United States Environmental Protection Agency

Augmenting Species Diversity in Water Quality Criteria Derivation using Interspecies Correlation Models

Mace G. Barron, Crystal R. Lilavois, Morgan M. Willming, Jill Awkerman, Sandy Raimondo

USEPA Office of Research and Development
Gulf Ecology Division

The Problem of Species Diversity

Most Commonly Reported Aquatic Toxicity Test Records in ECOTOX

Taxa	Test Type	Number of Records[a]
Fish	Acute	10,566
	Chronic	4,184
	Bioconcentration	796
Arthropods	Acute	8,134
	Chronic	698
Mollusk	Acute	1,722
	Bioconcentration	239
Plant	Acute	933
Algae	Acute	468
	Chronic	571
Amphibian	Acute	393
	Chronic	323
Annelid	Acute	234
	Chronic	121
Rotifer	Acute	210
Echinoderm	Acute	74

Species	Common Name	Percentage of Records[a]
Oncorhynchus mykiss	Rainbow trout	7.7
Daphnia magna	Water flea	6.2
Pimephales promelas	Fathead minnow	5.3
Lepomis macrochirus	Bluegill	2.8
Cyprinus carpio	Common carp	2.0
Danio rerio	Zebra danio	1.8
Oryzias latipes	Japanese medaka	1.4
Ceriodaphnia dubia	Water flea	1.3
Pseudokirchneriella subcapitata	Green algae	1.3
Ictalurus punctatus	Channel catfish	1.2

2012 Download: Fairbrother, Barron, Johnson 2015

Web-ICE developed to address problem of species diversity

ICE (Interspecies Correlation Estimation)
- log-linear models of the relationship between the acute toxicity (LC50) of chemicals tested in two species

Web-ICE
- internet application containing suite of ICE models
- predict acute toxicity to species, genus or family level
- fish/invertebrate/amphibian; algae; wildlife
- modules for SSD generation, batch T&E taxa prediction
- peer reviewed technical basis (publications, SAP)

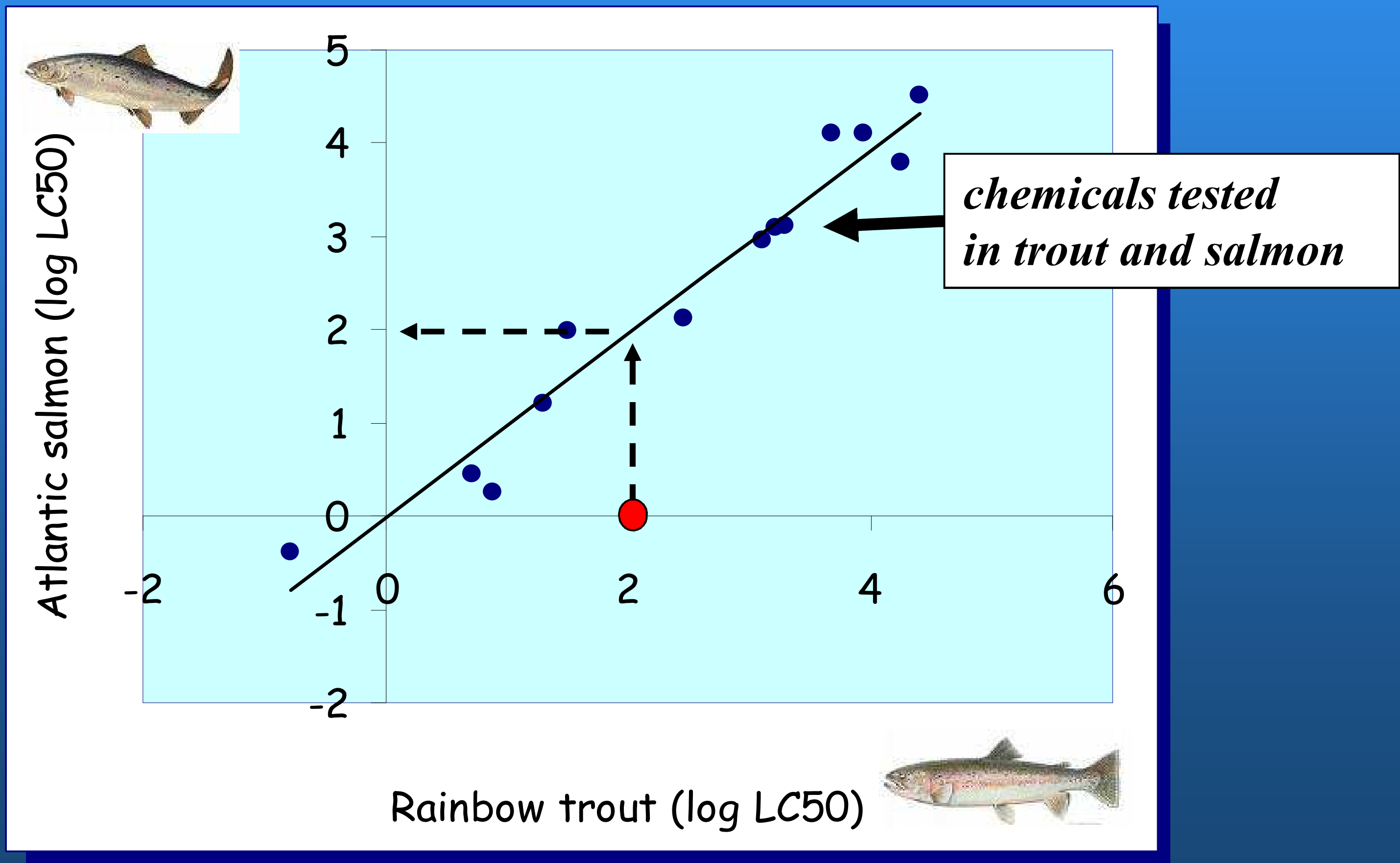
Regression models built from standardized toxicity values
- chemical identity/purity; CAS/name curation
- water quality, test conditions, species/life stage

