Application of Logistic Regression Model Predictions of Toxicity From Sediment Chemistry To Benthic Injury Assessment

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IQA Disclaimer

- "My agency pays me to do this job and entrusts me with a lot of responsibility, but what I say should be considered only my personal opinion and observations, should not be interpreted as agency policy, and if you don't like what I say they'll claim they never heard of me" – Robert A. Taylor, 2006

Why Predictive Models?

- Models provide a continuous response from 0 to 1, rather than individual thresholds, which allow users to establish the level of effect (probability of toxicity, magnitude of effect) to meet their objectives
- Models can take into account site-specific mixtures, and model output can be calibrated to site-data
- Calibrated models can be applied to other sediment chemistry data from the site/region without matching toxicity data

Approaches to Predicting Risk From Sediment Mixtures

- Mechanistic approach (EqP, SEM/AVS):
  - Mechanistically-based approaches are designed to predict sediment toxicity based on an understanding of the chemical and biological processes that influence toxicity.
  - Requires understanding bioavailability and toxicity of all constituents, common mode of action, contaminant interactions to address mixtures (e.g., PAH toxic unit approach)
- Empirical approach:
  - Derived from field-collected environmental sediment samples with matching measures of chemistry and biological effects
  - Requires association between concentrations and effects, where each constituent is considered an estimator of the toxicity of the mixture

Outline of Presentation

- Overview of logistic regression model (LRM) derivation and approach
- Application of LRM predictions of toxicity to Site- or Regional-specific assessments
- Using predictive models to scale benthic injury

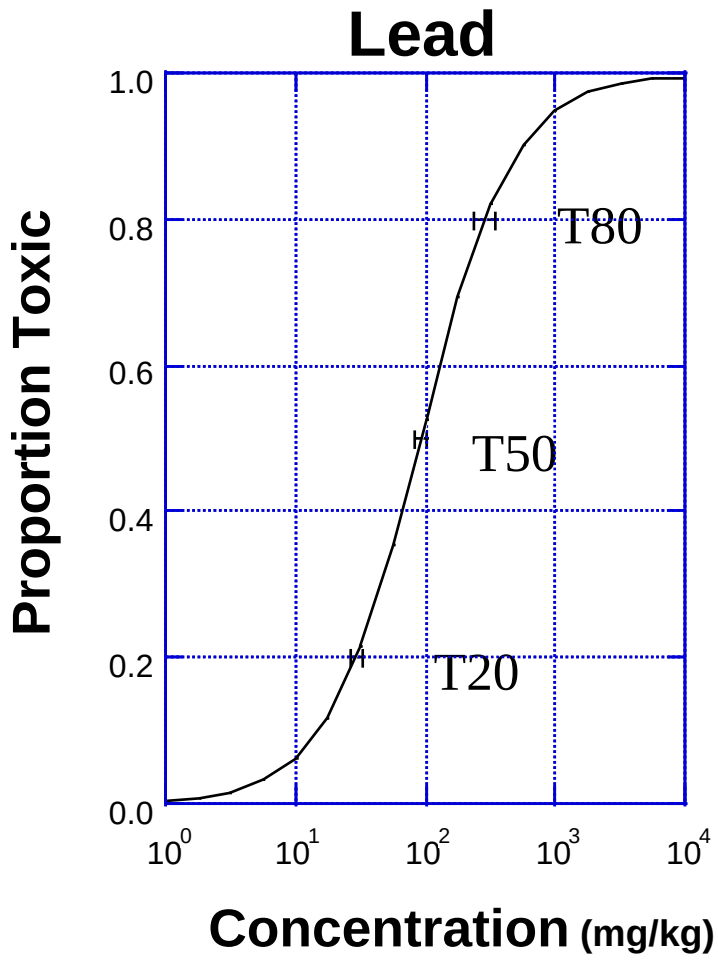
Logistic Regression Modeling Development Approach

- Compile/standardize/QA database of matching sediment chemistry and toxicity for specific test endpoints
- Derive and evaluate individual chemical-specific logistic regression models that estimate the probability of toxicity for a given chemical concentration
- Combine acceptable individual models into single mixture model for estimating probability and magnitude of toxicity on a per sample basis

