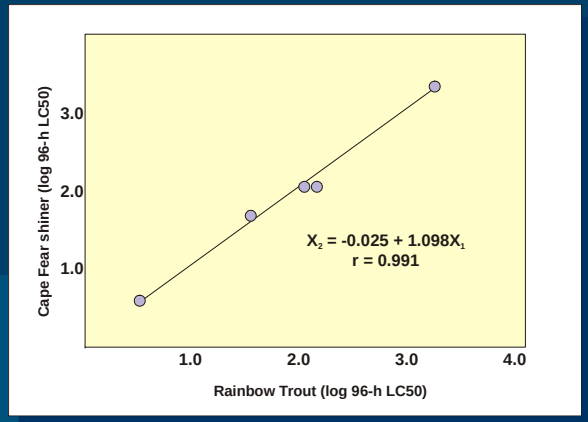
EPA
United States
Environmental Protection
Agency

Aquatic and Wildlife Species Sensitivity Modeling using Web-ICE

Mace Barron

USEPA/ORD/NHEERL/GED



Office of Research and Development
NHEERL, Gulf Ecology Division, Gulf Breeze, FL 32561

With the invaluable assistance of…

GED Coauthors: Sandy Raimondo, Deborah N. Vivian, Jill Awkerman

USEPA/ORD/NHEERL/GED

Sonny Mayer (retired)
Carl Litzinger
Marion Marchetto
Larry Goodman
Anthony DiGirolamo
Brandon Jarvis
Christel Chancy
Nathan Lemoine
Nicole Allard
Laura Dobbins
Cheryl McGill
Sarah Kell
Michael Murrell
Raymond Wilhour
Susan Yee
Crystal Jackson
Sorci Soriano

USEPA/ORD/NHEERL

Chris Russom (MED)
Rick Bennett (MED)
Glen Thursby (AED)
Anne Fairbrother (WED)

USEPA/ORD/NERL/ERD

Candida West
Tim Rowen
Luis Suárez

Proctor & Gamble

Scott Dyer
Don Versteeg
Joel Chaney
Scott Belanger

USEPA/OPPTS

Thomas Steeger (OPP)
Brian Montague (OPP)
Don Rodier (OPPT)
Vince Nabholz (OPPT)

Environment Canada

Pierre Mineau
Alain Baril
Brian Collins

USGS

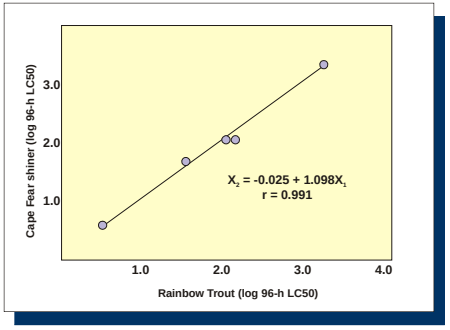
Christopher Ingersoll
Ning Wang

Computer Sciences Corporation

Wally Schwab
Derek Lane
Mike Galvin
David Owens

What is Web-ICE?

- Web-ICE: Web-based Interspecies Correlation Estimation
- User friendly internet-based acute toxicity estimation tool
- ICE models estimate toxicity to a species, genus, family, or multiple species from a single known toxicity value
- Consists of modules to predict acute toxicity to aquatic and wildlife species using ICE models and generate species sensitivity distributions (SSDs)
- Validated and published models and methodologies:
  ES&T (2006,2007, 2008), ETC (2007, 2008)



Presentation Outline

Model Development

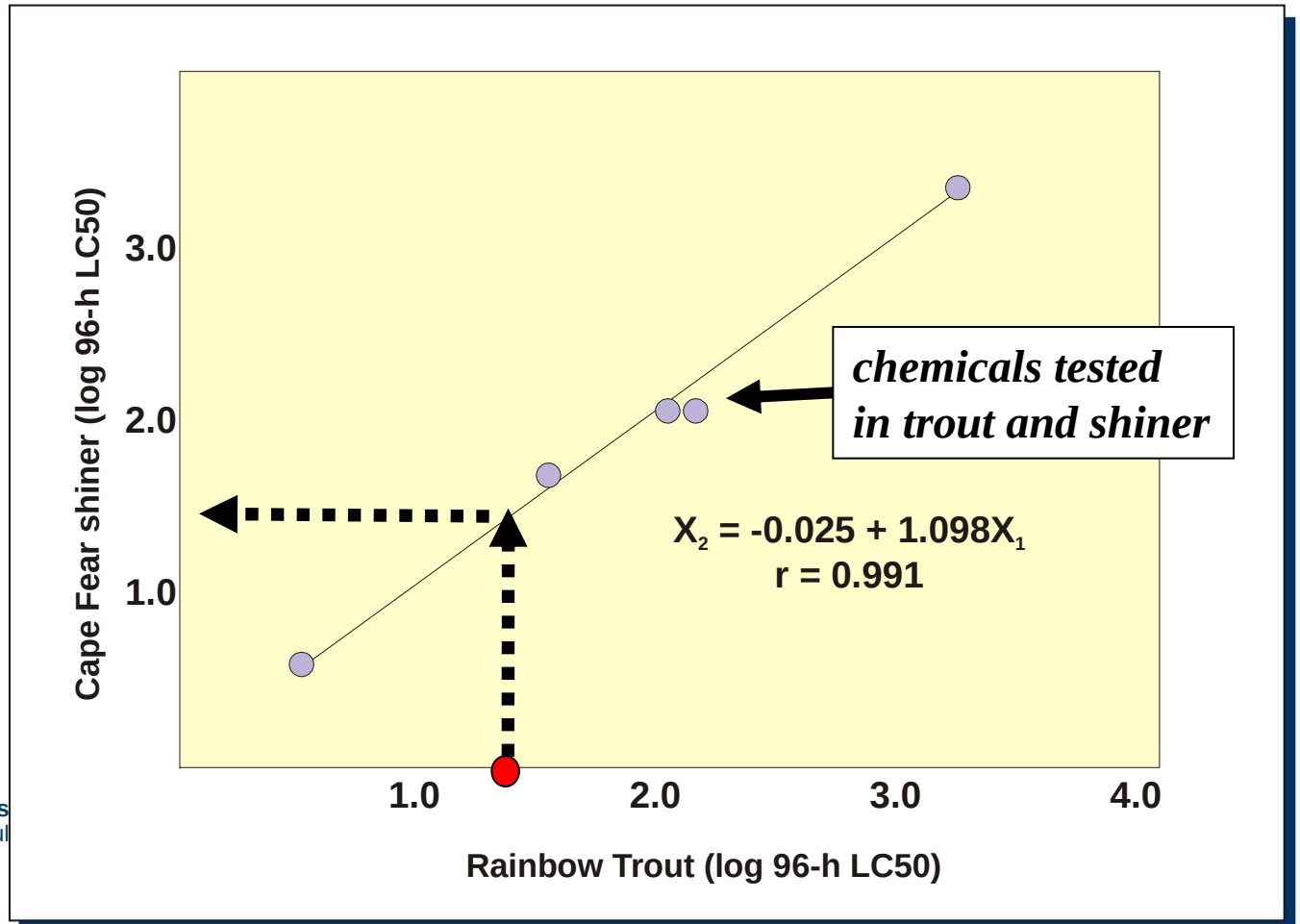
- Background on ICE models
- Database expansion & QC
- Model validation & uncertainty analysis
- User guidelines

Tour of Web-ICE

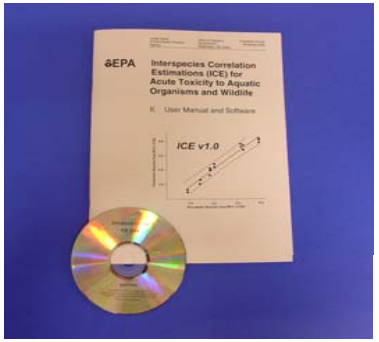
- Introduction to Web-ICE
- User-friendliness
- Species Sensitivity Distribution (SSD) Module
- Applications, Future development

What is an ICE Model?