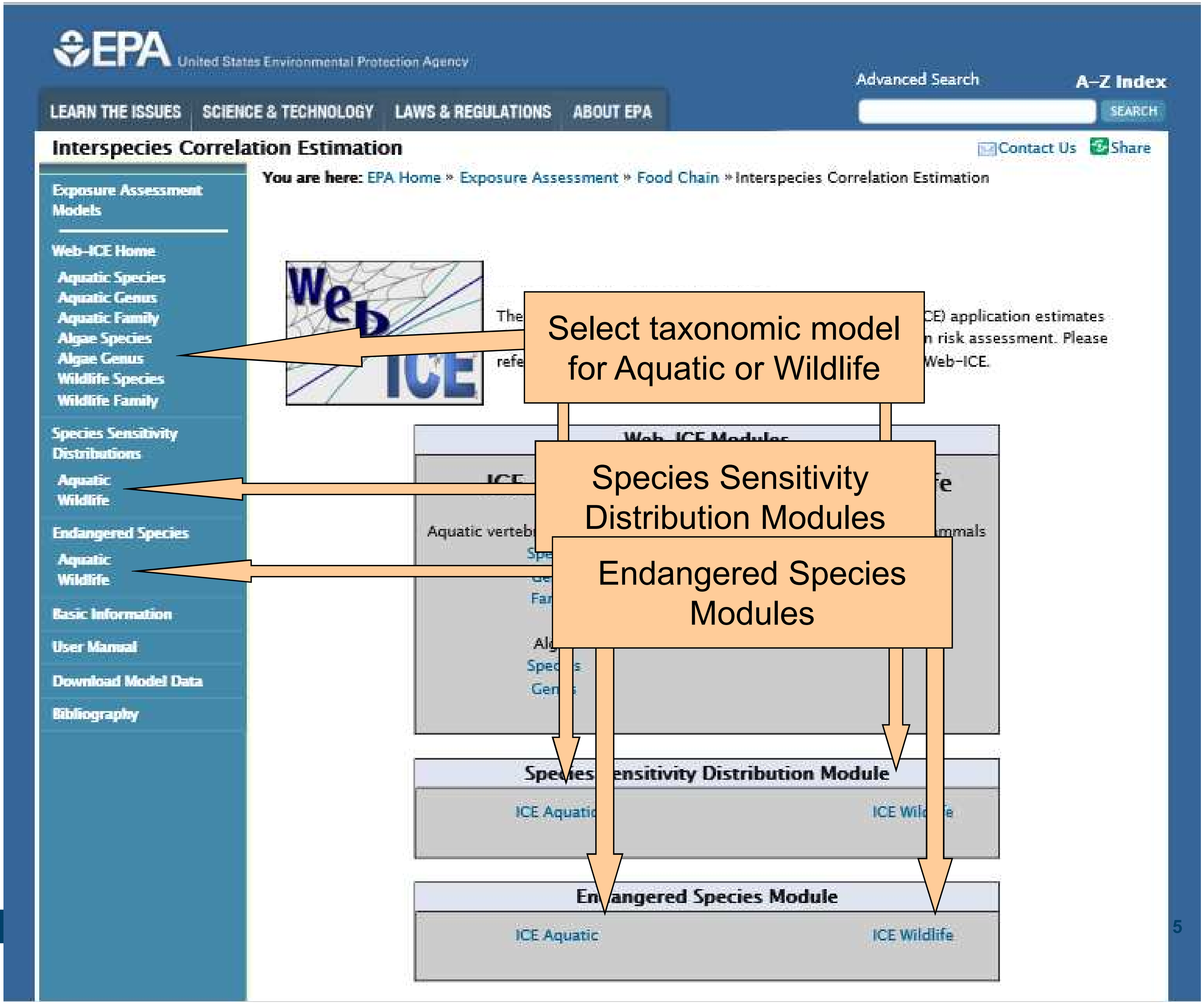
2015 Update
- increased taxa diversity
- change from geomean genus/family level models to minimum toxicity models
- ORD website migration (in progress)

What are ICE models?

Interspecies Correlation Estimation (ICE)

Log-linear models of the relationship between the acute toxicity (LC50) of chemicals tested in two species

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Web-ICE Aquatic Data Sources

Acute toxicity: fish, amphibians, and aquatic invertebrates

- ECOTOX
- OPP: ecotox database
- OPPT: PMN, HPV
- OW: AWQC
- USGS (RM grant)
- P&G (CRADA)
- Open literature (T&E, molluscs)

QA/QC:

- centralized data management system
- data transcription thoroughly reviewed
- CAS/chemical curation
- species name consistency
- reviewed each source for quality
- duplicate records removed

