

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

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Water quality criteria (WQC) designate the maximum concentrations of water-borne toxicants that do not adversely affect specific protection goals under certain natural conditions. As the foundation of water quality standards, WQC provide a critical scientific basis for environmental protection agencies to protect aquatic ecosystems. The vast majority of WQC are derived using assessment factors and/or species sensitivity distributions (SSD). The SSD is the preferred method for derivation of WQCs as they are cumulative distribution functions of toxicity values for multiple species that estimate a hazard level that is protective of most species within the distribution. While SSDs based on measured toxicity values can provide a strong level of confidence for environmental protection, there is still some uncertainty in their applicability for untested species. Additionally, SSD development has been limited to a relatively few chemicals because of the requirement for toxicity data for a broad diversity of taxa. Interspecies correlation estimations (ICE) models may provide great assistance for addressing the development of WQC that are protective of species that cannot be tested.

ICE models were first developed by the U.S. Environmental Protection Agency (USEPA) to extrapolate acute toxicity of aquatic and wildlife species to taxa with acute toxicity data for a chemical.<sup>1</sup> ICE models were developed to fill in data gaps for

species that could not be tested (e.g., endangered species) as well as supplement databases for SSDs. The accuracy of ICE models to predict chemical toxicity to tested species has been shown to be within an order of magnitude.<sup>2,4</sup> The development of WQCs generally require a minimum of 8 or 10 species toxicity data that compose all major trophic levels (e.g., algae, invertebrates, fish) or perhaps even focus on the most sensitive species or trophic level. For example, in USEPA guidelines of WQC, three phyla and eight families are required in the derivation of WQC.<sup>3</sup> The use of ICE to estimate supplemental taxa sensitivity data, including that for rare or endangered species, for a particular toxicant can be useful for both filling data gaps and/or adding more weight of evidence for environmental protection goals. For some chemicals with limited toxicity data, such as a new emerging pollutant (e.g., polybrominated diphenyl ethers, nanomaterials, perfluorooctanoic acid), ICE models can be used to estimate additional toxicity data that may help to derive WQC of these chemicals.

To date, ICE models have had limited usage in the derivation of WQC throughout the world, but have been used extensively for estimating the relative sensitivity of rare, threatened and/or endangered species. Basically, ICE could potentially be used in the development of WQC by two different means. First, the prediction tool could be used to predict acute toxicity values for single species for which experimental data are unavailable. This application could fulfill minimum data requirements or be used to estimate the toxicity of a chemical to a specific species of interest. Second, ICE models could be used to construct SSDs and calculate hazard concentrations (e.g., HC5) from both experimentally determined and estimated acute values. Until now, ICE models have been employed in toxicity extrapolation of aquatic invertebrates and fishes, and the accuracy has been validated.<sup>4</sup> For example, Dyer et al.<sup>2</sup> introduced the use of ICE models to generate SSDs and recommended additional assessment and validation of ICE-based HC5s. The applications of ICE for wildlife, such as birds and mammals have also been investigated,<sup>1</sup> indicating that ICE models can also be used to generate SSDs comparable to those derived from measured wildlife toxicity data. In our previous study, the application of ICE models to generate species sensitivity distribution for zinc has been demonstrated, suggesting that ICE could be used to

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derive potential water quality criteria for diverse chemicals in China.<sup>5</sup>

For ecological risk assessment (ERA) in China, researchers are exploring the use of predicted ICE toxicities in ERA. Potential applications of ICE include the problem formulation phase of an ERA to screen for contaminants of potential concern and in the analysis phase to characterize effects to a larger number of species. We recommend that the estimation of species-specific toxicity values using ICE be as an alternative to safety factors typically applied when extrapolating toxicity or risks to taxa with limited chemical and toxicity data. The estimated hazard concentration by ICE-based SSDs could be used in ERA in place of species-specific toxicity values or as a component of the uncertainty analysis.

ICE is a methodology which can help establish WQC or facilitate specific chemical risk assessment for a diversity of chemicals. Currently, the Internet-based Web-ICE tool ([www.epa.gov/ceampubl/fchain/webice/](http://www.epa.gov/ceampubl/fchain/webice/)) can be used to predict both aquatic and wildlife species toxicity, and provides modules to construct SSDs and compute hazard concentration values of chemicals. Still, some challenges exist using ICE models. For example, the uncertainty of each model prediction needs to be evaluated prior to inclusion in SSDs. If the surrogate toxicity value entered into an ICE model is far outside the range of data used to develop the model, the predicted values should not be used. This is because each ICE model can only be validated for the range of data in the model training set and input data that are far outside this range generally result in low prediction confidence. As such, model confidence intervals need to be evaluated for each prediction. Moreover, the current ICE application has primarily North American species represented. Including these species data to apply ICE models for non-North American regions may introduce additional uncertainty. Other considerations include testing model stability, evaluating sample size considerations, and assessing impacts of taxonomic distance. Currently, Web-ICE provides interspecies extrapolation models for acute toxicity in a user-friendly Internet platform, which can be widely used all over the world.

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### Notes

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