Log-linear model of the relationship between the acute toxicity (LC50/LD50) of chemicals tested in two taxa



A Brief History of ICE



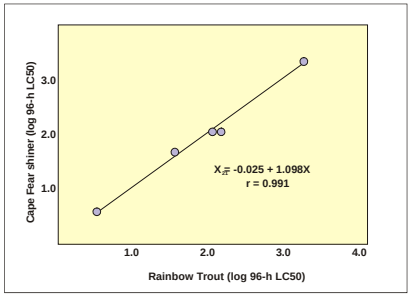
- **2003 - ICE version 1.0**
  - Sonny Mayer (USEPA/ORD/NHEERL/GED)
  - Mark Ellersieck & Amha Asfaw (Univ. Missouri)
  - CD-based platform

- **2007 - Web-ICE**
  - Sandy Raimondo, Deborah Vivian, Mace Barron (USEPA/ORD/NHEERL/GED)

- **2008-2010** – Continued development of Web-ICE
  - database expansion (>12000 records)
  - new modules (endangered species, algae)
  - improved functionality (SSDs, etc)

ICE Models – the basics

1. ICE models start with large database of acute toxicity
   - e.g. ICE v1.0 aquatic database = 4708 LC50 values; 661 chemicals; 247 species
2. All possible pairings of species by common chemical
   - e.g. 247*247 = 61009 potential pairings
3. ICE model = Log-linear least squares regression of common chemicals tested in two species
   - some pairings will not yield any ICE model
   - some models will not be significant (p>0.05)
4. Suite of ICE models dependent on toxicity database



Web-ICE Database Sources

Aquatic (fish and invertebrates):

- US EPA Office of Pesticide Programs Ecotoxicity Database
- US EPA Office of Pollution Prevention & Toxics (HPV, PMN)
- ECOTOX/Aquire: 250,000 records
- US Geologic Survey
- AWQC
- Mayer 1987
- Mayer and Ellersieck 1986
- other literature sources for taxa of interest
  - endangered species
  - Molluscs

Web-ICE Database Sources

Wildlife (birds and mammals):

- US EPA Office of Pesticide Programs Ecotoxicity Database
- Environment Canada (Baril et al. 1994)
- Hudson et al. 1984
- Schafer et al. 1983
- Shafer and Bowles 1985
- Safer and Bowles 2004
- Smith 1987

Test Data Standardization

Aquatic data

- Test Duration/endpoint:
  - 96-hr LC50/EC50 (immobilization): fish, most invertebrates
  - 48-hr LC50/EC50: daphnids, midges, copepods, mosquito
- Life stage: juvenile
- Chemical purity/formulation: ≥ 90%
- Concentrations: ug/L
- Test conditions: ASTM or similar
- Metals, PCP, HCN, ammonia: normalized according to AWQC docs

Wildlife data

- Single oral dose, 14 d acute LD50 (mg/kg)
- Adults only
- Chemical purity/formulation: ≥ 90%

Web-ICE Aquatic Expansion

1) Compile records from all sources (>250,000)
2) Filter out records not meeting test standardization criteria
3) Assign and QC age classes (juvenile only on Web)
4) QC chemical names and CAS
5) Screen out duplicate records
6) Assign and QC MOAs
7) Build ICE and QC ICE Models
8) Validate models
9) Upload to Web

Web-ICE Database

	# Records	# Chemicals	# Species
Aquatic 2007	4706	695	217
T&E species	1043	465	22
Aquatic 2009	> 10,000	> 1600	> 300
T&E species	~ 2000	~ 550	~ 25
Wildlife	4329	951	156

Additional data sources added
AWQC
new Ecotox
OPPT PMN & HPV
endangered species

Quality Assurance

In house

- centralized data management system
- data transcription thoroughly reviewed
- chemical and species name consistency
- duplicate records removed

Extraneous factors

- reviewed each source for quality
- multiple records for same species and chemical were removed if min and max were > 10-fold

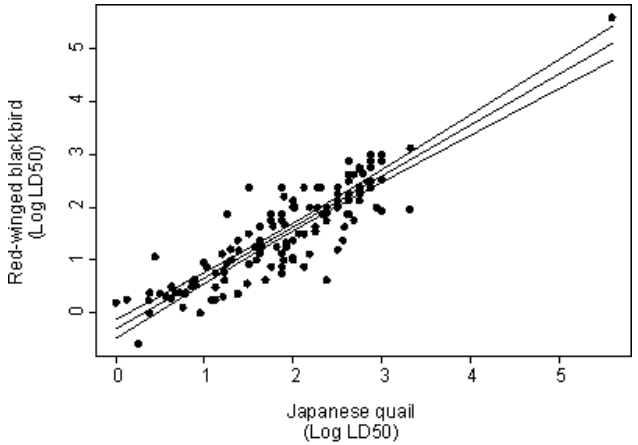
	A	B	C	D	G	H
1	data source	chemical	cas	species	type	toxicity (ug/L)
2	OPP	(S)-Dimethenamid	163515148	Cyprinodon variegatus	F	12000
3	OPP	(S)-Dimethenamid	163515148	Daphnia magna	F	12000
4	OPP	(S)-Dimethenamid	163515148	Lepomis macrochirus	F	10000
5	OPP	(S)-Dimethenamid	163515148	Oncorhynchus mykiss	F	6300
6	ECOTOX	1,1,2,2-tetrachloroethane	79345	Paratanytarsus dissimilis	S	30800
7	ECOTOX	1,1,2,2-tetrachloroethane	79345	Pimephales promelas	F	13400
8	ECOTOX	1,1,2,2-tetrachloroethane	79345	Pimephales promelas	F	20300
9	ECOTOX	1,1-Dichloroethene	75354	Menidia beryllina	S	250000
10	ECOTOX	1,2,4-trichlorobenzene	120821	Oncorhynchus mykiss	F	1530
11	OPP	1,2-Benzenedicarboxaldehyde	643798	Daphnia magna	SR	87
12	OPP	1,2-Benzenedicarboxaldehyde	643798	Daphnia magna	S	90
13	OPP	1,2-Benzenedicarboxaldehyde	643798	Oncorhynchus mykiss	SR	20
14	OPP	1,2-Benzenedicarboxaldehyde	643798	Oncorhynchus mykiss	F	72
15	ECOTOX	1,2-dichlorobenzene	95501	Lepomis macrochirus	S	27000
16	ECOTOX	1,2-dichlorobenzene	95501	Lepomis macrochirus	S	320000
17	ECOTOX	1,2-dichlorobenzene	95501	Menidia beryllina	S	7300
18	ECOTOX	1,2-dichlorobenzene	95501	Menidia beryllina	S	240000
19	ECOTOX	1,2-dichlorobenzene	95501	Oncorhynchus mykiss	F	1580
20	ECOTOX	1,2-dichlorobenzene	95501	Paratanytarsus dissimilis	S	12000
21	OPP	1,3 Dichloropropene	542756	Crassostrea virginica	F	640
22	OPP	1,3 Dichloropropene	542756	Cyprinodon variegatus	F	870
23	OPP	1,3 Dichloropropene	542756	Daphnia magna	S	90
24	OPP	1,3 Dichloropropene	542756	Lepomis macrochirus	F	3700
25	OPP	1,3 Dichloropropene	542756	Lepomis macrochirus	S	6700
26	OPP	1,3 Dichloropropene	542756	Micropterus salmoides	S	3650
27	OPP	1,3 Dichloropropene	542756	Pimephales promelas	S	4100
28	OPP	1,3 Dichloropropene	542756	Sander vitreus	S	1080
29	OPP	1,3,5-Triethylhexahydro-s-triazin	7779273	Daphnia magna	S	15300
30	OPP	1,3,5-Triethylhexahydro-s-triazin	7779273	Daphnia magna	F	26000
31	OPP	1,3,5-Triethylhexahydro-s-triazin	7779273	Lepomis macrochirus	S	30800
32	OPP	1,3,5-Triethylhexahydro-s-triazin	7779273	Oncorhynchus mykiss	S	23300
33	OPP	1,3,5-Triethylhexahydro-s-triazin	7779273	Oncorhynchus mykiss	F	35000
34	OPP	1,4-dichlorobenzene	106467	Lepomis macrochirus	S	6400
35	OPP	1,4-dichlorobenzene	106467	Oncorhynchus mykiss	S	880
36	ECOTOX	1,4-dichlorobenzene	106467	Oncorhynchus mykiss	F	1120
37	ECOTOX	1,4-dichlorobenzene	106467	Paratanytarsus dissimilis	S	13000
38	OPP	1,4-dichlorobenzene	106467	Salvelinus fontinalis	S	1670
39	Boogard	2-(digeranylamino)-ethanol	001	Carassius auratus	S	290
40	Boogard	2-(digeranylamino)-ethanol	001	Cyprinus carpio	S	50.7
41	Boogard	2-(digeranylamino)-ethanol	001	Fundulus diaphanus	S	792
42	Boogard	2-(digeranylamino)-ethanol	001	Lepomis cyanellus	S	640
43	Boogard	2-(digeranylamino)-ethanol	001	Lepomis macrochirus	S	720
44	Boogard	2-(digeranylamino)-ethanol	001	Micropterus dolomieu	S	237
45	Boogard	2-(digeranylamino)-ethanol	001	Micropterus salmoides	S	360

EcoToxdata

Web-ICE Model Development

Model II least square regression of log-transformed toxicity data for all possible species pairs

Included only models significant at the $p<0.05$ level



# ICE Models:	Species	Genus	Family
Aquatic 2007	1074	481	526
Wildlife	560	n/a	292

Model Validation & Uncertainty Analysis

- **Only included models significant at the p<0.05 level**

- **Leave-1-out cross-validation**
  - only conducted for models N ≥ 4
  - models excluded if removal of data resulted in non-significant model
    - degrees of freedom < 8 (N < 10)
    - 0.05 ≥ p-value ≥ 0.01
  - "N-fold difference" of each removed data point categorized
    - 5-fold, 10-fold, 50-fold, >50-fold
  - Cross-validation success rate for each model
    - percentage of model datapoints predicted within 5-fold of actual value

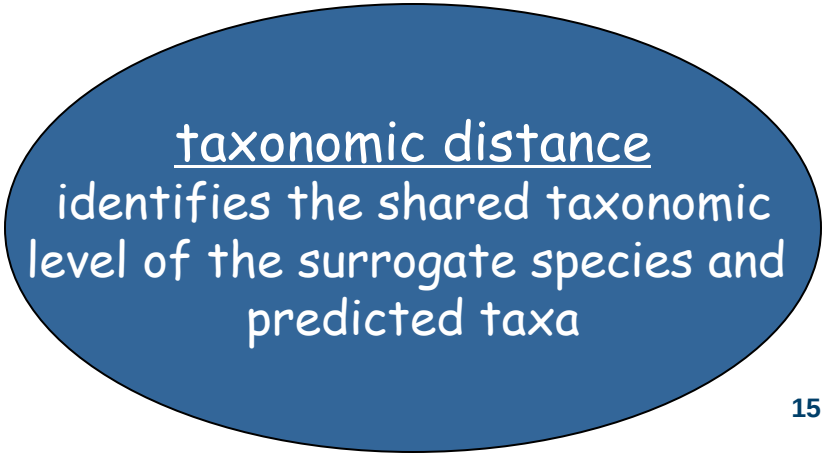
leave-1-out cross-validation

Each data point is removed, one at a time, and the model is rebuilt with remaining data. Removed surrogate data are used to estimate removed predicted data from rebuilt model.