Database Used to Derive LRMs

- >3200 samples of matching sediment chemistry and marine amphipod toxicity from coastal North America
- 10-day lethality endpoint for two species of marine amphipods: *Ampelisca abdita* (N=2012) and *Rhepoxynius abronius* (N=1211)
- Most of data from large programs with standardized methods

Individual Chemical Logistic Regression Models



- Logistic model estimates the proportion of samples expected to be toxic at a given concentration
- Normalized chi-square statistic provides a relative measure of the goodness-of-fit for the individual chemical models
- Point estimates (e.g., T20, T50, T80) represent the concentration at which 20, 50, or 80% of the samples would be predicted to be toxic

Individual Chemical Models

Metals

Antimony
Arsenic
Cadmium
Chromium
Copper
Lead
Mercury
Nickel
Silver
Zinc

PCBs/ Pesticides

Total PCBs
Dieldrin
p,p'-DDD
p,p'-DDE
p,p'-DDT

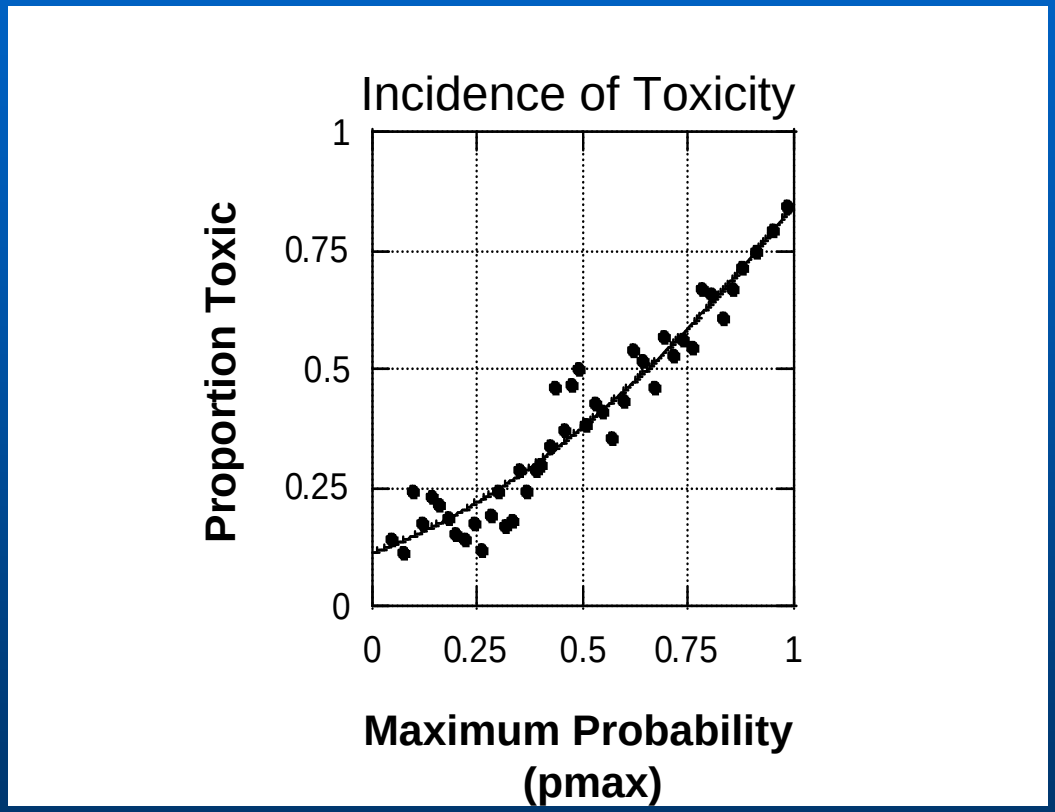
PAHs

1-Methylnaphthalene
1-Methylphenanthrene
2,6-Dimethylnaphthalene
2-Methylnaphthalene
Acenaphthene
Acenaphthylene
Anthracene
Benz(a)anthracene
Benzo(a)pyrene
Benzo(b)fluoranthene
Benzo(g,h,i)perylene
Benzo(k)fluoranthene
Biphenyl
Chrysene
Dibenz(a,h)anthracene
Fluoranthene
Fluorene
Indeno(1,2,3-c,d)pyrene
Naphthalene
Perylene
Phenanthrene
Pyrene