	EXPERIMENTAL	LOG	SPECIES	CHEMICAL	GLOCHIDIA LAB	JUVENILE LAB
Metallic stress	(>363, 272)	(>2.6, 2.4)	Lampsilis siliquoidea	Lead	CERC	CERC
	(>107, 99)	(>2.0, 2.0)	Villosa iris	Mercury	VPI	VPI
	(>247, 19)	(>2.4, 1.3)	Lampsilis siliquoidea	Cadmium	CERC	CERC
	(>330, 28)	(>2.5, 1.4)	Lampsilis cardium	Cadmium	CERC	SU
	(31, 23)	(1.5, 1.4)	Utterbackia imbecillis	Cadmium	UGA	CU
	(10, 11)	(1.0, 1.1)	Lampsilis abrupta	Copper	CERC	CERC
	(14, 7.0)	(1.1, 0.84)	Lampsilis fasciola	Copper	CERC, Univ. of Guelph, VPI	CERC
	(12, 9.6)	(1.1, 0.98)	Lampsilis rafinesqueana	Copper	CERC	CERC
	(14, 11)	(1.2, 1.0)	Lampsilis siliquoidea	Copper	ASU, CERC, Univ. of Guelph	CERC
	(57, 13)	(1.8, 1.1)	Megalonaias nervosa	Copper	ASU	CERC
	(23, 25)	(1.4, 1.4)	Utterbackia imbecillis	Copper	UGA	ASU, CERC, CU, UGA
	(11, 7.6)	(1.1, 0.88)	Villosa iris	Copper	CERC	ARRC, CERC
	(411, 200)	(2.6, 2.3)	Actinonaias pectorosa	Zinc	VPI	VPI
	(2779, 182)	(3.4, 2.3)	Lampsilis siliquoidea	Zinc	CERC	CERC
	(724, 250)	(2.9, 2.4)	Villosa iris	Zinc	VPI	VPI
Narcosis	(6000, 6300)	(3.8, 3.8)	Lampsilis siliquoidea	2-Propanol	NCSU	NCSU
	(390, 375)	(2.6, 2.6)	Utterbackia imbecillis	Nonylphenol	UGA	UGA
	(5900, 7200)	(3.8, 3.9)	Lampsilis siliquoidea	Glyphosate isopropylamine salt	NCSU	NCSU
	(20750, 10010)	(4.3, 4.0)	Lampsilis siliquoidea	Propiconazole	NCSU	NCSU
	(480, 30)	(2.7, 1.5)	Lampsilis siliquoidea	Pyraclostrobin	NCSU	NCSU
Respiratory toxicity	(72, >100)	(1.9, >2)	Lampsilis siliquoidea	Chlorine	CERC	CERC
	(103, 80)	(2.0, 1.9)	Epioblasma capsaeformis	Chlorine	VPI	VPI
	(1333, 1082)	(3.1, 3.0)	Utterbackia imbecillis	Chlorine	UGA	UGA
	(220, 68)	(2.3, 1.8)	Villosa iris	Chlorine	VPI	CERC
	(544025, 3980000)	(5.7, 6.6)	Lampsilis fasciola	Sodium chloride	NCSU, Univ. of Guelph	NCSU
	(1437900, 3750799)	(6.2, 6.6)	Lampsilis siliquoidea	Sodium chloride	CERC, NCSU, Univ. of Guelph	CERC, NCSU
	(2760000, 4503332)	(6.4, 6.7)	Villosa constricta	Sodium chloride	NCSU	CERC
	(3310000, 5230000)	(6.5, 6.7)	Villosa delumbis	Sodium chloride	NCSU	NCSU
	(13090, 11526)	(4.1, 4.1)	Lampsilis fasciola	Ammonia	CERC	CERC, VPI
	(14793, 18323)	(4.2, 4.3)	Lampsilis rafinesqueana	Ammonia	CERC	CERC
	(19416, 8750)	(4.3, 3.9)	Lampsilis siliquoidea	Ammonia	CERC	CERC, Purdue Univ.
	(8235, 6441)	(3.9, 3.8)	Utterbackia imbecillis	Ammonia	UGA	CERC, EPA, TVA, UGA
	(7619, 9296)	(3.9, 4.0)	Villosa iris	Ammonia	CERC, VPI	CERC, VPI
	(636514, 669666)	(5.8, 5.8)	Alasmidonta raveneliana	Sodium fluoride	EPA	EPA
	(775751, 517168)	(5.9, 5.7)	Utterbackia imbecillis	Sodium fluoride	EPA	EPA
Other MOAs	(164400, >500000)	(5.2, >5.7)	Lampsilis siliquoidea	Perfluorooctanoic acid	NCSU	NCSU
	(16100, >500000)	(4.2, >5.7)	Ligumia recta	Perfluorooctanoic acid	NCSU	NCSU
	(16500, 158100)	(4.2, 5.2)	Lampsilis siliquoidea	Perfluorooctanesulfonic acid	NCSU	NCSU
	(13500, 141700)	(4.1, 5.2)	Ligumia recta	Perfluorooctanesulfonic acid	NCSU	NCSU
	(625, 62)	(2.8, 1.8)	Lampsilis siliquoidea	Fluoxetine hydrochloride	NCSU	NCSU
	(293, 97)	(2.5, 2.0)	Ligumia recta	Fluoxetine hydrochloride	NCSU	NCSU
	(500, 250)	(2.7, 2.4)	Lampsilis siliquoidea	Chlorpyrifos	NCSU	NCSU
	(90, 280)	(2.0, 2.4)	Lampsilis siliquoidea	Chlorothalonil	NCSU	NCSU

Open-ended value
Multiple Laboratories

Data Standardization

Chemical
- CAS/name curation
- single compound tested; a.i. $\geq$ 90%
- chemical & element specific AWQC normalizations

Species-Specific Test Conditions
- no sed, diet, mixture exposures or phototoxicity results
- ASTM/OCSPP standards or equivalent
- temperature (6 ^{o}C range); D.O. (>40-60%); Salinity (FW:<1ppt; SW:$\geq$15ppt)

Endpoint = mortality/immobilization
- 24-48 h EC50 – fairy shrimp
- 48h EC/LC50 - daphnids, midges and mosquitoes
- 96h EC/LC50 – fish, amphibians and other invertebrates

Life stage
- fish, decapods: juvenile only
- mollusc: juvenile, spat
- amphibians, insects: immature
- all other species: all life stages except embryo/egg

- T&E listing (**ecos.fws.gov/ecos/home.action**)

Peer Reviewed ICE Research

Environ. Sci. Technol. 2008, 42, 3447–3452

Development of Species Sensitivity Distributions for Wildlife using Interspecies Toxicity Correlation Models

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Taylor & Francis

Estimation of Wildlife Hazard Levels Using Interspecies Correlation Models and Standard Laboratory Rodent Toxicity Data

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Hazard/Risk Assessment

AUGMENTING AQUATIC SPECIES SENSITIVITY DISTRIBUTIONS WITH INTERSPECIES TOXICITY ESTIMATION MODELS

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Environ. Sci. Technol. 2007, 41, 5888–5894

Estimation of Chemical Toxicity to Wildlife Species Using Interspecies Correlation Models

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PROTECTIVENESS OF SPECIES SENSITIVITY DISTRIBUTION HAZARD CONCENTRATIONS FOR ACUTE TOXICITY USED IN ENDANGERED SPECIES RISK ASSESSMENT

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Ecotoxicology (2009) 18:918–928
DOI 10.1007/s10646-009-0353-y

Standardizing acute toxicity data for use in ecotoxicology models: influence of test type, life stage, and concentration reporting

Sandy Raimondo · Deborah N. Vivian · Mace G. Barron

Environ. Sci. Technol. 2010, 44, 7711–7716

Influence of Taxonomic Relatedness and Chemical Mode of Action in Acute Interspecies Estimation Models for Aquatic Species

SANDY RAIMONDO,* CRYSTAL R. JACKSON, AND MACE G. BARRON
US Environmental Protection Agency, National Health and