Model Validation & Uncertainty Analysis

Cross-validation results used to identify sources of model uncertainty:

- Aquatic
  - 2007: taxonomic distance
  - final: model parameters, chemical MOA/class
- Wildlife
  - taxonomic distance
  - chemical MOA/class
  - model parameters (MSE, R^2)



How well do ICE models work?

Model uncertainty related to taxonomic distance

Aquatics in same order ~ 90% within 5-fold, 95% within 10-fold

Percentage of all datapoints in cross-validation category

Common level	Number datapoints	5-fold	10-fold	50-fold	> 50 fold
genus (1)	372	92	3	4	1
family (2)	1042	92	6	2	0
order (3)	280	89	6	4	1
class (4)	5622	79	9	8	4
phylum (5)	854	52	17	21	10
kingdom (6)	4524	50	16	22	12

How well do ICE models work?

Model uncertainty related to taxonomic distance

Wildlife in same order ~ 90% within 5-fold, 97% within 10-fold

Percentage of all datapoints in cross-validation category

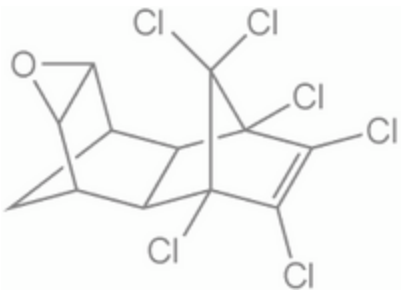
Common level	Number datapoints	5-fold	10-fold	50-fold	> 50 fold
genus (1)	48	100	0	0	0
family (2)	1452	92	6	2	0
order (3)	2238	90	7	3	0.3
class (4)	5706	85	10	5	0.2
phylum (5)	2402	76	13	9	1.5

Raimondo et al. 2003 Environmental Science and Technology (ES&T)

ICE Model Uncertainty: Chemical Mode of Action (MOA)

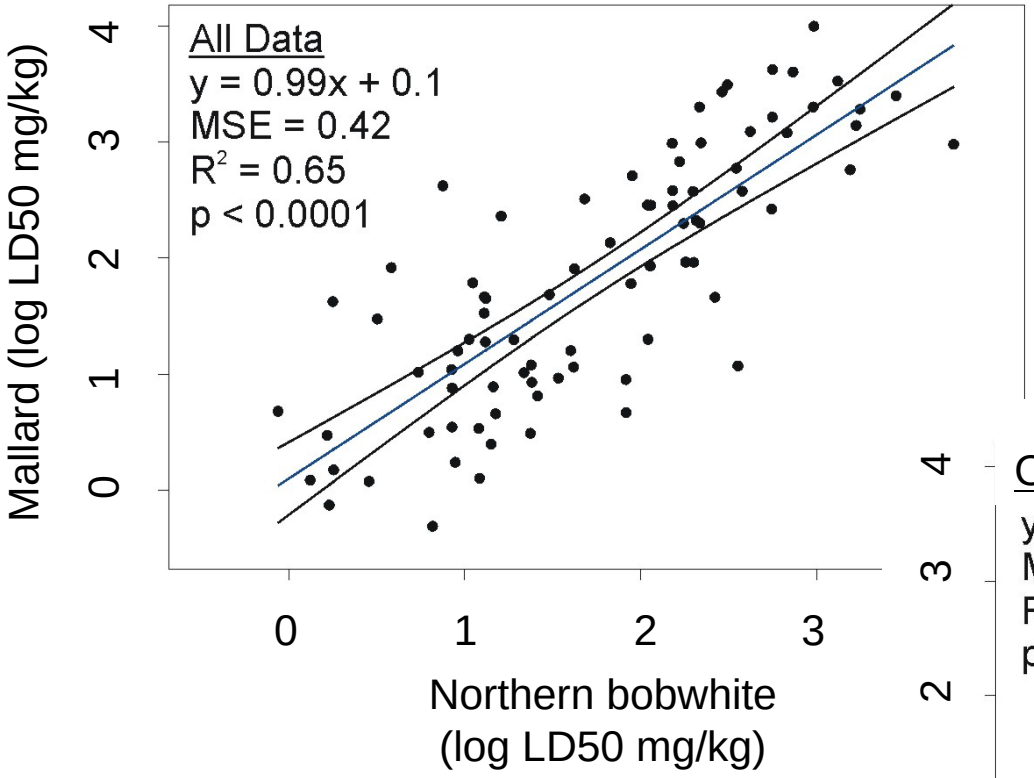
- Each chemical assigned a chemical MOA based on ASTER assignment, assessment of chemical structure, mechanism of acute toxicity, therapeutic category and pesticidal activity

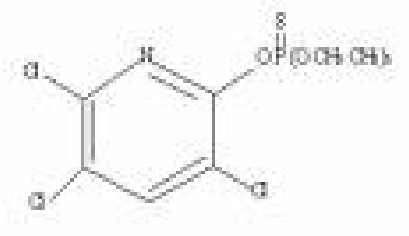
- Wildlife complete; aquatics in progress

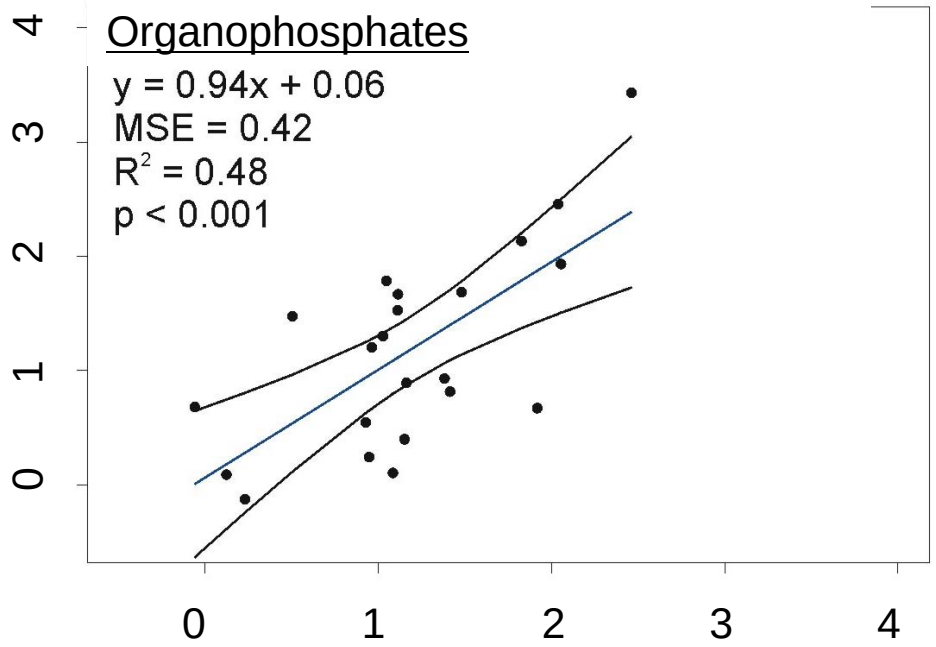


Model Uncertainty: Chemical MOA

Wildlife models



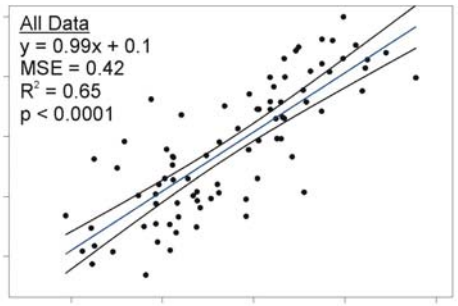


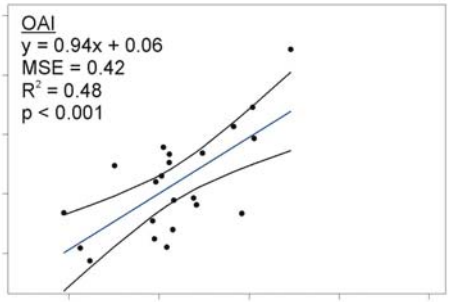


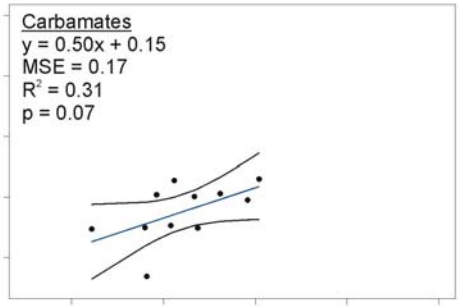
Model Uncertainty: Chemical MOA

Wildlife models

- Models were improved when built from data subsets for half of MOAs compared with models built from all data
- Many models built with MOA data subsets lost statistical significance
  - related to reduced degrees of freedom
  - signifies lack of model robustness
- Models may be improved by using MOA-specific data
- Abundant data is necessary to ensure model robustness preserved







User Guidance: Selecting a Model with Low Uncertainty

No one attribute defines model robustness!

