-40			> 40			Grageda et al. 2004; Froese and Pauly 2008
Cyprinodontidae	<i>Cyprinodon sp.</i>	< 12		< 0.1	12-30		0.1-0.5	> 30		> 0.5	Hardy 1978a, personal communication Gerry Cripe EPA, GED 2008
	<i>Jordanella floridae</i>	>4	<8 d		<25	>8 d	<0.3 g	>25		>0.3g	Nasuti 2006; Holdway and Dixon 1986
Fundulidae	<i>Fundulus sp.</i>	< 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
	<i>Poecilia reticulata</i>	6			<20		<.58	>20	>1 m	>.58	Reznick 1983, Reznick et al. 1990, Froese and Pauly 2008

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
	<i>Xiphophorus maculatus</i>							>31		0.7	Froese and Pauly 2008
Esocidae	<i>Esox sp.</i>	< 20		< 0.1	20-200		0.1-55	> 200		> 55	Jones et al. 1978, Scott and Chapman 1979, Froese and Pauly 2008
Umbridae	<i>Umbra pygmaea</i>	< 8.5		<.01	8.5-37		.01-.44	>37		>.44	Froese and Pauly 2008
Gasterosteidae		< 15			15-45			> 45			Hardy 1978a, Able and Fahay 1998
	<i>Culaea inconstans</i>	< 26			26-38			>38	>1 y		Acere 1986
	<i>Gasterosteus aculeatus</i>	< 16	<9 d	<.03	16-45	>9 d-1 yr	.03-.94	>45	>1 yr	>.94	Norenburg and Ritgers 2015, Froese and Pauly 2008
Mugilidae		< 35		< 0.2	35-350		0.2-300	> 350		> 300	Martin and Drewry 1978, Froese and Pauly 2008
Anabantidae	<i>Anabas testudineus</i>	< 10		< 0.1	10-110		0.1-25	> 110		> 25	Mookerjee and Mazumdar 1946, Froese and Pauly 2008
Centrarchidae	<i>Lepomis sp.</i>	< 13		< 0.1	13-125		0.1-25	> 125		> 25	Hardy 1978b, Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008
	<i>Lepomis macrochirus</i>	<26		<.32	26-72	<1 y	.32-7.93	>72	>1 y	>7.93	Belk 1998, Froese and Pauly 2008
	<i>Micropterus sp.</i>	< 17		< 0.2	17-250		0.2-175	> 250		> 175	Hardy 1978b, Scott and Chapman 1979, Ross 2001, Froese and Pauly 2008
	<i>Micropterus salmoides</i>	<9		<.01	9-285	<9 m-1 y	.01-358.06	>285	>9 m-1 y	>358.06	Froese and Pauly 2008
	<i>Pomoxis sp.</i>	< 15		< 0.1	15-200		0.1-70	> 200		> 70	Hardy 1978b, Froese and Pauly 2008
Channidae	<i>Channos channos</i>	<13		<.03	13-918		.03-5890	>918		>5890	Froese and Pauly 2008
	<i>Channa orientalis</i>							>201			Froese and Pauly 2008
	<i>Channa punctata</i>	<40		<.99	10-120		.99-23.27	>120		23.27	Froese and Pauly 2008, Dehadrai and Tripathi 1976