Environmental Science & Technology
Article
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Development and Practical Application of Petroleum and Dispersant Interspecies Correlation Models for Aquatic Species

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Interspecies Correlation Estimation—Applications in Water Quality Criteria and Ecological Risk Assessment

Chenglian Feng,† Fengchang Wu,*,† Yunsong Mu,† Wei Meng,† Scott D. Dyer,‡ Ming Fan,‡ Sandy Raimondo,§ and Mace G. Barron§

Environ. Sci. Technol. 2008, 42, 3076–3083

Comparison of Species Sensitivity Distributions Derived from Interspecies Correlation Models to Distributions used to Derive Water Quality Criteria

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Predicting the Toxicities of Chemicals to Aquatic Animal Species

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Anita Pease[2]
Sandy Raimondo[3]

Aquatic Toxicology 116–117 (2012) 1–7
Contents lists available at SciVerse ScienceDirect
Aquatic Toxicology
journal homepage: www.elsevier.com/locate/aquatox
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Evaluation of in silico development of aquatic toxicity species sensitivity distributions

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Web-ICE 2015 Update (v. 3.3; October)

Increased taxa diversity and expanded T&E:

- new data developed for mussel and fairy shrimp (USGS/FWS collaboration (ms accepted, in prep)
- overall: 1.5x records, 1.8x species, 2x models
- T&E: 1.3x records; 1.5x species, 2x models

Genus and family level changed to minimum toxicity models:

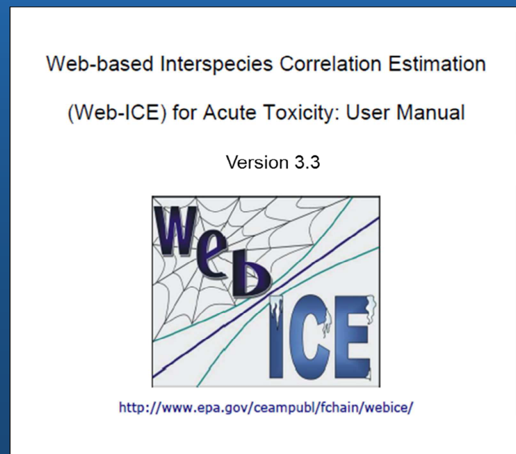
- fit to minimum genus or family value (no longer geomean)

Other updates:

- 2015 User Guidance, Database Documentation, Bibliography
- new MOA specific models (based on MOAtox v. 1.0)

Updated rules of thumb:

- MSE $\leq$ 0.95
- $R^2 > 0.6$
- slope $\geq$ 0.6
- predicted value CI within 10x


Web-based Interspecies Correlation Estimation

(Web-ICE) for Acute Toxicity: User Manual

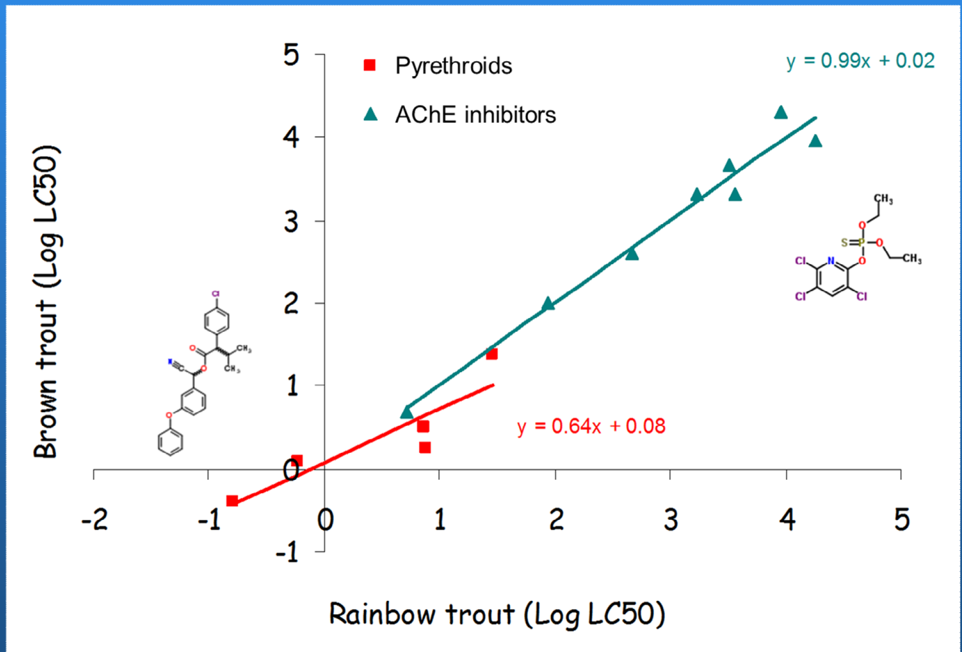
Version 3.3

Web ICE

http://www.epa.gov/ceampubl/fchain/webice/

Web-ICE v3.3: Updated MOA-specific models

- standard ICE models have chemicals of mixed mode of action (MOA)
- MOA-specific models developed using MOAtox (Barron et al. 2015)
- improved prediction accuracy for high taxa distance species pairs
- MOA-specific models downloadable via Web-ICE



MOAtox v. 1.0 database

- **AChE inhibition** (285)
  - Carbamate (74)
  - Organophosphate (211)
- **Electron transport inhibition** (91)
  - Arsenical respiratory inhibition (22)
  - Oxidative phosphorylation inhibition (14)
  - Uncoupling oxidative phosphorylation (55)
- **Iono/Osmoregulatory/Circulatory impairment** (51)
  - Anticoagulation (25)
  - Metallic iono/osmoregulatory impairment (14)
  - Methemoglobinemia (6)
  - Other osmoregulatory (6)
- **Narcosis** (465)
  - Ester (48)
  - Unknown (9)
  - Nonpolar (347)
  - Polar (61)
- **Neurotoxicity** (201)
  - Alicyclic GABA antagonism (42)
  - Diphenyl sodium channel modulation (11)
  - GABA agonism (16)
  - nAChR agonism (8)
  - Other (9)
  - Pyrazole GABA antagonism (6)
  - Pyrethroid sodium channel modulation (102)
  - Sodium channel blocking (3)
  - Strychnine (4)
- **Reactivity** (111)
  - Acrylate (8)
  - Alkylation (38)
  - Carbonyl (13)
  - Chromate (3)
  - Cyanate/nitrile (9)
  - Di/trinitroaromatic (14)
  - Hydrazine (4)
  - Other (19)
  - Phosphide (3)