Rules of Thumb:

(based on uncertainty analysis of Wildlife models)

- close taxonomic distance (within order)
- low MSE (< ~0.22)
- high R^2 (> ~0.6)
- high cross-validation success rate
- low p-value (< 0.01)
- high degrees of freedom (d.f. > 8; N > 10)

- input value should be relatively close to the range of surrogate data used to create the model

Tour of Web-ICE

Available on EPA's Center for Exposure Assessment Modeling (CEAM)

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

Office of Research and Development
NHEERL, Gulf Ecology Division, Gulf Breeze, FL 32561

U.S. Environmental Protection Agency

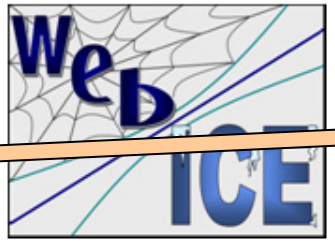
Interspecies Correlation Estimation

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information
User Manual
Download Model Data
Bibliography



The W... acute... to th... Web-ICE) application estimates ...use in risk assessment. Please refer ...Web-ICE.

Select taxonomic model for Aquatic or Wildlife

Web-ICE Modules

ICE Aquatic
Aquatic vertebrates / invertebrates
- Species
- Genus
- Family

ICE Wildlife
Terrestrial Birds / Mammals
- Species
- Family

Species Sensitivity Distribution Module

- ICE Aquatic
- ICE Wildlife

Wildlife Species/Family Taxa Selection | Interspecies Correlation Estimation | US EPA - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address http://www.epa.gov/ceampubl/fchain/webice/getPredSurr.htm?file=as

Go Links

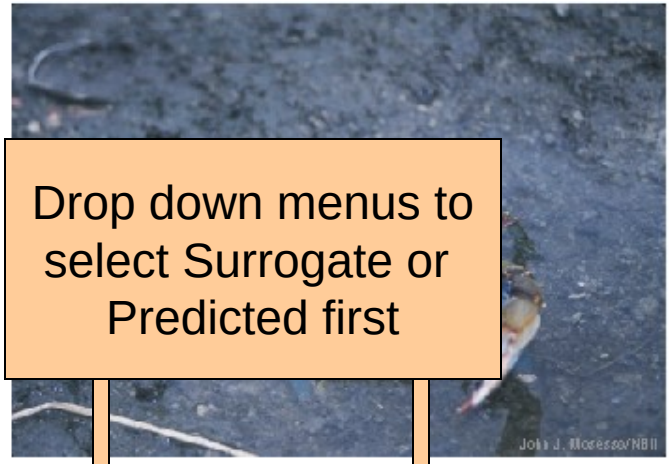
U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Recent Additions | Contact Us Search: All EPA This Area Go

You are here: EPA Home » Exposure Assessment » Food Chain » Web-ICE Home » Aquatic Species

Aquatic Species - Taxa Selection Page



Drop down menus to select Surrogate or Predicted first

Exposure Assessment Models

Web-ICE Home
- Aquatic Species
- Aquatic Genus
- Aquatic Family
- Wildlife Species
- Wildlife Family

Species Sensitivity Distributions
- Aquatic
- Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Surrogate:

Predicted:

Downy rainbow (Villosa villosa)
Eastern mud snail (Nassarius obsoletus)
Eastern oyster (Crassostrea virginica)
Fathead minnow (Pimephales promelas)
Fiddler crab (Uca pugilator)
Flagfish (Jordanella floridae)
Fountain darter (Etheostoma fonticola)
Fowlers toad (Bufo fowleri)
Gila topminnow (Poeciliopsis occidentalis)
Goldfish (Carassius auratus)
Green crab (Carcinus maenas)

Continue

ments and questions to the webmaster
and Environmental Effects Research Laboratory | Gulf Ecology Division

Local intranet

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

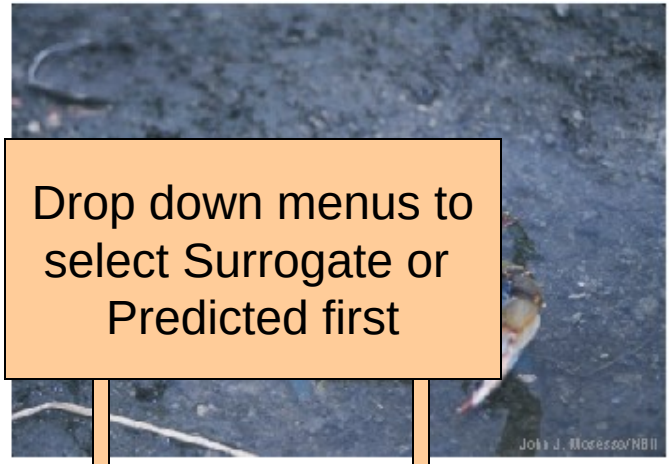
Basic Information

User Manual

Download Model Data

Bibliography

Aquatic Species - Taxa Selection Page



Drop down menus to select Surrogate or Predicted first

Surrogate:

Predicted:

Sort By: Common Name

Reset

California grunion (Leuresthes tenuis)
Cape Fear shiner (Notropis mekistocholas)
Channel catfish (Ictalurus punctatus)
Chinook salmon (Oncorhynchus tshawytscha)
Coho salmon (Oncorhynchus kisutch)
Colorado pikeminnow (Ptychocheilus lucius)
Common carp (Cyprinus carpio)
Copepod (Acartia clausi)
Copepod (Acartia tonsa)
Copepod (Eurytemora affinis)
Crayfish (Orconectes nais)

Wildlife Species/Family Taxa Selection | Interspecies Correlation Estimation | US EPA - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address http://www.epa.gov/ceampubl/fchain/webice/getPredSurr.htm?file=as Go Links

U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Recent Additions | Contact Us Search: All EPA This Area Go

You are here: EPA Home » Exposure Assessment » Food Chain » Web-ICE Home » Aquatic Species

Exposure Assessment Models

Web-ICE Home
- Aquatic Species
- Aquatic Genus
- Aquatic Family
- Wildlife Species
- Wildlife Family

Species Sensitivity Distributions
- Aquatic
- Wildlife

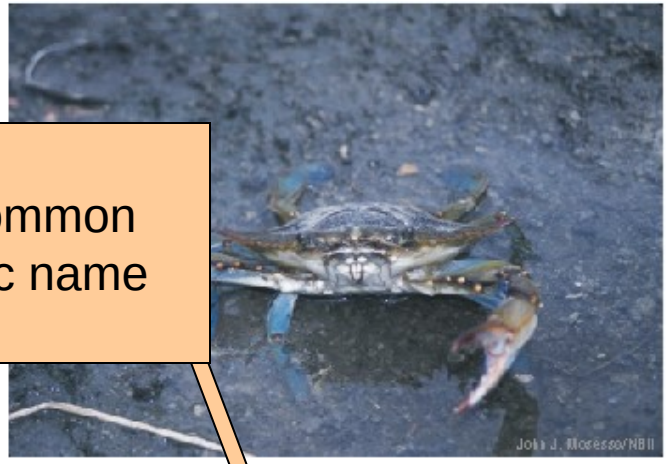
Basic Information

User Manual

Download Model Data

Bibliography

Aquatic Species - Taxa Selection Page



Sort by common or scientific name

Surrogate: Predicted:

Sort By: Scientific Name

Reset

Acartia clausi (Copepod)
Acartia tonsa (Copepod)
Acipenser brevirostrum (Shortnose sturgeon)
Actinonaias pectorosa (Pheasantshell)
Ameiurus melas (Black bullhead)
Americamysis bahia (Mysid)
Argopecten irradians (Bay scallop)
Anguilla rostrata (American eel)
Aplexa hypnorum (Snail)
Asterias forbesi (Starfish)

Please address all comm

Office of Research and Development | National Health ... ivision

Done Local intranet

U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Exposure Assessment Models
Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family
Species Sensitivity Distributions
Aquatic
Wildlife
Basic Information
User Manual
Download Model Data
Bibliography

Aquatic Species - Taxa Selection Page

Only offers significant ($p<0.05$) models for chosen taxon

Surrogate:

Americamysis bahia (Mysid
Carcinus maenas (Green crab)
Homarus americanus (American lobster)
Mytilus edulis (Blue mussel)

Predicted:

Acartia tonsa (Copepod)

Continue

Rainbow trout -Brook trout | Wildlife Species/Family ICE Calculator | Interspecies Correlation - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address http://www.epa.gov/ceampubl/fchain/webice/iceCalculate.htm?Surrogate=Rainbow+trout+%28Oncorhynchus+mykiss%29&Predicted=Brook+trout+%28Salvelinus+fontin

Go Links

Exposure Asse
Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity
Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Surrogate toxicity input