Mixture Models

- Predict the probability of observing toxicity in samples that contain a mixture of chemicals (most environmental samples)
- LRM approach uses the maximum probability of observing toxicity taken from the set of probabilities calculated for each individual chemical in a sample (P_Max model)

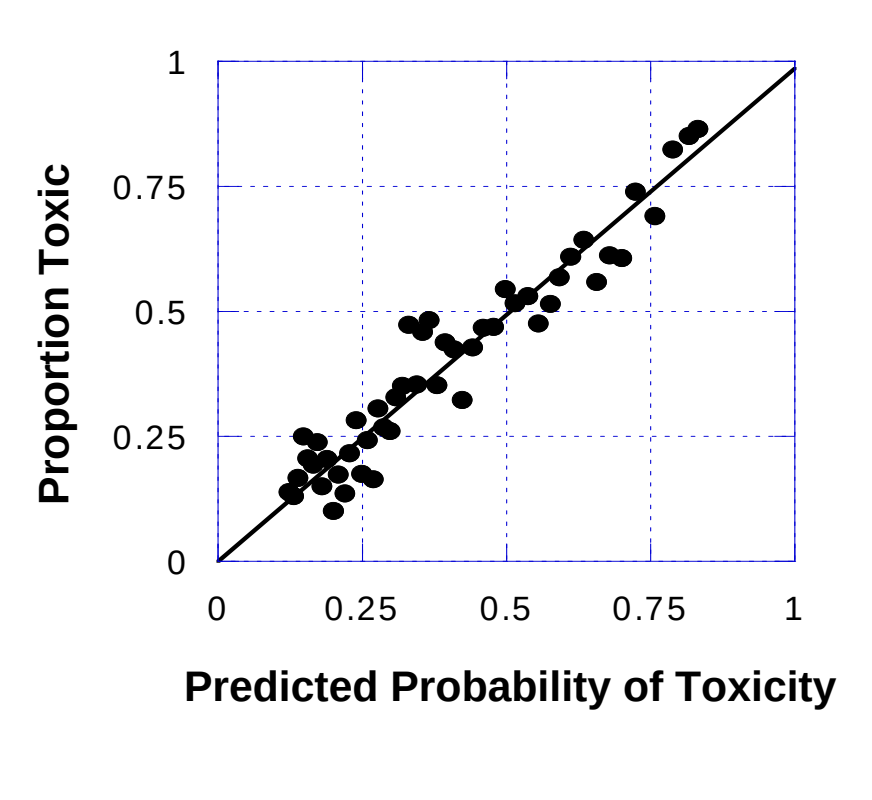
Mixture Model



$Y = 0.11+0.33x+0.40x^2$

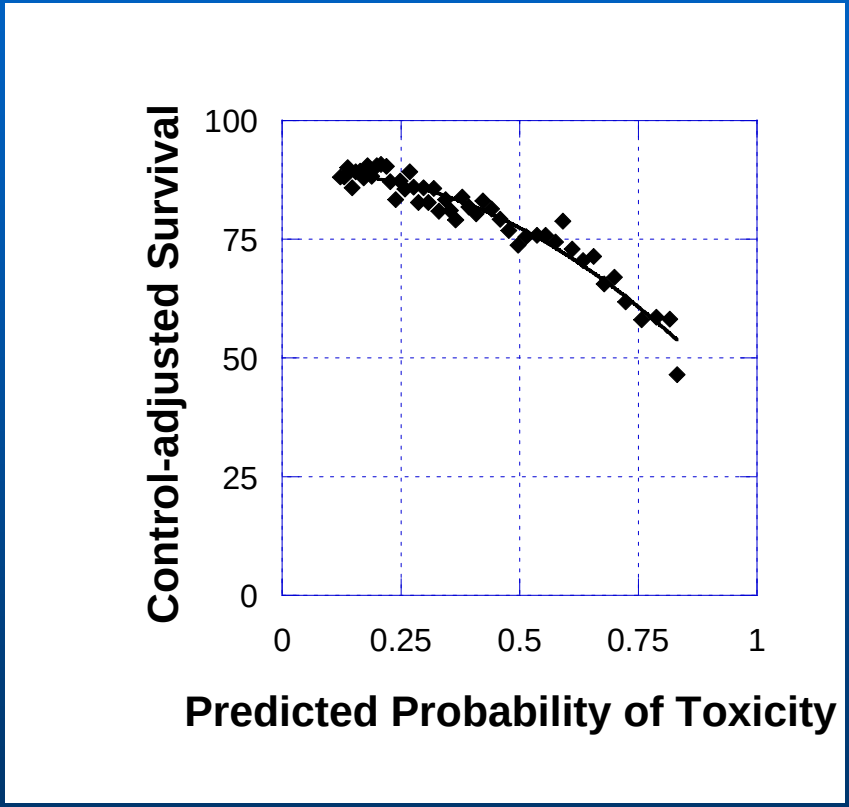