Contents lists available at ScienceDirect

Aquatic Toxicology

journal homepage: www.elsevier.com/locate/aquatox

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MOAtox: A comprehensive mode of action and acute aquatic toxicity database for predictive model development

M.G. Barron[a,*], C.R. Lilavois[a], T.M. Martin[b]

Web-ICE October 2015 Update:
increased T&E and taxa diversity

All Species						
Web-ICE Database	Database Attributes			Number of models		
	Records	Species	Chemicals	Species	Genus	Family
v. 3.3 (2015)	8203	314	1501	1544	854	887
v. 3.2 (2013)	5501	180	1266	780	289	374

U.S. Threatened and Endangered Species						
Web-ICE Database	Database Attributes			Number of models		
	Records	Species	Chemicals	Species	Genus	Family
v. 3.3 (2015)	1591	32	492	379	428	547
v. 3.2 (2013)	1272	21	449	230	168	267

Web-ICE October 2015 Update:
prediction accuracy; all species models

Cross-validation results; n>3	Percentage within prediction category					
	Taxonomic Distance	Significant Models (N)	5-fold	10-fold	50-fold	>50-fold
genus	1	444	95	4	1	0
family	2	1144	92	6	2	0
order	3	430	87	11	3	0
class	4	5734	77	10	10	3
phylum	5	1658	62	14	16	8
kingdom	6	8006	55	15	19	11

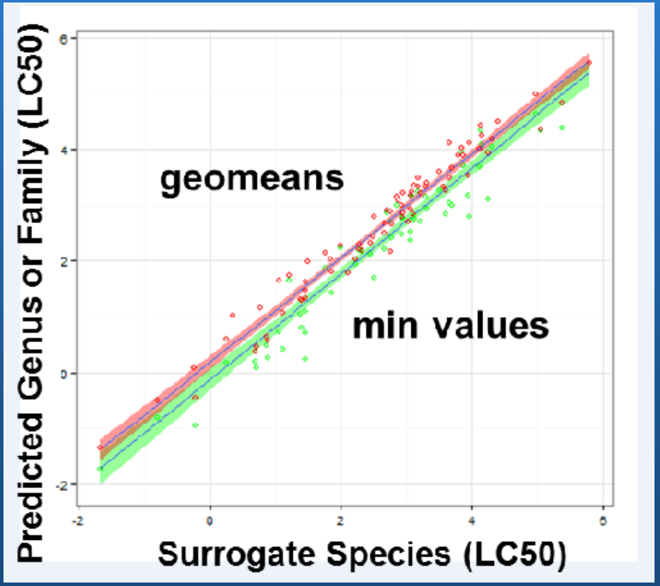
Genus and Family Level Minimum Models
Web-ICE v3.3

Genus and Family Level Models:

• used when species-specific ICE models not available
• need to be protective of T&E species within the Genus or Family
• previous ICE models (v. 3.2) based on geomean had limited conservatism
• min models in Web-ICE (v. 3.3)

What are minimum toxicity models:

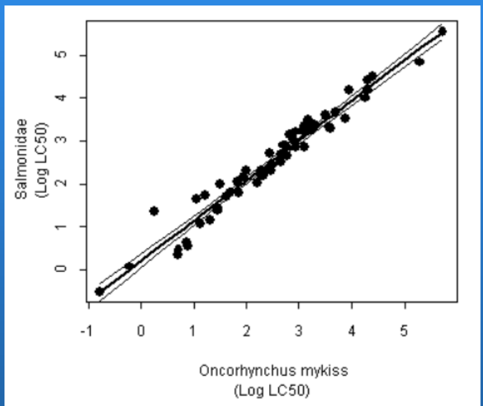
• use lowest observed LC50 for the predicted taxa (rather than geomean)
• objective is to provide more conservative estimate of toxicity to taxa containing listed species