Select confidence interval

Predicted toxicity and confidence interval

Surrogate Acute Toxicity (log value)	Predicted Acute Toxicity (log value)	
400 µg/L (2.60)	454.50 µg/L (2.65)	
Select Confidence Interval:	Lower Limit	Upper Limit
95%	288.03 µg/L	717.18 µg/L
Calculate		

Aquatic graphs coming in 2009

Model Information

Intercept:	-0.316554
Slope:	1.14
Degrees of Freedom (N-2):	15
R^2:	0.923529
p-value:	0.000000

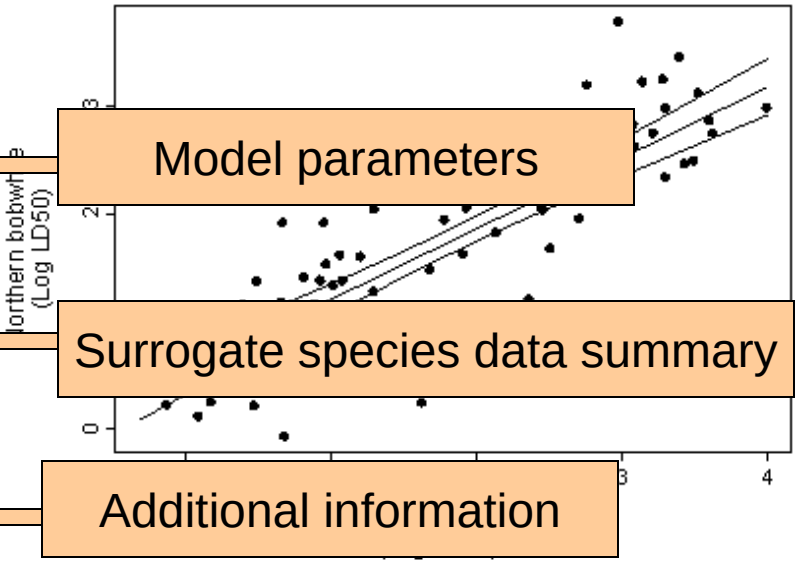
Model parameters

Average value of surrogate (log value):	302.23 (2.48)
Minimum value of surrogate (log value):	3.80 (0.580881)
Maximum value of surrogate (log value):	19208.68 (4.28)

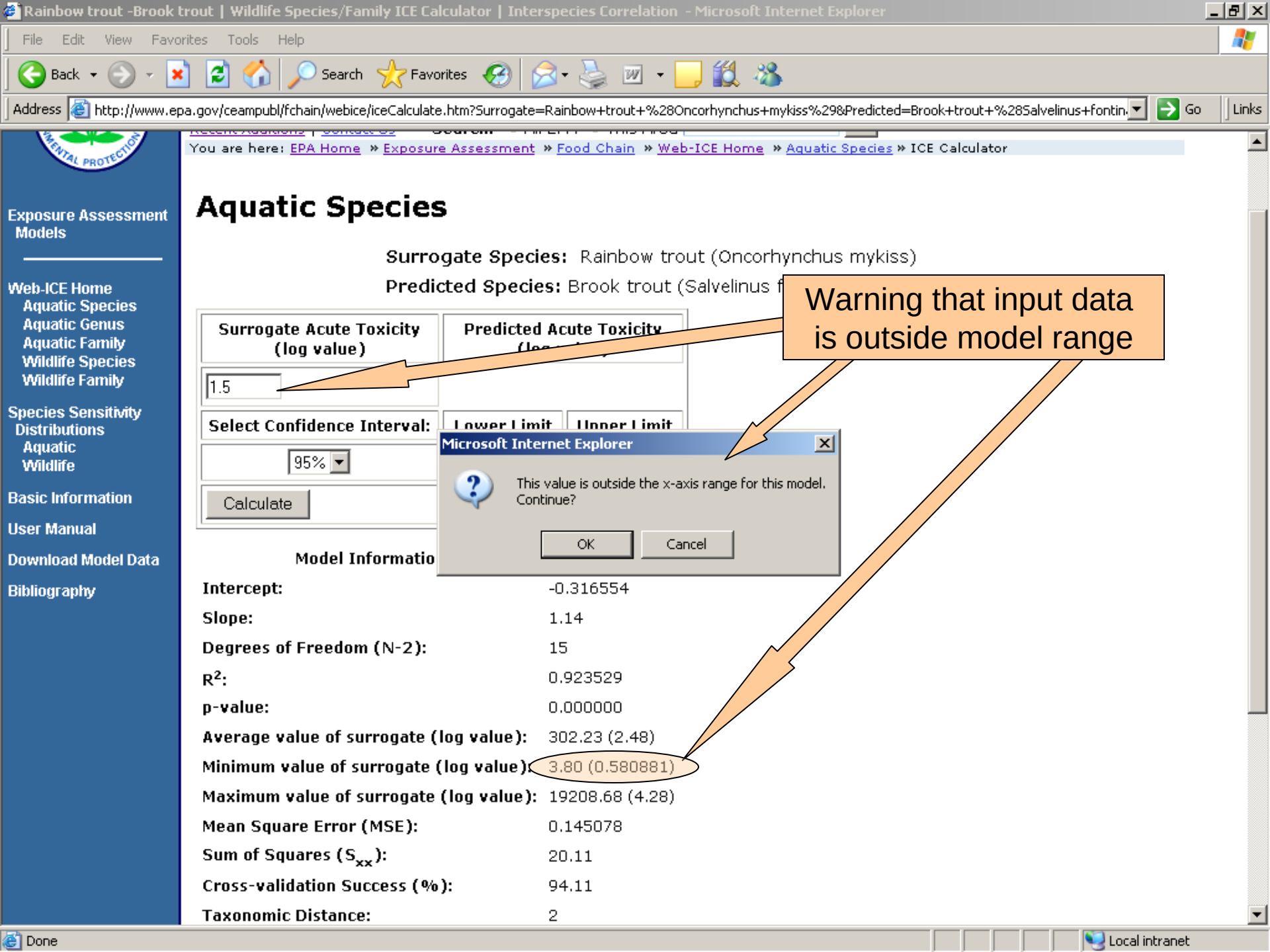
Surrogate species data summary

Mean Square Error (MSE):	0.145078
Sum of Squares (S_{xx}):	20.11
Cross-validation Success (%):	94.11
Taxonomic Distance:	2

Additional information



Local intranet


Rainbow trout -Brook trout | Wildlife Species/Family ICE Calculator | Interspecies Correlation - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites
Address http://www.epa.gov/ceampubl/fchain/webice/iceCalculate.htm?Surrogate=Rainbow+trout+%28Oncorhynchus+mykiss%29&Predicted=Brook+trout+%28Salvelinus+fontin
Go Links
You are here: EPA Home » Exposure Assessment » Food Chain » Web-ICE Home » Aquatic Species » ICE Calculator
Exposure Assessment Models
Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family
Species Sensitivity Distributions
Aquatic
Wildlife
Basic Information
User Manual
Download Model Data
Bibliography
Aquatic Species
Surrogate Species: Rainbow trout (Oncorhynchus mykiss)
Predicted Species: Brook trout (Salvelinus f
Surrogate Acute Toxicity (log value)
Predicted Acute Toxicity
1.5
Select Confidence Interval:
Lower Limit
Upper Limit
95%
Calculate
Warning that input data is outside model range
Microsoft Internet Explorer
This value is outside the x-axis range for this model. Continue?
OK
Cancel
Model Informatio
Intercept: -0.316554
Slope: 1.14
Degrees of Freedom (N-2): 15
R2: 0.923529
p-value: 0.000000
Average value of surrogate (log value): 302.23 (2.48)
Minimum value of surrogate (log value): 3.80 (0.580881)
Maximum value of surrogate (log value): 19208.68 (4.28)
Mean Square Error (MSE): 0.145078
Sum of Squares (Sxx): 20.11
Cross-validation Success (%): 94.11
Taxonomic Distance: 2
Done
Local intranet

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Aquatic Species

Surrogate Species: Rainbow trout (Oncorhynchus mykiss)

Predicted Species: Brook trout (Salvelinus fontinalis)

Surrogate Acute Toxicity (log value)	Predicted Acute Toxicity (log value)	
1.5 µg/L (0.176)	0.766 µg/L (-0.115)	
Select Confidence Interval:	**Lower Limit**	**Upper Limit**
95%	0.265 µg/L	2.21 µg/L
Calculate	Surrogate toxicity outside model range.	

Review confidence intervals for prediction certainty

Warning that input data is outside model range

Model Information

Intercept:	-0.316554
Slope:	1.14
Degrees of Freedom (N-2):	15
R^2:	0.923529
p-value:	0.000000
Average value of surrogate (log value):	302.23 (2.48)
Minimum value of surrogate (log value):	3.80 (0.580881)
Maximum value of surrogate (log value):	19208.68 (4.28)
Mean Square Error (MSE):	0.145078
Sum of Squares (S_{xx}):	20.11
Cross-validation Success (%):	94.11
Taxonomic Distance:	2

U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

The Web-based Interspecies Correlation Estimation (Web-ICE) application estimates acute toxicity to aquatic and terrestrial organisms for use in risk assessment. Please refer to the User Manual for detailed instructions on using Web-ICE.