$R^2 = 0.93$

Predicted Probability of Toxicity vs. Observed Proportion of Toxic Samples



The probability of toxicity is predicted using the P_Max model. Each point represents the median predicted probability of a minimum of 50 individual samples within the interval (n=3223)

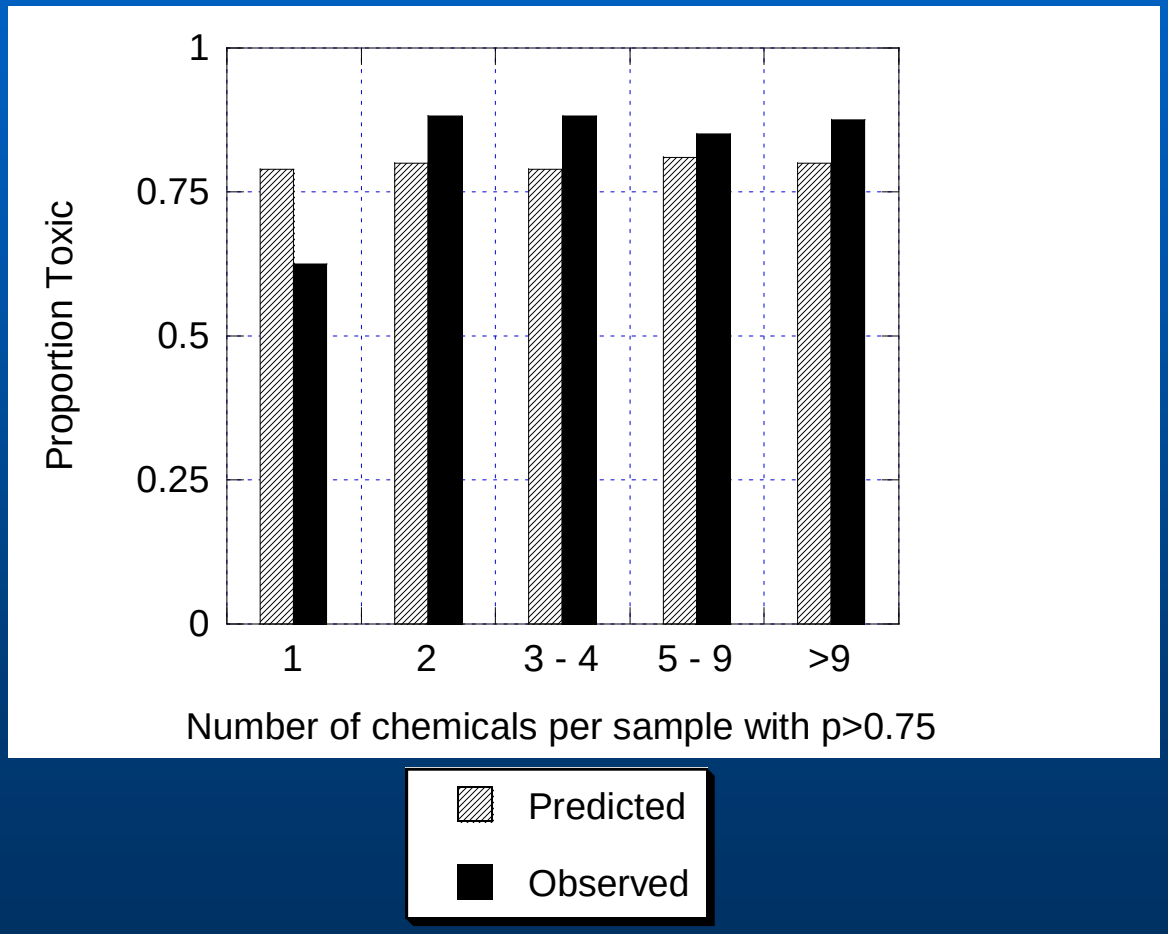
As the Predicted Probability of Toxicity Increases, Control-Adjusted Survival Decreases