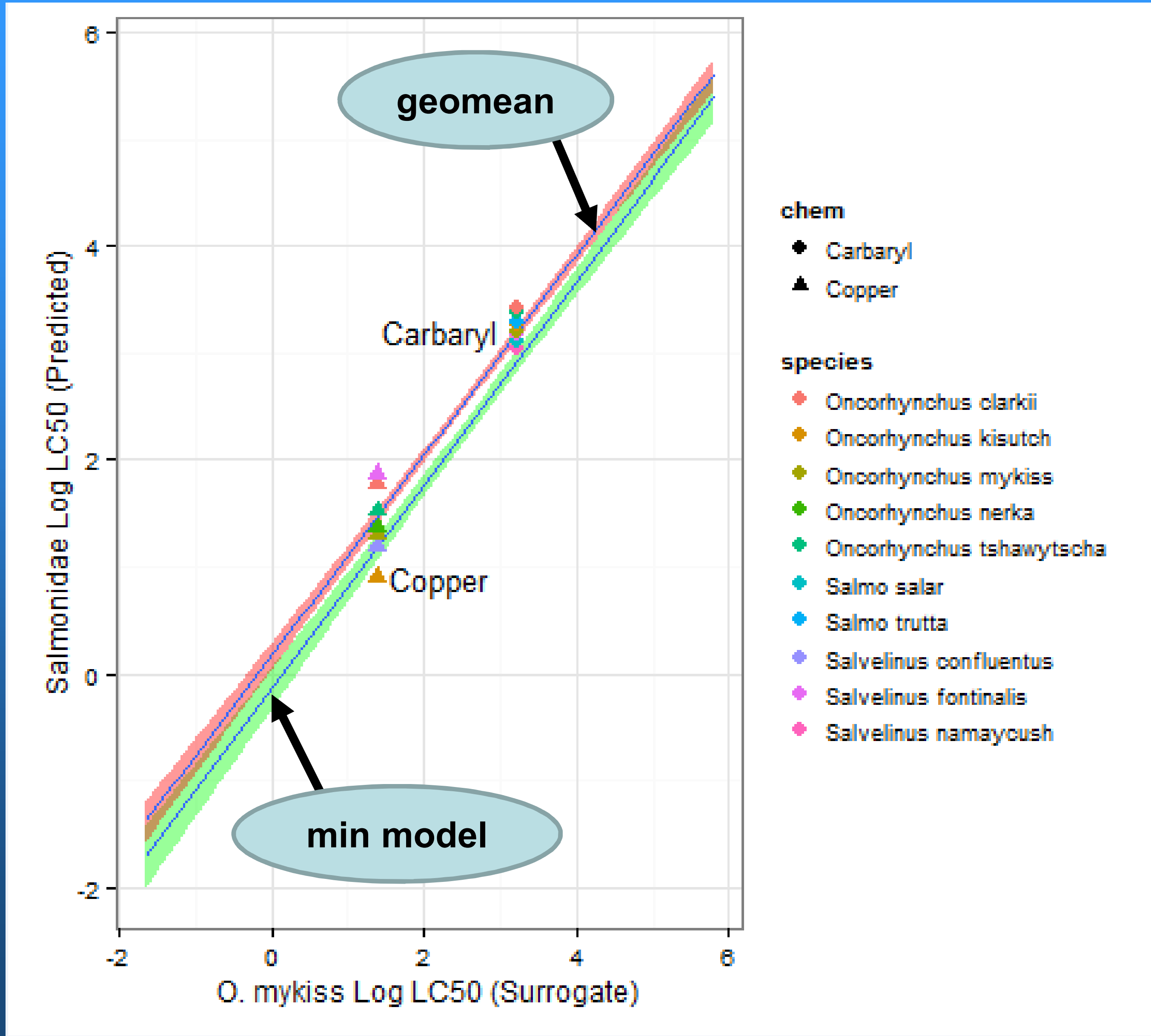


How min models derived:

• fit to minimum measured species toxicity value within the predicted taxa (genus or family)
• no longer geomean

Trout-Salmonidae Family Level Models





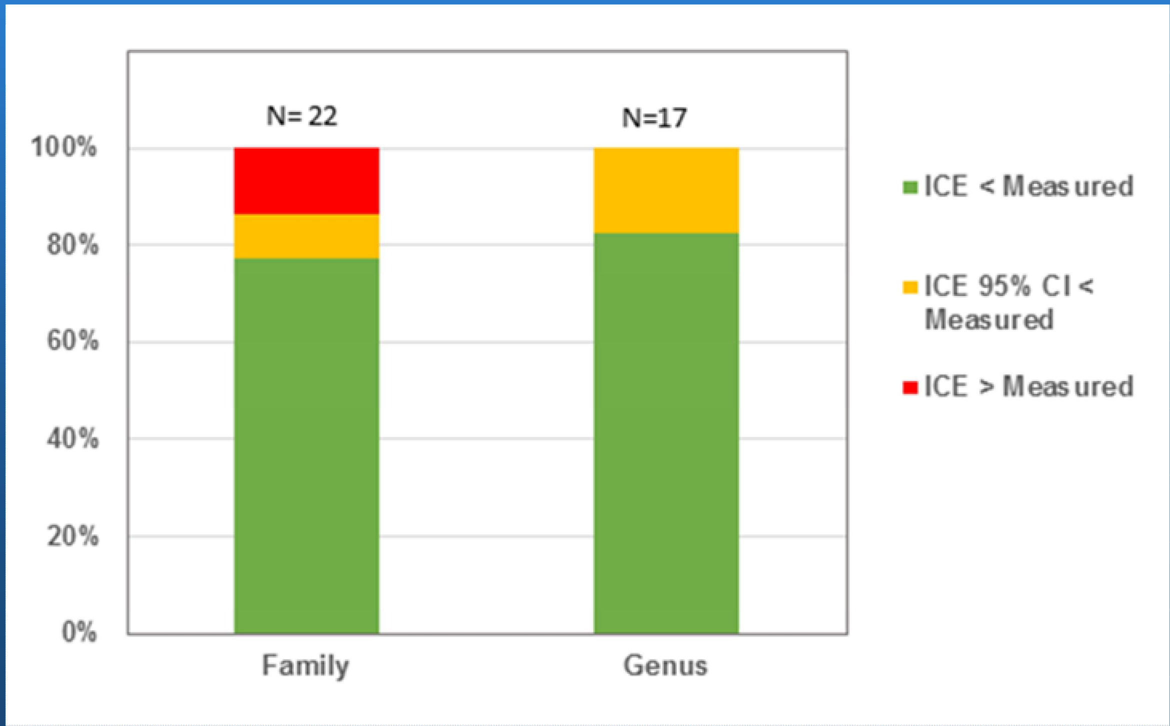
Web-ICE Prediction to Listed Taxa using Min Models

Case Study based on San Francisco Delta (Hoogeweg et al. 2012*):

- 13 priority chemicals
- 5 Families containing listed species
- toxicity predicted to Genus and Family level using Web-ICE (v. 3.3) min models
- selected best model for each species:chemical pair using new rules of thumb
- determined percentage of ICE predicted value protective of listed species

Case Study Chems
ATRAZINE
Carbaryl
Chlorpyrifos
COPPER
Cypermethrin
Diazinon
Fipronil
GLYPHOSATE
Imidacloprid
Malathion
Methomyl
Permethrin
Thiobencarb

Case Study Taxa
Acipenseridae
Branchinectidae
Ranidae
Salmonidae
Unionidae



**Pesticide Regulation and the Endangered Species Act Chap 22. ACS Symposium Series Vol. 1111

Augmenting species diversity

Comparison of Web-ICE v. 3.3 (2015) and 3.2 (2013)

- selected 10 representative surrogates (e.g., standard test species)
- determined number of models predicting to specific taxa groups

Surrogate
Americamysis bahia
Ceriodaphnia dubia
Cyprinodon variegatus
Daphnia magna
Hyalella azteca
Ictalurus punctatus
Lampsilis siliquoidea
Lepomis macrochirus
Oncorhynchus mykiss
Pimephales promelas

Total Freshwater Web-ICE Species Models	1985 Freshwater Taxa Requirements (# models predicting to:)							
	salmonid species	any non-salmonid fish species	amphibian species	planktonic crustaceans (cladocern, copepods)	benthic crustaceans (ostracod, isopod, amphipod, crayfish, decapods)	insects	non-arthropoda or chordata (rotifer, annelid)	molluscs
v3.3	49	115	17	29	53	34	8	58
v3.2	34	79	3	15	21	21	1	0