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
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, personal communication M.Peterson
Embiotocidae	<i>Micrometrus minimus</i>							>106		>20	Schultz et al. 1991, Froese and Pauly 2008
Gobiidae	<i>Gobiosoma bosc</i>	< 7			7-30			> 30			Ruple 1984, Froese and Pauly 2008
Moronidae	<i>Morone americana</i>	< 20			20-150			> 150			Hardy 1978b, Froese and Pauly 2008
	<i>Morone chrysops</i>	<17.2			17.2-280	>4 w	>5.9	>280	>1 y	>250g	Denson and Smith 1996, Froese and Pauly 2008, Smith 1995
	<i>Morone saxatilis</i>	< 25	5-30 d		25-400	30 d-2 y		> 400	>2 y		Hardy 1978b, Froese and Pauly 2008, Fay et al. 1983
Percidae	<i>Etheostoma sp.</i>	< 18		< 0.1	18-35		0.1-0.4	> 35		> 0.4	Johnson 1984, Fisher 1990, Froese and Pauly 2008
	<i>Perca flavescens</i>	< 20		< 0.1	20-125		0.1-20	> 125		> 20	Hardy 1978b, Froese and Pauly 2008
	<i>Sander vitreus</i>	< 20		< 0.1	20-250		0.1-177	> 250		> 177	Hardy 1978b, Froese and Pauly 2008
Sciaenidae	<i>Leiostomus xanthurus</i>	< 15		< 0.1	15-200		0.1-90	> 200		> 90	Johnson 1978, Froese and Pauly 2008
Sparidae	<i>Lagodon rhomboides</i>	< 15		< 0.1	15-120		0.1-60	> 120		> 60	Johnson 1978, Froese and Pauly 2008
Terapontidae	<i>Bidyanus bidyanus</i>	3.6						>238		>412.7	Rowland 2004
	<i>Terapon jarbua</i>	< 23		< 0.3	23-130		0.3-46.92	>130		>46.92	Froese and Pauly 2008
Pleuronectidae	<i>Platichthys sp.</i>	< 7		< 0.1	7-200		0.1-80	> 200		> 80	Ahlstrom et al. 1984, Froese and Pauly 2008
Salmonidae	<i>Oncorhynchus sp.</i>	< 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
	<i>Oncorhynchus mykiss</i>	<40		<0.3	40-192	>19 d	0.3-70	>192		>70	Froese and Pauly 2008; USEPA 1996

Family	Species	Larvae ^a			Juvenile ^b			Adult			Source
		Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	Lengths (mm)	Age	weights (g)	
	<i>Prosopium williamsoni</i>	<60			60-200			>200	>2 y	>100g	McPhail and Troffe 1998, Stalnaker and Gresswell 1974
	<i>Salmo sp.</i>	< 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
	<i>Salvelinus sp.</i>	<20		< 0.2	20-200		0.2-100	> 200		> 100	Kendall and Behnke 1984, Froese and Pauly 2008, Ueberschar and Froese 2008
	<i>Salvelinus fontinalis</i>	<18		<.1	18-150		0.1-42.1	>150		>42.1	Froese and Pauly 2008
Cottidae	<i>Cottus bairdii</i>	<9			9-41			>41			Grossman et al. 2002, Froese and Pauly 2008
Ariidae	<i>Ariopsis felis</i>	<45			68-88			>126			Froese and Pauly 2008, Merriman 1940
Bagridae		< 10			10-90			> 90			Rahman et al. 2004, Froese and Pauly 2008
Clariidae	<i>Heterobranchus longifilis</i>	>3.1		0.2	3.1-597		0.2-1588	>597		1588	Froese and Pauly 2008, Legendre 1986
Heteropneustidae		< 12			12-120			> 120			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
	<i>Ameiurus nebulosus</i>	4-22		<.13	22-178		0.13-71.06	>178		>71.06	Froese and Pauly 2008
Mastacembilidae	<i>Macrogathus aculeatus</i>	<10.8	<30 d	< 0.1	10.8-160		0.1-14.6	>160		14.6	Das and Kalita 2003, Froese and Pauly 2008
	<i>Monopterus albus</i>							>400		>60.2	Froese and Pauly 2015
Syngnathidae	<i>Syngnathus fuscus</i>	9+						>99		>1.1	Froese and Pauly 2015, Campbell and Able 1998
Monacanthidae	<i>Stephanolepis hispidus</i>	< 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)

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Appendix A-7. Temperature ranges used to standardize species in the model data subset.