$Y = 88.75+6.75x-58.73x^2$

$R^2 = 0.94$

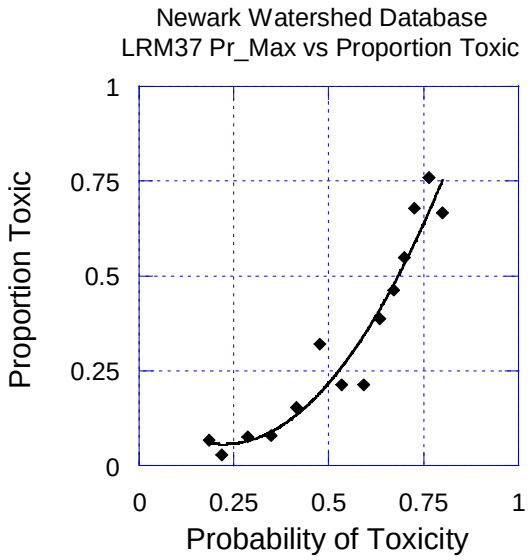
Effect of the Number of Chemicals in a Sample with High Predicted Probability of Toxicity (p>0.75)



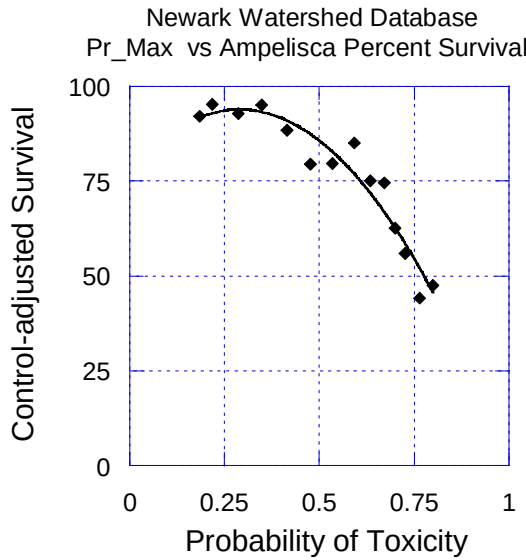
Application of LRMs to Specific Sites or Regions

- Site-specific matching chemistry-toxicity data to evaluate model performance always recommended
- If limited available data, model output predicting incidence and/or magnitude of toxicity can be used to establish framework for scaling benthic injury