Total Salt Water Web-ICE Species Models	Salt Water Taxa (# models predicting to:)				
	fish	arthropods	echinoderms	molluscs	polychaetes, oligochaetes
v3.3	25	24	0	8	2
v3.2	16	12	1	6	0

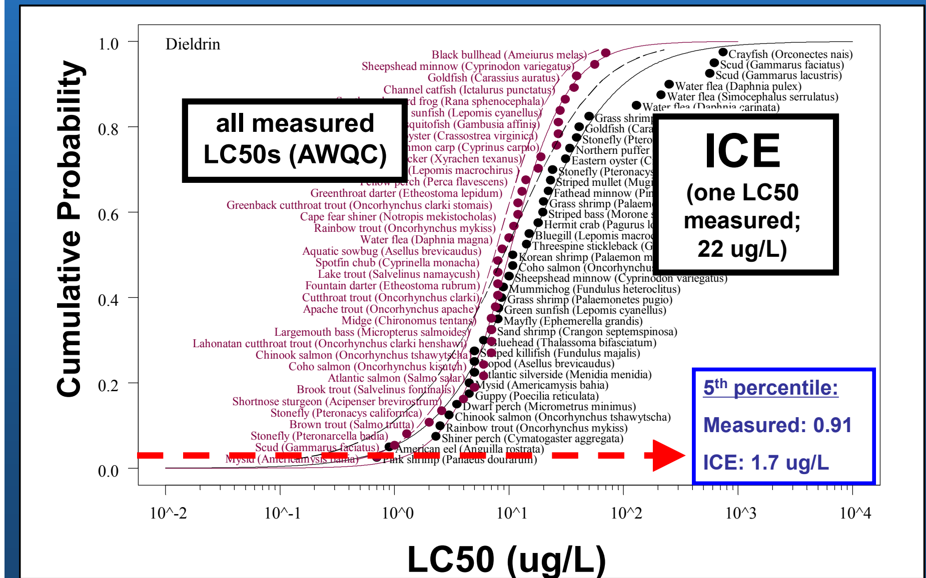
Estimating Taxa Toxicity using Web-ICE

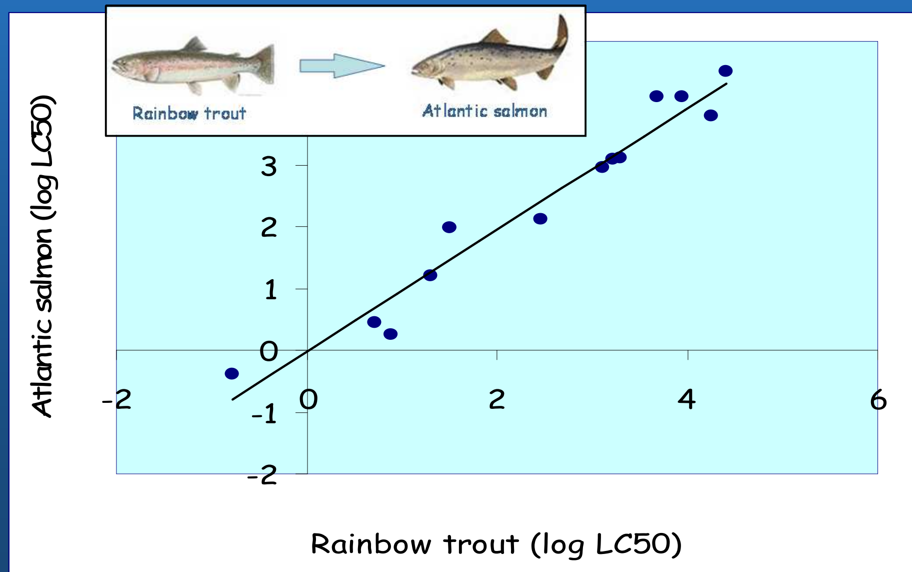
Direct toxicity estimation:

- estimation at species, genus, or family level
- model statistics/uncertainty
- cross validation, taxonomic distance
- single surrogate or multiple surrogates (best estimate)

SSD approach:

- Hazard Concentration (HC1, HC5)
- single surrogate or multiple surrogates (augmentation)





SSD Approach

<u>Rare species similar sensitivity as non-listed species</u>

- species composition affects HC5 more than geography/habitat of assemblage

<u>Raimondo et al. 2008</u>

- HC5s and HC1s lower than 97 and 99.5% of listed species LC50s
- HC5s less than levels derived from 10x safety factors for rainbow trout
- SSD generally protective of listed species

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PROTECTIVENESS OF SPECIES SENSITIVITY DISTRIBUTION HAZARD CONCENTRATIONS FOR ACUTE TOXICITY USED IN ENDANGERED SPECIES RISK ASSESSMENT

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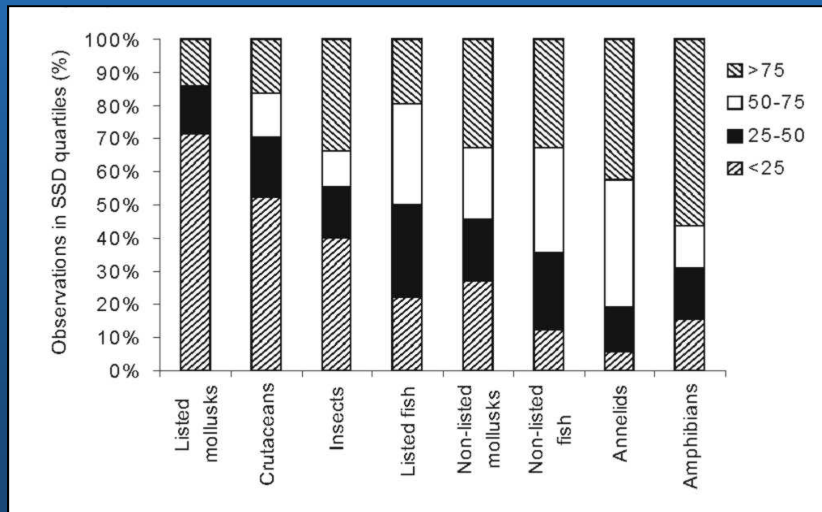