Species	ICE Temp Acceptance Range	Species from Guidelines	ASTM ¹	OPP ²	OPPTS 1996 ³	OECD 203 ⁴	EPA 1975 ⁵	EPA 1993 ⁶
<i>Acartia tonsa</i>	20-26	x	x	x	x	x	x	x
<i>Actinonaias pectorosa</i>	20-26	x	x	x	x	x	x	x
<i>Aedes aegypti</i>	22-28	x	x	x	x	x	x	x
<i>Aldrichetta forsteri</i>	19-25	x	x	x	x	x	x	x
<i>Ameiurus melas</i>	18-24	x	x	x	x	x	x	x
<i>Ameiurus nebulosus</i>	18-24	x	x	x	x	x	x	x
<i>Americamysis bahia</i>	21-27	<i>Americamysis bahia</i>	25-29	21-23	23-27	x	x	19-21, 24-26
<i>Ampelisca abdita</i>	20-26	x	x	x	x	x	x	x
<i>Asellus sp.</i>	18-24	x	x	x	x	x	x	x
<i>Asellus aquaticus</i>	13-19	x	x	x	x	x	x	x
<i>Astropecten sp.</i>	19-25	x	x	x	x	x	x	x
<i>Baetis sp.</i>	15-21	x	x	x	x	x	x	x
<i>Bidyanus bidyanus</i>	20-26	x	x	x	x	x	x	x
<i>Bufo bufo</i>	16-22	x	x	x	x	x	x	x
<i>Caecidotea brevicauda</i>	15-21	x	x	x	x	x	x	x
<i>Carassius auratus</i>	17-23	<i>Carassius auratus</i>	15-24	x	x	x	20-24	x
<i>Catostomus commersonii</i>	10-16	x	x	x	x	x	x	x
<i>Ceriodaphnia dubia</i>	21-27	<i>Ceriodaphnia dubia</i>	23-27	x	x	x	x	19-21, 24-26
<i>Chironomus sp.</i>	17-23	<i>Chironomus sp.</i>	20-24	x	x	x	20-24	x
<i>Chironomus plumosus</i>	17-23	<i>Chironomus sp.</i>	20-24	x	x	x	20-24	x
<i>Chironomus riparius</i>	17-23	<i>Chironomus sp.</i>	20-24	x	x	x	20-24	x
<i>Chironomus tentans</i>	19-25	<i>Chironomus sp.</i>	20-24	x	x	x	20-24	x
<i>Chironomus zealandicus</i>	17-23	<i>Chironomus sp.</i>	20-24	x	x	x	20-24	x
<i>Clarias batrachus</i>	20-26	x	x	x	x	x	x	x
<i>Coregonus fera</i>	8-14	x	x	x	x	x	x	x
<i>Corophium volutator</i>	9-15	x	x	x	x	x	x	x
<i>Crangonyx pseudogracilis</i>	8-14	x	x	x	x	x	x	x
<i>Crassostrea virginica</i>	19-25	<i>Crassostrea virginica</i>	20-24	x	x	x	x	x
<i>Ctenopharyngodon idella</i>	19-25	x	x	x	x	x	x	x

Species	ICE Temp Acceptance Range	Species from Guidelines	ASTM ¹	OPP ²	OPPTS 1996 ³	OECD 203 ⁴	EPA 1975 ⁵	EPA 1993 ⁶
<i>Culicoides furens</i>	19-25	x	x	x	x	x	x	x
<i>Cyclops</i> sp.	18-24	x	x	x	x	x	x	x
<i>Cymatogaster aggregata</i>	12-18	x	x	x	x	x	x	x
<i>Cyprinodon variegatus</i>	20-26	<i>Cyprinodon variegatus</i>	20-24	21-23	20-24	x	20-24	19-21, 24-26
<i>Cyprinus carpio</i>	18-24	<i>Cyprinus carpio</i>	x	x	20-24	20-24	x	x
<i>Daphnia carinata</i>	18-24	x	x	x	x	x	x	x
<i>Daphnia magna</i>	18-24	<i>Daphnia magna</i>	18-22	x	18-22	x	15-19	19-21, 24-26
<i>Daphnia pulex</i>	15-21	<i>Daphnia pulex</i>	18-22	x	18-22	x	15-19	19-21, 24-26
<i>Diaptomus clavipes</i>	16-22	x	x	x	x	x	x	x
<i>Esox lucius</i>	12-18	x	x	x	x	x	x	x
<i>Eurytemora affinis</i>	19-25	x	x	x	x	x	x	x
<i>Farfantepenaeus duorarum</i>	19-25	<i>Farfantepenaeus duorarum</i>	20-24	x	x	x	20-24	x
<i>Fenneropenaeus indicus</i>	23-29	x	x	x	x	x	x	x
<i>Gambusia affinis</i>	14-20	x	x	x	x	x	x	x
<i>Gammarus fasciatus</i>	15-21	<i>Gammarus fasciatus</i>	15-19	x	17-19	x	15-19	x
<i>Gammarus lacustris</i>	14-20	<i>Gammarus lacustris</i>	15-19	x	17-19	x	15-19	x
<i>Gammarus pseudolimnaeus</i>	15-21	<i>Gammarus pseudolimnaeus</i>	15-19	x	17-19	x	15-19	x
<i>Gammarus pulex</i>	13-19	x	x	x	x	x	x	x
<i>Gasterosteus aculeatus</i>	18-24	<i>Gasterosteus aculeatus</i>	15-19	x	10-14	x	20-24	x
<i>Gibellion catla</i>	24-30	x	x	x	x	x	x	x
<i>Heteropneustes fossilis</i>	20-26	x	x	x	x	x	x	x
<i>Hexagenia bilineata</i>	18-24	x	x	x	x	x	x	x
<i>Hyaella azteca</i>	18-25	x	x	x	x	x	x	x
<i>Ictalurus punctatus</i>	17-23	<i>Ictalurus punctatus</i>	15-24	x	20-24	x	20-24	x
<i>Ischnura</i> sp.	13-19	x	x	x	x	x	x	x
<i>Ischnura verticalis</i>	15-21	x	x	x	x	x	x	x
<i>Labeo rohita</i>	24-30	x	x	x	x	x	x	x
<i>Lagodon rhomboides</i>	20-26	<i>Lagodon rhomboides</i>	20-24	x	x	x	20-24	x
<i>Lates calcarifer</i>	24-30	x	x	x	x	x	x	x
<i>Leiostomus xanthurus</i>	21-27	x	x	x	x	x	x	x
<i>Lepomis cyanellus</i>	17-23	<i>Lepomis cyanellus</i>	15-24	x	x	x	x	x
<i>Lepomis macrochirus</i>	18-24	<i>Lepomis macrochirus</i>	15-24	x	20-24	21-25	20-24	x
<i>Lepomis microlophus</i>	18-24	x	x	x	x	x	x	x
<i>Lestes congener</i>	19-25	x	x	x	x	x	x	x