Web-ICE Modules

ICE Aquatic

Aquatic vertebrates / invertebrates
- Species
- Genus
- Family

ICE Wildlife

Terrestrial Birds / Mammals
- Species
- Family

Species Sensitivity Distribution Module

- ICE Aquatic
- ICE Wildlife

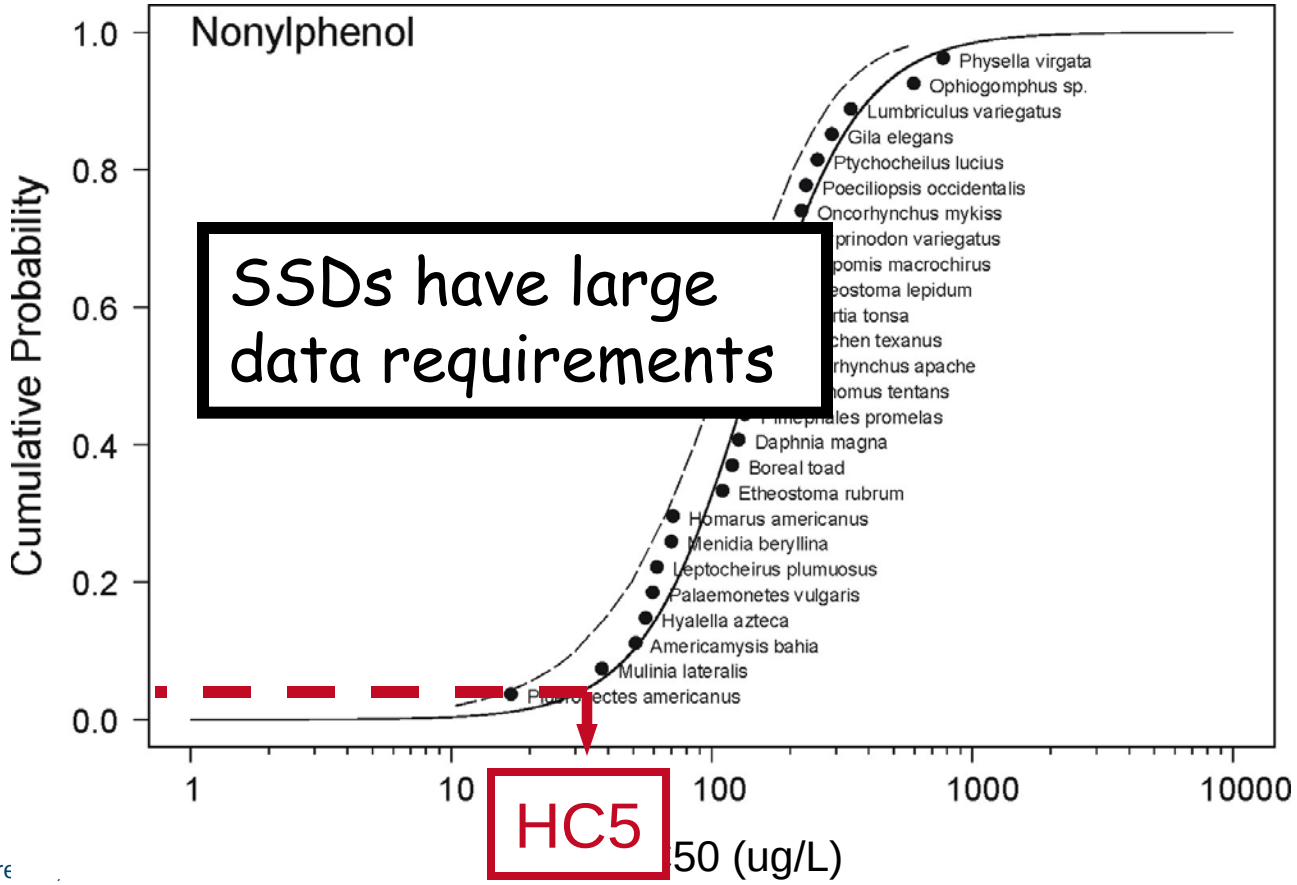
Please address all ... and questions to the webmaster
Office of Research and Development | National Health and Environmental Effects Research Laboratory | Gulf Ecology Division

Species Sensitivity Distributions (SSDs)

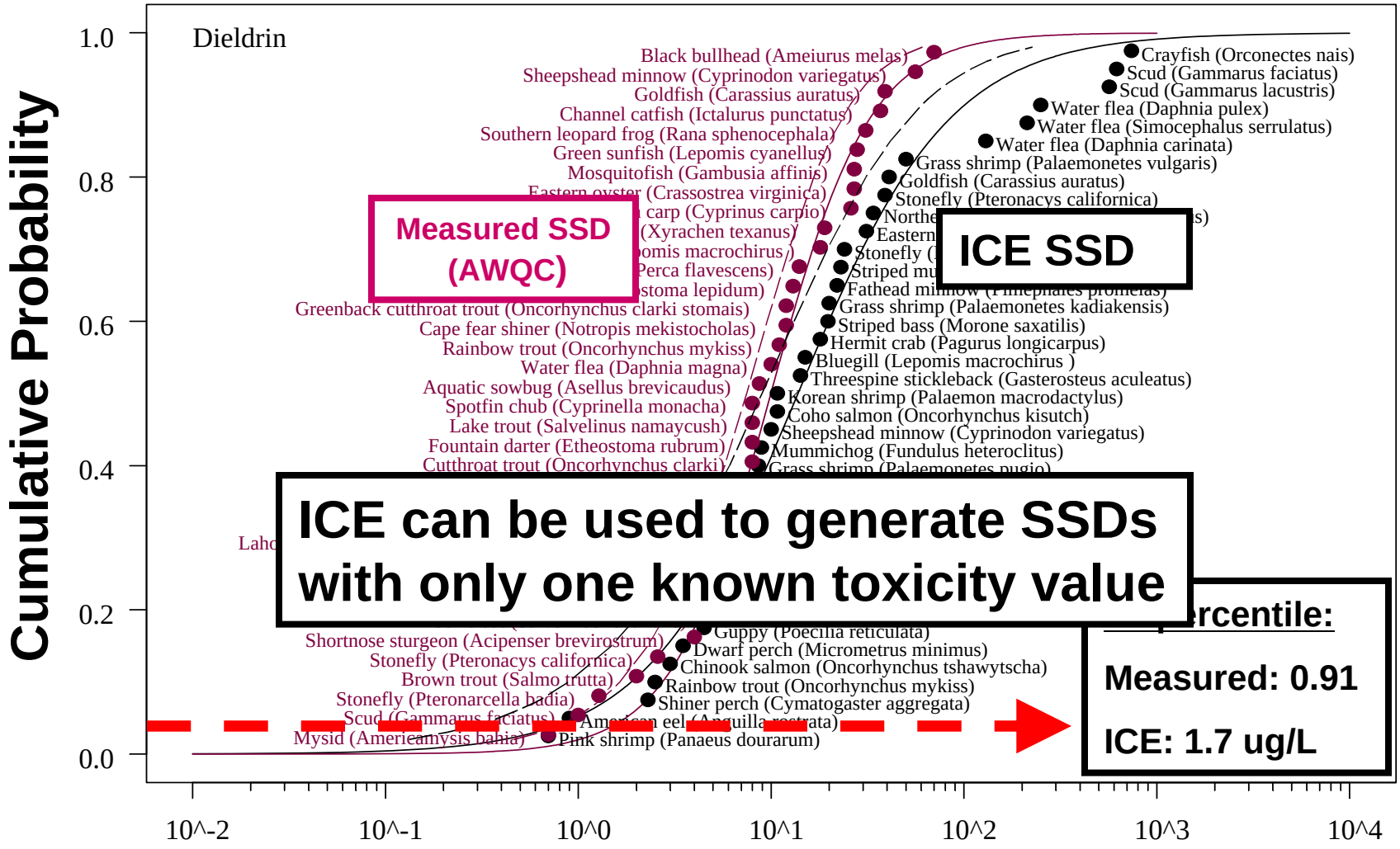
- **Cumulative probability distribution of species sensitivity**

Used widely in ecological risk assessment to determine hazard level (e.g., HC5)