Application of LRM to Newark Bay Watershed Data: Ampelisca 10-d Survival

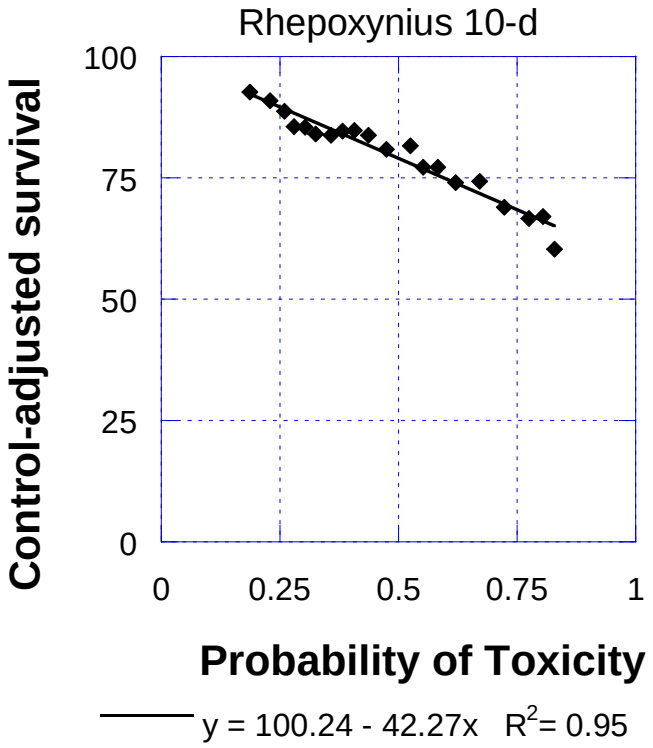


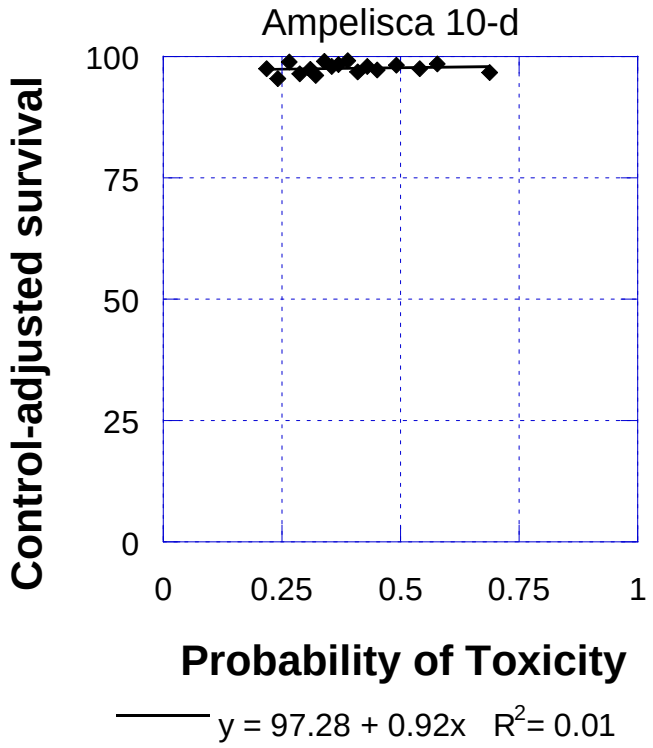
$Y = M0 + M1*x + ... M8*x^8 + M9*x^9$	
M0	0.16
M1	-0.92
M2	2.09
R^2	0.93