Species	ICE Temp Acceptance Range	Species from Guidelines	ASTM ¹	OPP ²	OPPTS 1996 ³	OECD 203 ⁴	EPA 1975 ⁵	EPA 1993 ⁶
<i>Limnodrilus hoffmeisteri</i>	20-26	x	x	x	x	x	x	x
<i>Lithobates catesbeianus</i>	17-23	x	x	x	x	x	x	x
<i>Lithobates clamitans</i>	17-23	x	x	x	x	x	x	x
<i>Lithobates pipiens</i>	17-24	x	x	x	x	x	x	x
<i>Lumbriculus variegatus</i>	19-25	x	x	x	x	x	x	x
<i>Menidia beryllina</i>	19-25	<i>Menidia</i> sp.	20-24	21-23	20-24	x	20-24	19-21, 24-26
<i>Menidia menidia</i>	22-28	<i>Menidia</i> sp.	20-25	21-24	20-25	x	20-25	19-21, 24-27
<i>Micropterus dolomieu</i>	17-23	x	x	x	x	x	x	x
<i>Micropterus salmoides</i>	17-23	x	x	x	x	x	x	x
<i>Morone saxatilis</i>	13-19	x	x	x	x	x	x	x
<i>Mystus vittatus</i>	22-28	x	x	x	x	x	x	x
<i>Neanthes arenaceodentata</i>	17-23	x	x	x	x	x	x	x
<i>Neomysis americana</i>	19-25	x	x	x	x	x	x	x
<i>Nereis diversicolor</i>	10-16	x	x	x	x	x	x	x
<i>Notemigonus crysoleucas</i>	16-22	x	x	x	x	x	x	x
<i>Notropis topeka</i>	19-25	x	x	x	x	x	x	x
<i>Oncorhynchus clarkii</i>	9-15	x	x	x	x	x	x	x
<i>Oncorhynchus gorbuscha</i>	9-15	x	x	x	x	x	x	x
<i>Oncorhynchus keta</i>	9-15	x	x	x	x	x	x	x
<i>Oncorhynchus kisutch</i>	9-15	<i>Oncorhynchus kisutch</i>	10-14	x	10-14	x	10-14	x
<i>Oncorhynchus mykiss</i>	9-15	<i>Oncorhynchus mykiss</i>	10-14	x	10-14	13-17	10-14	11-13
<i>Oncorhynchus nerka</i>	7-13	x	x	x	x	x	x	x
<i>Oncorhynchus tshawytscha</i>	9-15	x	x	x	x	x	x	x
<i>Ophiogomphus</i> sp.	15-21	x	x	x	x	x	x	x
<i>Orconectes nais</i>	15-21	<i>Orconectes</i> sp.	15-24	x	x	x	20-24	x
<i>Oreochromis mossambicus</i>	23-29	x	x	x	x	x	x	x
<i>Oryzias latipes</i>	19-25	<i>Oryzias latipes</i>	x	x	x	21-25	x	x
<i>Palaemonetes</i> sp.	19-25	x	x	x	x	x	x	x
<i>Palaemonetes kadiakensis</i>	15-21	x	x	x	x	x	x	x
<i>Paratanytarsus dissimilis</i>	18-24	x	x	x	x	x	x	x
<i>Pelophylax nigromaculata</i>	15-21	x	x	x	x	x	x	x
<i>Penaeus merguensis</i>	29-35	x	x	x	x	x	x	x
<i>Penaeus monodon</i>	23-29	x	x	x	x	x	x	x
<i>Penaeus semisulcatus</i>	18-24	x	x	x	x	x	x	x