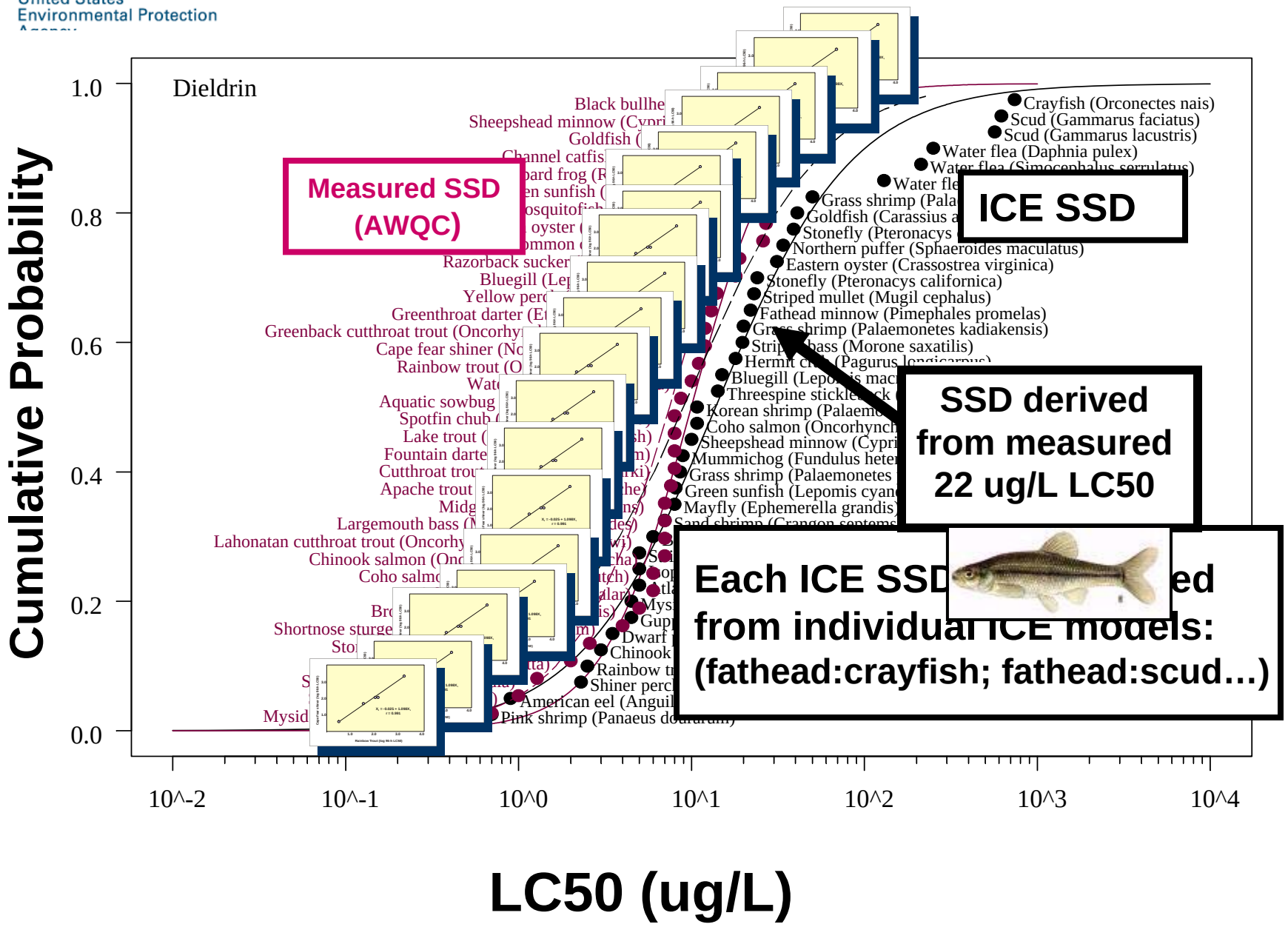
SSDs protective of endangered species (Raimondo et al. 2008. ETC 27:2599-2607)



ICE and Measured SSDs



ICE and Measured SSDs



How Do ICE and Measured SSDs Compare?

- **Aquatic Species Proof of Concept** (Dyer et al. 2006. ES&T 40:3102–3111)
  - ICE-based SSDs had HC5s within an order of magnitude of measured HC5s
- **Aquatic Species, Expanded Study** (Dyer et al. 2008. ES&T 42:3076–3083)
  - 55 AWQC chemicals
  - using fish surrogate to predict fish and invertebrate surrogate to predict invertebrates yielded SSDs similar to measured
- **Wildlife ICE SSD study** (Awkerman et al. 2008. ES&T 42:3447–3452)
  - > 90% of ICE HD5s within 5-fold of measured HD5

Web-ICE SSD Modules

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

U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information
User Manual
Download Model Data
Bibliography

The Web-based Interspecies Correlation Estimation (Web-ICE) application estimates acute toxicity to aquatic and terrestrial organisms for use in risk assessment. Please refer to the User Manual for detailed instructions on using Web-ICE.

Species Sensitivity Distribution Modules

ICE A dlife
Aquatic vertebrates invertebrates
• Spec s
• Gen s
• Fam y
Terrestrial B rds / Mammals
• S ecies
• amily

Species Sensitivity Distribution Module
• ICE Aquatic
• ICE Wildlife

Please address all comments and questions to the webmaster
Office of Research and Development | National Health and Environmental Effects Research Laboratory | Gulf Ecology Division

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Species Sensitivity Distrib

Pick a surrogate
Enter known toxicity

Single Surrogate SSD

Pick your Surrogate	Enter Toxicity (µg/L)
(•) Fathead minnow (Pimephales promelas)	75
( ) Sheepshead minnow (Cyprinodon variegatus)	
( ) Bluegill (Lepomis macrochirus)	
( ) Channel catfish (Ictalurus punctatus)	
( ) Rainbow trout (Oncorhynchus mykiss)	

Reset Continue

If toxicity data for a chemical is available for both a vertebrate and an invertebrate species, SSDs can be improved by using two surrogates. The two surrogate SSD uses the vertebrate surrogate to estimate toxicity to all vertebrate species and the invertebrate surrogate to estimate toxicity to all invertebrate species. Data generated from both surrogates are combined to create one SSD. See the user manual for more on this method.

Two Surrogate SSD

Pick your vertebrate Surrogate	Enter Toxicity (µg/L)
( ) Fathead minnow (Pimephales promelas)	
( ) Sheepshead minnow (Cyprinodon variegatus)	
( ) Bluegill (Lepomis macrochirus)	
( ) Channel catfish (Ictalurus punctatus)	
( ) Rainbow trout (Oncorhynchus mykiss)	

U.S. Environmental Protection Agency

Interspecies Correlation Estimation

Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Species Sensitivity Distributions

Calculates hazard level confidence interval

Surrogate Species: Fathe minnow (Pimephales pr melas)

Input Toxicity: 75 g/L

HC5 3.56 µg/L 95% Confidence Interval: 0.547 - 7.77

Unclick boxes to exclude species

Simultaneously calculates toxicity & confidence intervals

Indicates potential uncertainty

Common Name Sort	Scientific Sort	Estimated Toxicity Sort ↓	95% Confidence Intervals Sort
Mysid	Americamysis bahia	0.825	0.020 - 32.47
Stonefly		1.37	0.567 - 3.3
Stonefly		2.48	1.36 - 4.5
Amphipo		3.30	0.695 - 15.7
Stonefly	eronarcys californica	5.83	1.60 - 21.2
Northern pike	Esox lucius	11.63	4.06 - 33.30
Atlantic s on	Salmo salar	13.39	3.61 - 49.68
Bro out	Salmo trutta	13.52	3.85 - 47.40
Shortnose sturgeon	Acipenser brevirostrum	14.83	7.05 - 31.20
Brook trout	Salvelinus fontinalis	18.98	6.65 - 54.17
Smallmouth bass	Micropterus dolomieu	19.66	4.35 - 88.92
Fountain darter	Etheostoma fonticola	20.64	10.63 - 40.09

* Input toxicity less than model minimum of 93.07

Pick your Surrogate	Enter Toxicity (µg/L)
○ Fathead minnow (Pimephales promelas)	
○ Sheepshead minnow (Cyprinodon variegatus)	
○ Bluegill (Lepomis macrochirus)	
○ Channel catfish (Ictalurus punctatus)	
○ Rainbow trout (Oncorhynchus mykiss)	

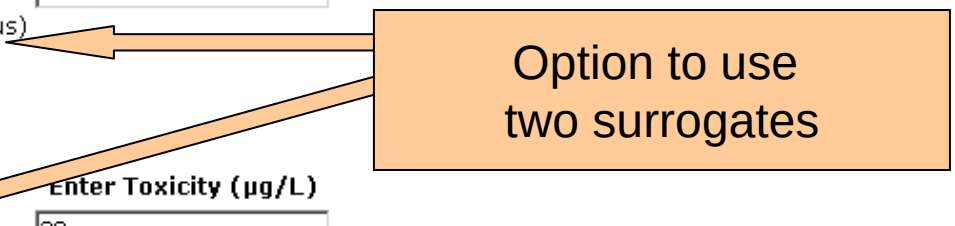
Reset Continue

If toxicity data for a chemical is available for both a vertebrate and an invertebrate species, SSDs can be improved by using two surrogates. The two surrogate SSD uses the vertebrate surrogate to estimate toxicity to all vertebrate species and the invertebrate surrogate to estimate toxicity to all invertebrate species. Data generated from both surrogates are combined to create one SSD. See the user manual for more on this method.