$Y = M0 + M1*x + ... M8*x^8 + M9*x^9$	
M0	78.35
M1	107.64
M2	-185.88
R^2	0.92

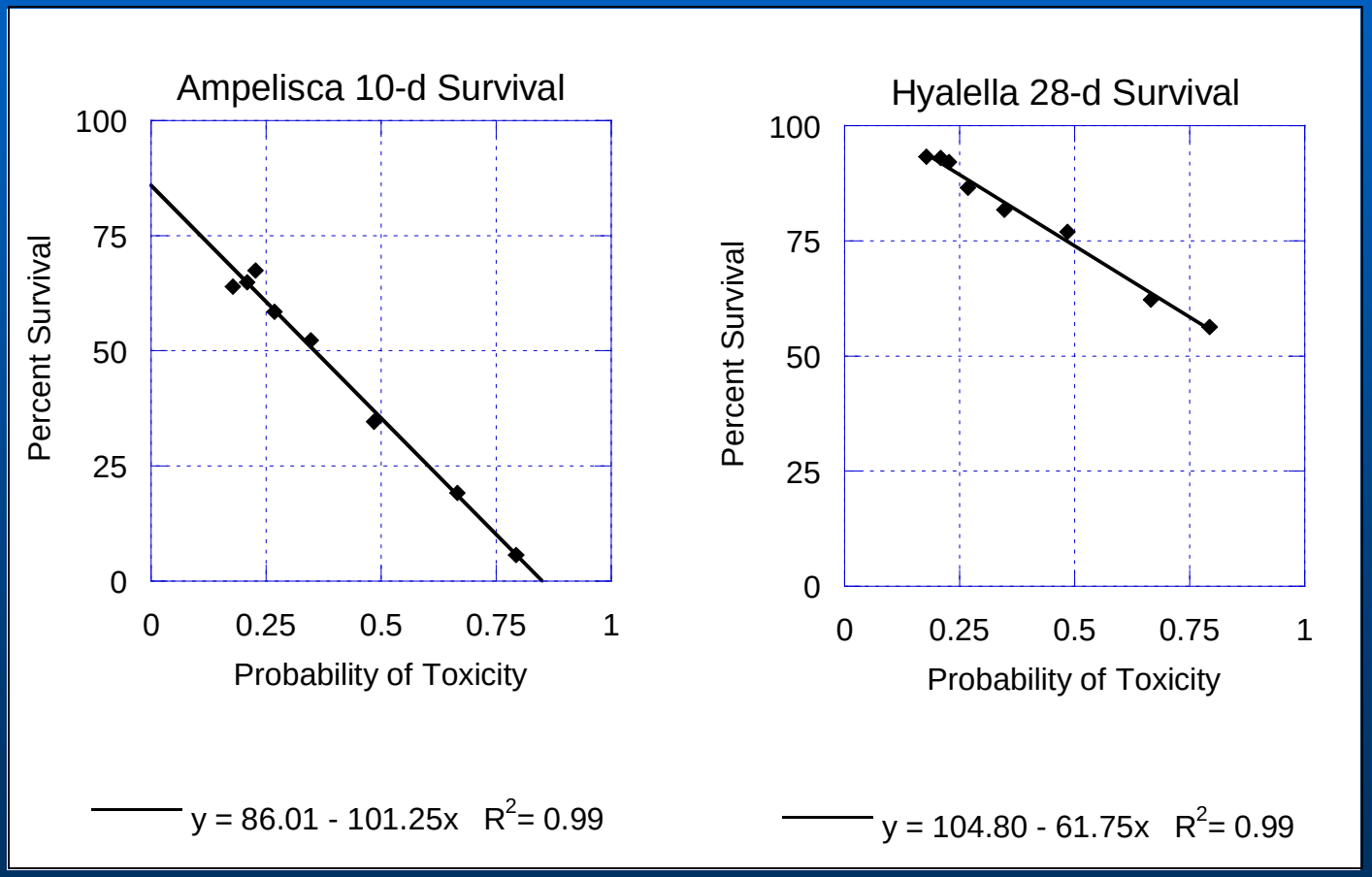
Application of LRM to Puget Sound Data for *Rhepoxynius abronius* and *Ampelisca abdita* 10-d Survival