Species	ICE Temp Acceptance Range	Species from Guidelines	ASTM ¹	OPP ²	OPPTS 1996 ³	OECD 203 ⁴	EPA 1975 ⁵	EPA 1993 ⁶
<i>Perca flavescens</i>	12-18	x	x	x	x	x	x	x
<i>Pimephales promelas</i>	20-26	<i>Pimephales promelas</i>	23-27	x	21-25	21-25	20-24	19-21, 24-26
<i>Poecilia reticulata</i>	23-29	<i>Poecilia reticulata</i>	x	x	21-25	21-25	x	x
<i>Polypedilum</i> sp.	18-24	x	x	x	x	x	x	x
<i>Praunus flexuosus</i>	9-15	x	x	x	x	x	x	x
<i>Pseudacris regilla</i>	17-23	x	x	x	x	x	x	x
<i>Pteronarcella badia</i>	10-16	x	x	x	x	x	x	x
<i>Pteronarcys californica</i>	10-16	<i>Pteronarcys</i> sp.	10-14	x	x	x	10-14	x
<i>Puntius conchonius</i>	13-19	x	x	x	x	x	x	x
<i>Salmo salar</i>	11-17	<i>Salmo salar</i>	x	x	10-14	x	x	x
<i>Salmo trutta</i>	11-17	x	x	x	x	x	x	x
<i>Salvelinus confluentus</i>	7-13	x	x	x	x	x	x	x
<i>Salvelinus fontinalis</i>	11-17	<i>Salvelinus fontinalis</i>	10-14	x	10-14	x	10-14	11-13
<i>Salvelinus namaycush</i>	9-15	x	x	x	x	x	x	x
<i>Sander vitreus</i>	12-18	x	x	x	x	x	x	x
<i>Scylla serrata</i>	23-29	x	x	x	x	x	x	x
<i>Simocephalus serrulatus</i>	15-21	x	x	x	x	x	x	x
<i>Simocephalus vetulus</i>	19-25	x	x	x	x	x	x	x
<i>Streptocephalus proboscideus</i>	19.5-25.5	x	x	x	x	x	x	x
<i>Tilapia nilotica</i>	21-27	x	x	x	x	x	x	x
<i>Tilapia zillii</i>	24-30	x	x	x	x	x	x	x
<i>Tubifex tubifex</i>	19-25	x	x	x	x	x	x	x
<i>Utterbackia imbecillis</i>	19-25	x	x	x	x	x	x	x
<i>Villosa iris</i>	19-25	x	x	x	x	x	x	x
<i>Villosa lienosa</i>	25-31	x	x	x	x	x	x	x
<i>Villosa villosa</i>	25-31	x	x	x	x	x	x	x
<i>Xenopus laevis</i>	22-28	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

Appendix A-8. 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)
Source citation	Citation of original source of data (i.e. the source listed in ECOTOX or AWQC for where they obtained the data)
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); 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, E = embryo)
Test duration	48h; 96h; NR (not recorded)
Dose Type	LC50; EC50; NR (not recorded)
Test Type	F (flow through); S (static); R (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	True/False field - does record meet ICE model standardization requirements
Comments	Any additional information from source that could be useful
MMR-False	If record does not meet model requirements (MMR), this column contains the reason(s) why record is false (e.g. age)

9 Appendix B. Algae ICE Module; 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 E_rC_{50} was based on growth rate while an E_bC_{50} 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
	Compound	CAS corresponds to single compound or element 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 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