Web-ICE SSDs vs measured

Single surrogate ICE generated SSDs

- 55 AWQC chemicals (Dyer et al. 2008)
- HC5s within 10x of measured
- within taxa surrogates (fish to fish; invert to invert)

Multiple surrogates

- augment species diversity
- > 90% within 5 fold (Awkerman et al. 2014)
- accuracy affected by species composition, MOA

Environ. Sci. Technol. 2008, 42, 3076–3083

Comparison of Species Sensitivity Distributions Derived from Interspecies Correlation Models to Distributions used to Derive Water Quality Criteria

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Introduction

Ecological risk assessments typically require characterizing the effects of multiple chemicals on a diversity of ecological receptors using toxicity data for only a limited number of species. Regulatory activities such as REACH (Registration, Evaluation and Authorization of Chemicals ((1, 2); http://europa.eu.int/comm/environment/chemicals/reach.htm), ICCA (International Council of Chemical Associations) High Production Volume (HPV) Chemicals Challenge (http://www.icca-chem.org/), and Canada's Domestic Substance List (3) will also create new demands for toxicity data. Note that the ICCA HPV Chemicals challenge is in cooperation with OECD and its member countries which then also include other HPV challenge programs such as those of the United

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Hazard/Risk Assessment

AUGMENTING AQUATIC SPECIES SENSITIVITY DISTRIBUTIONS WITH INTERSPECIES TOXICITY ESTIMATION MODELS

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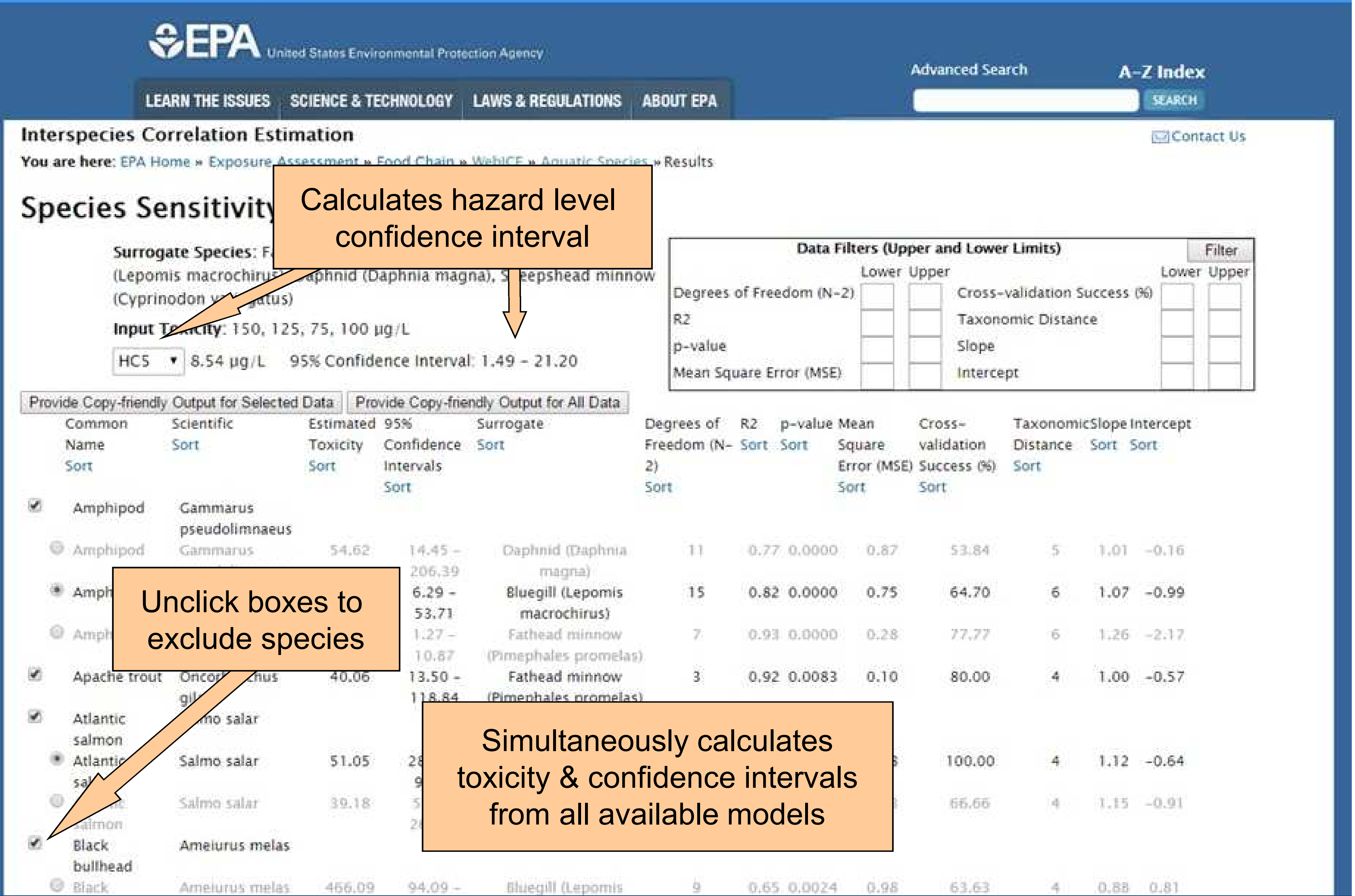
Web-ICE v3.3 SSD Generator



Summary

- NRC (2013) recommended ICE models as alternative to generic safety factors
- Web-ICE platform: data, models, modules for SSDs and T&E extrapolation
  - models for 250 U.S. federally listed T&E; 120 surrogate species
  - most models predict to genus and family
  - mollusc models expand family level predictions to 87 unionids
  - SSD generation additional approach for T&E protective levels
- peer reviewed technical basis (journal articles; FIFRA Science Advisory Panel)
- Web-ICE toxicity estimates and ICE-SSD HCs demonstrated high accuracy for closely related taxa (within same order)
- Web-ICE toxicity extrapolation: increase taxa diversity in SSDs for development of AWQC with reasonable uncertainty

EPA United States Environmental Protection Agency

QUESTIONS?

www.epa.gov/ceampubl/fchain/webice/