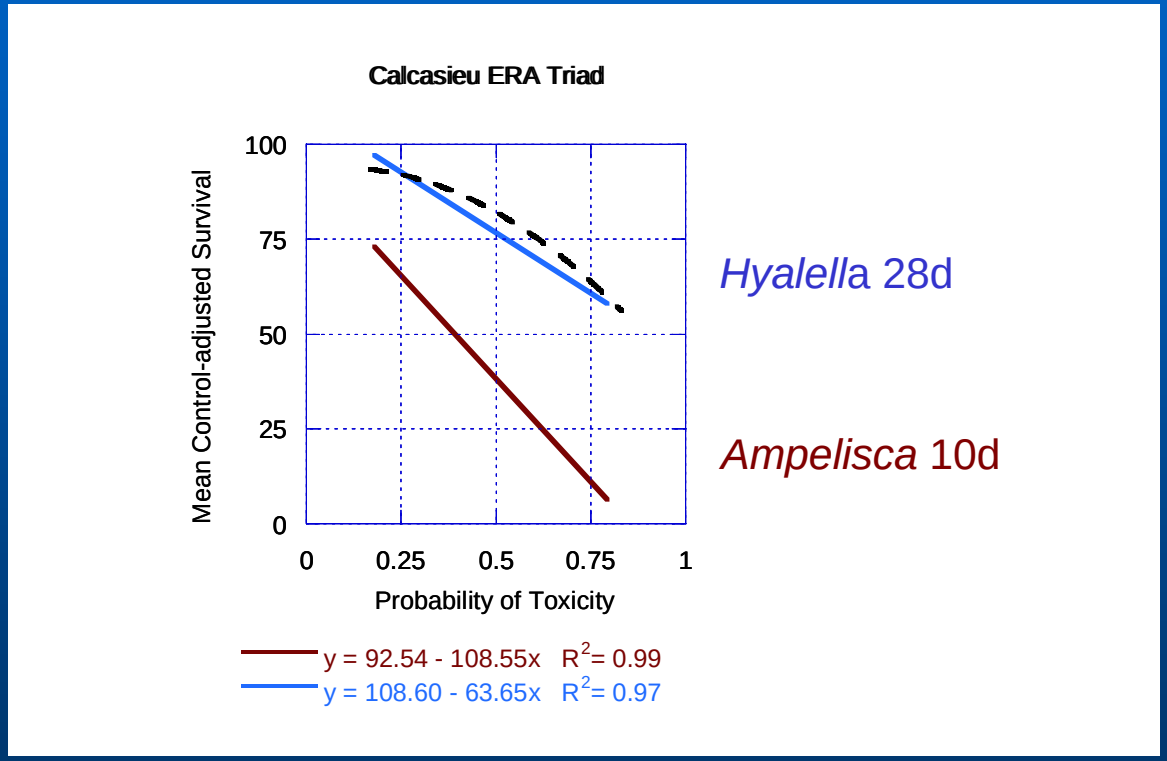


Each point represents the median sample probability of toxicity for samples within the interval

Application of LRM to Calcasieu Estuary for Ampelisca 10-d and Hyalella 28-d Survival



Calcasieu Estuary
Comparison with original PMax Model



Approaches to Using LRM Models to Scale Benthic Injury

- Interpolated surface
  - LRM model output of predicted probability of toxicity or percent survival
  - Spatial weighting of individual data points
  - Use of numeric values vs defined levels of injury
- Grid
  - allows weighting of multiple lines of evidence (eg., LRM predictions and sediment bioassay results)

Advantages of LRM Approach

- Defined scale of probability from 0 – 1
- Less affected by number of chemicals analyzed than mean quotient approaches
- Model output can be used to define scale of injury based on incidence of toxicity or magnitude of response
- Models can be calibrated to site-specific data

Limitations of LRM Approach

- Bioavailability not explicitly accounted for
- Causality not directly attributable to individual chemicals without additional evidence
- Based on acute lethality endpoint
- Successful development of LRMs typically requires large database representing multiple chemical gradients

Spiked-sediment Amphipod Bioassay LC50 Values and Probability of Toxicity from Chemical-specific LRMs

Chemical	LC_{50}	Probability of Toxicity	Source
Cadmium (mg/kg)	9.81	0.90	Mearns et al.1986
	8.8 - 10.0	0.88 - 0.90	Kemp et al. 1986
	8.2 - 11.5	0.88 - 0.91	Robinson et al.1988
	6.9	0.85	Swartz et al.1985
Mercury (mg/kg)	13.1	0.97	Swartz et al. 1988
Zinc (mg/kg.)	276	0.54	Swartz et al. 1988
Fluoranthene (mg/kg)	4.2	0.71	Swartz et al. 1988
	3.3 - 10.5	0.68 - 0.82	Swartz et al. 1987
Phenanthrene (mg/kg)	3.68	0.82	Swartz et al. 1989
Total PCBs (mg/kg)	8.8	0.87	Swartz et al. 1988
p,p'-DDT (ng/g)	11.2 - 125	0.50 - 0.85	Word et al. 1987

From U.S. EPA (2005). Predicting toxicity to amphipods from sediment chemistry. NCEA. Washington, DC; EPA/600/R-04/030

Summary

- The LRM approach provides a consistent basis for evaluating environmental sediment mixtures
- The models are not dose-response relationships for individual chemicals, but can be considered indicators of toxicity based on field-collected sediment chemical mixtures.
- Site- or regional-specific applications of the models should include an evaluation with matching sediment chemistry and toxicity data
- The LRM approach enables users to select the level of protectiveness (as measured by the probability of toxicity and/or the magnitude of toxicity) appropriate for their objectives.

Additional Information on LRM Approach

- U.S. EPA (2005). Predicting toxicity to amphipods from sediment chemistry. National Center for Environmental Assessment, Washington, DC; EPA/600/R-04/030.
- Field LJ, MacDonald DD, Norton SB, Ingersoll CG, Severn CG, Smorong D, Lindskoog R. 2002. Predicting amphipod toxicity from sediment chemistry using logistic regression models. Environ Toxicol Chem 21(9): 1993-2005.
- Field LJ, MacDonald DD, Norton SB, Severn CG, Ingersoll CG. 1999. Evaluating sediment chemistry and toxicity data using logistic regression modeling. Environ Toxicol Chem 18:1311-1322.