

# DEVELOPMENT OF INTERSPECIES CORRELATION ESTIMATION (ICE) MODELS FOR PETROLEUM HYDROCARBONS

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## Abstract

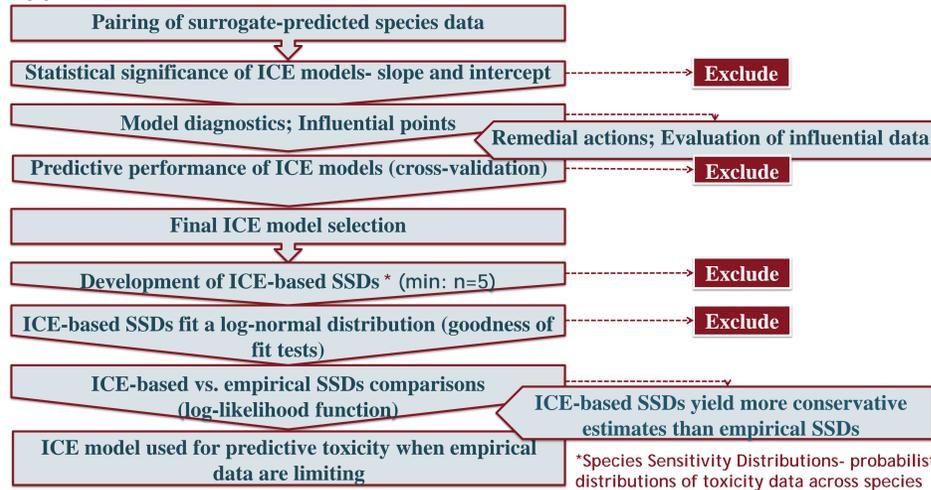
Estimating the consequences of petroleum products to water column organisms is hampered by limited acute toxicity data. We developed petroleum-specific Interspecies Correlation Estimation (ICE) models between surrogate and predicted test species, facilitating toxicity predictions to a broader number of species.

## Methods

The development of ICE models used petroleum hydrocarbon toxicity data (LC50|EC50; measured concentrations) from a recently developed database<sup>[1]</sup>. Linear regression models were developed for predicted-surrogate species pairs with at least 4 data points. Linear models are described by  $\text{Log } P_i = B_0 + B_1 \cdot \text{Log } S_i$ .  $P_i$ : acute toxicity of the predicted species,  $B_0$ : slope,  $B_1$ : intercept,  $S_i$ : acute toxicity of the surrogate species

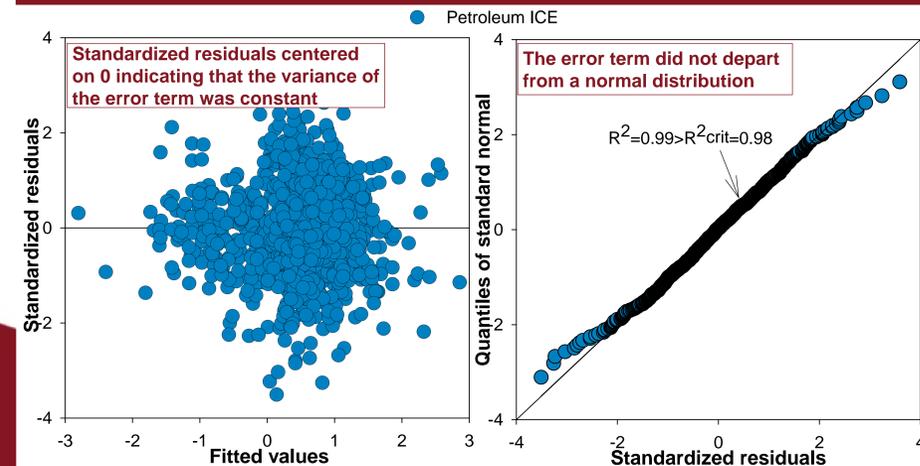
## Model Development

Steps involved in the development, selection, verification and application of ICE models see [2] for details