Two Surrogate SSD

Pick your vertebrate Surrogate	Enter Toxicity (µg/L)
◉ Fathead minnow (Pimephales promelas)	75
○ Sheepshead minnow (Cyprinodon variegatus)	
○ Bluegill (Lepomis macrochirus)	
○ Channel catfish (Ictalurus punctatus)	
○ Rainbow trout (Oncorhynchus mykiss)	
Pick your invertebrate Surrogate	**Enter Toxicity (µg/L)**
◉ Daphnid (Daphnia magna)	20
○ Mysid (Americamysis bahia)	

Reset Continue



Exposure Assessment Models

Web-ICE Home
Aquatic Species
Aquatic Genus
Aquatic Family
Wildlife Species
Wildlife Family

Species Sensitivity Distributions
Aquatic
Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Species Sensitivity Distributions - Aquatic

Surrogate Species: Fathead minnow (Pimephales promelas) ; Daphnid (Daphnia magna)

Input Toxicity: 75;20 µg/L

HC5 7.88 µg/L 95% Confidence Interval: 1.87 - 17.23

Common Name Sort	Scientific Sort	Estimated Toxicity Sort ↓	95% Confidence Intervals Sort
Mysid	Americamysis bahia	9.40	
Northern pike	Esox lucius	11.63	4.06 - 33.30
Atlantic salmon	Salmo salar	13.39	3.61 - 49.68
Brown trout	Salmo trutta	13.52	3.85 - 47.40
Shortnose sturgeon	Acipenser brevirostrum	14.83	7.05 - 31.20
Pink shrimp	Farfantepenaeus duorarum	15.61	0.398 - 612.31
Amphipod	Gammarus pseudolimnaeus	16.70	6.02 - 46.33
Brook trout	Salvelinus fontinalis	18.98	
Daphnid	Simocephalus serrulatus	19.10	7.87 - 46.34
Smallmouth bass	Micropterus dolomieu	19.66	4.35 - 88.92
Fountain darter	Etheostoma fonticola	20.64	10.63 - 40.09

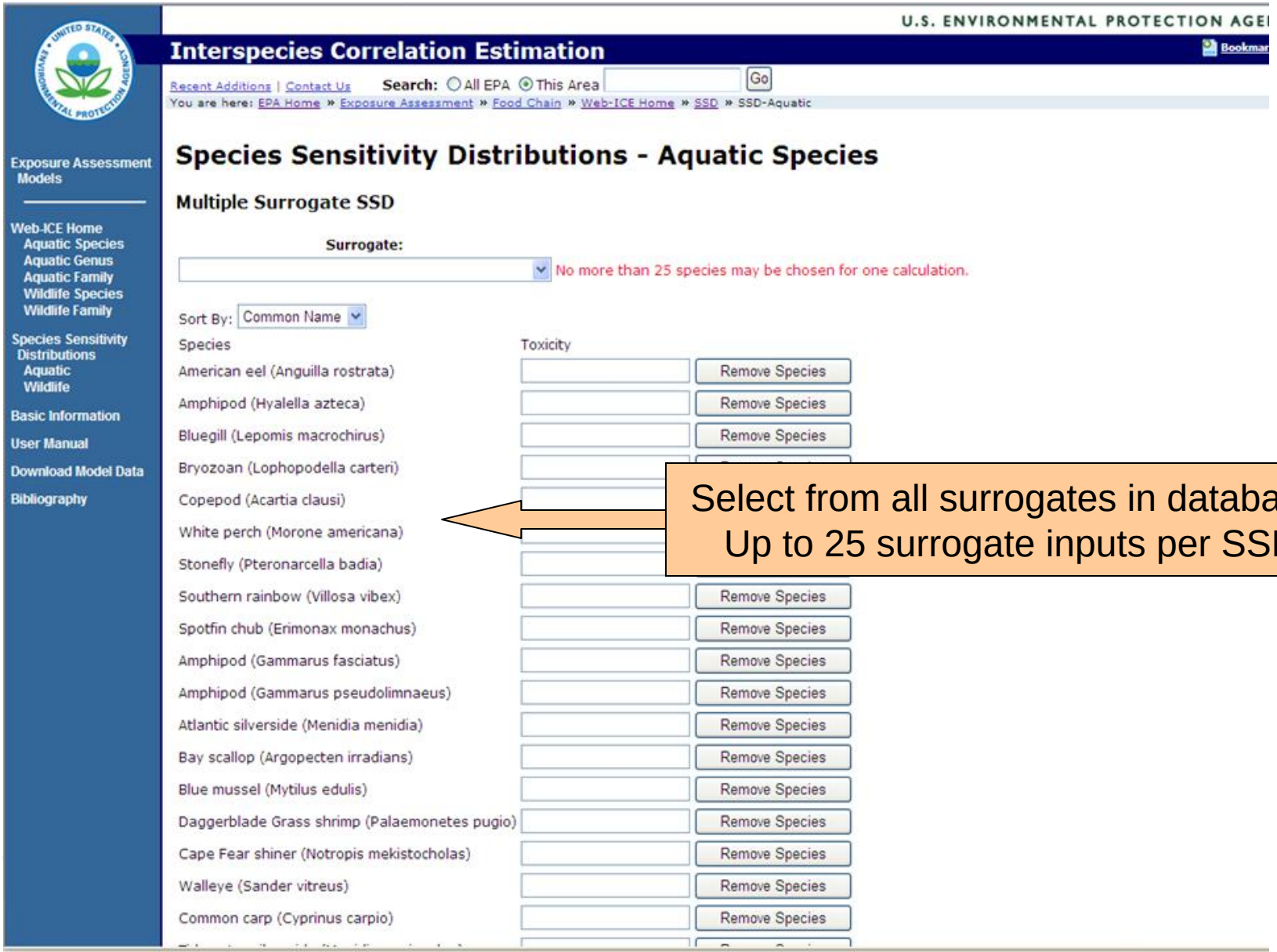
Predicted from invertebrate

* Input toxicity less than model minimum of 93.07

predicted from fish

United States Environmental Protection Agency

2009 update: Improved SSD surrogate choices



2009 update: Improved SSD output

United States Environmental Protection Agency

U.S. ENVIRONMENTAL PROTECTION AGENCY

Interspecies Correlation Estimation

Bookmark

Recent Additions | Contact Us Search: All EPA This Area Go

You are here: EPA Home » Exposure Assessment » Food Chain » Web-ICE Home » SSD » SSD-Aquatic » SSD-Aquatic Results

Exposure Assessment Models

Web-ICE Home
- Aquatic Species
- Aquatic Genus
- Aquatic Family
- Wildlife Species
- Wildlife Family

Species Sensitivity Distributions
- Aquatic
- Wildlife

Basic Information

User Manual

Download Model Data

Bibliography

Species Sensitivity Distributions - Aquatic

Surrogate Species: Blue crab (Callinectes sapidus), Channel catfish (Ictalurus punctatus), Rainbow trout (Oncorhynchus mykiss)

Input Toxicity: 150, 200, 250 µg/L

HC5 30.58 µg/L 95% Confidence Interval: 7.41 - 57.81

Common Name Sort	Scientific Sort	Estimated Toxicity Sort ↓	95% Confidence Intervals Sort	Show Data: Surrogate Sort
Stonefly	Claassenia sabulosa	1.94	0.805 - 4.68	Channel catfish (Ictalurus punctatus)
Stonefly	Pteronarcella badia	3.46	1.80 - 6.67	Channel catfish (Ictalurus punctatus)
Amphipod	Gammarus lacustris	12.14	4.72 - 31.19	Rainbow trout (Oncorhynchus mykiss)
Stonefly	Pteronarcys californica	30.44	13.44 - 68.94	Rainbow trout (Oncorhynchus mykiss)
Daphnid	Daphnia pulex	43.79	1(	
Pink shrimp	Farfantepenaeus duorarum	47.16	2	
Mysid	Americamysis bahia	49.87	12.59 - 197.51	mykiss)
Northern pike	Esox lucius	50.39	21.07 - 120.47	Channel catfish (Ictalurus punctatus)
Amphipod	Gammarus pseudolimnaeus	68.03	25.20 - 183.64	Rainbow trout (Oncorhynchus mykiss)

Estimate based on best fit ICE model of input surrogate species

Attributes of Web-ICE

Defensibility

- cross-validation of models provides user with estimate of model performance
- all models significant

User guidance

- clearly outlined
- uncertainty analyses identify “Rules of Thumb” (Aquatic complete in 2009)
- Web-ICE alerts users to potentially poor-fitting data

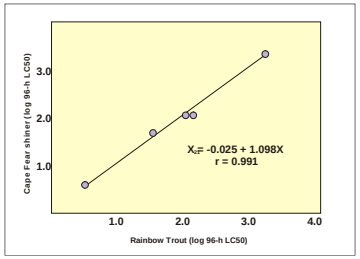
Dynamic application easy to update

- updated & new models with new toxicity data
- update user-friendliness through user feedback
- new modules to meet ecorisk needs

Applications: Ecological Risk Assessment

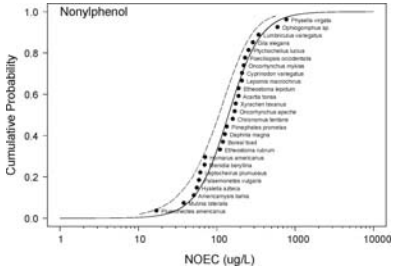
Direct toxicity estimation

- >14,000 standardized QC'd acute tox records
- 2000+ chemicals, 400+ species
- 2000 interspecies models



Species Sensitivity Distributions

- populate SSDs and derive HC5/HD5
- high accuracy, easy to use
- link to QSAR



Endangered species risk assessment

- Web-ICE module in development
- Direct toxicity estimation
- SSD approach: 97% T&E >HC5; 99% T&E >HC1
  (Raimondo et al. 2008. ETC 27:2599-2607)

Web-ICE Future Research Directions

- **Internet platform allows for dynamic product**
  - updates of latest model development
  - continuous improvement of user-friendliness
  - updates occur in short time frame
- **Expand SSD Module**
  - include option to select distribution type
  - include model information on output screen
- **2009-2010 Research**
  - QSAR to ICE linkage
  - ICE chronic toxicity models
  - Algal models
  - MOA specific aquatic models
- **FUTURE Modules**
  - Endangered Species module (2009)
  - Algal ICE (2009)

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