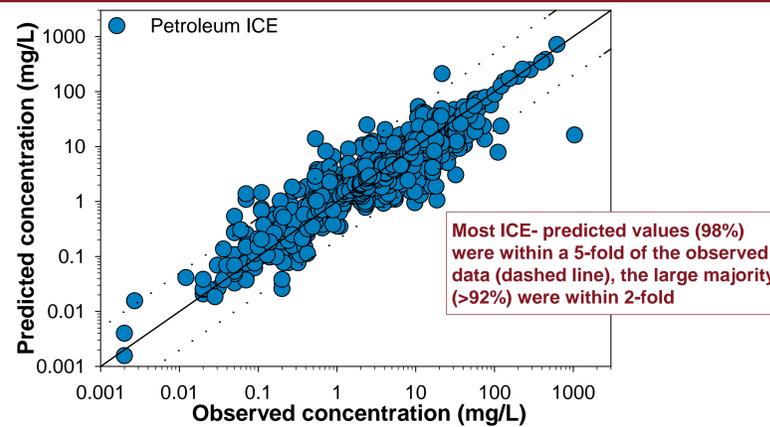


## Results

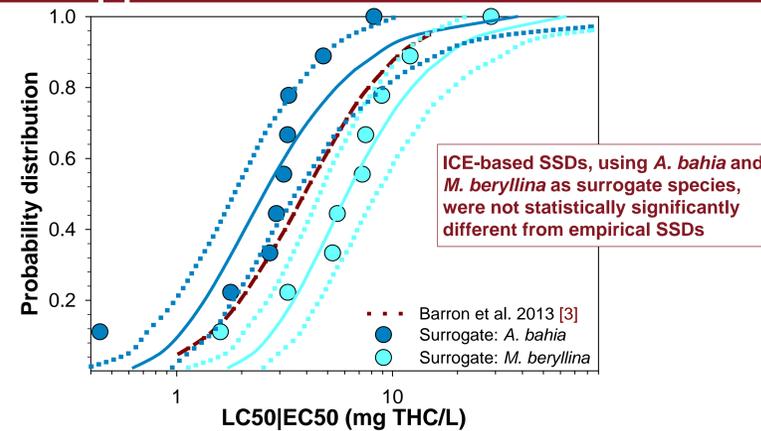
### Model Verification



### Observed vs. Predicted Values



### Practical Application

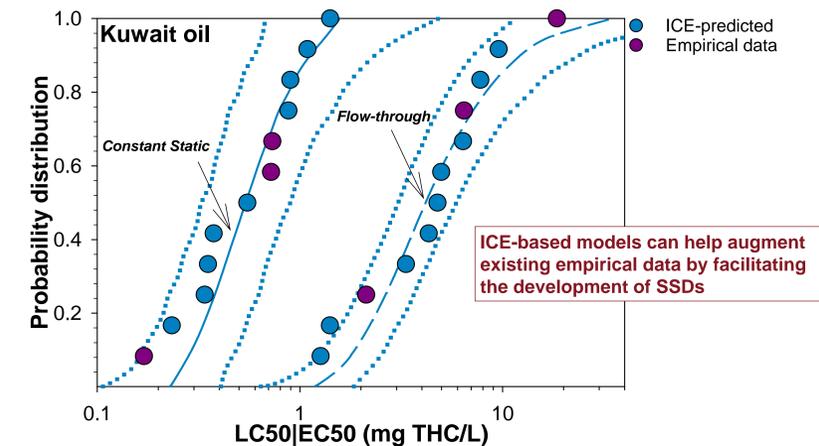
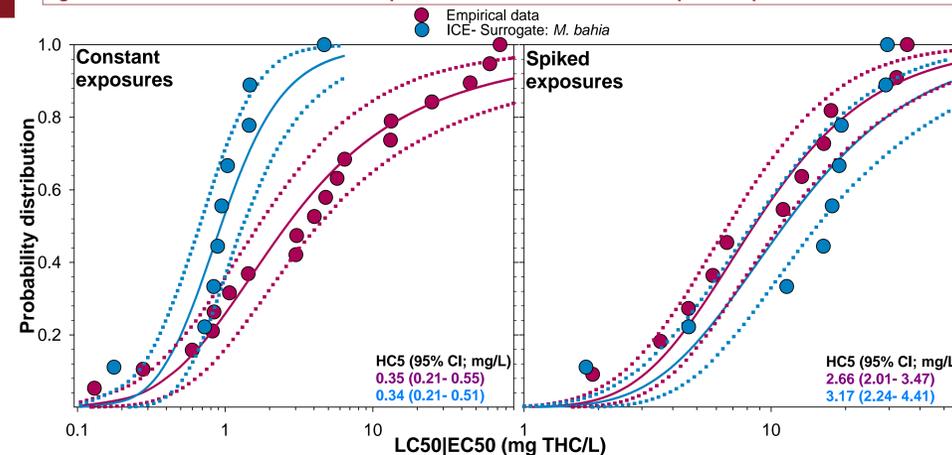


Petroleum hydrocarbon HC5s\* from ICE-based SSDs were in agreement with those derived from empirical SSDs<sup>[3]</sup>

Petroleum product	HC5 (95% PI) [3]	HC5 (95% CI) surrogate: <i>A. bahia</i>	HC5 (95% CI) surrogate: <i>M. beryllina</i>
All crudes	1.03 (0.80-1.34)	0.84 (0.59-1.12)	2.25 (1.68-2.95)
Alaska North Slope/Prudhoe Bay	1.36 (1.04-1.77)	0.82 (0.58-1.10)	4.32 (3.20-5.83)
South Louisiana	3.53 (2.61-4.77)	0.82 (0.58-1.10)	1.43 (1.06-1.87)
Fuel oil #2	0.285 (0.20-0.40)	0.33 (0.23-0.45)	1.18 (0.88-1.54)
Bunker C	0.561 (0.39-0.80)	0.33 (0.23-0.45)	0.56 (0.41-0.73)

\*Hazard concentration assumed to be protective of 95% of the species on the SSD

Petroleum hydrocarbon HC5s\* from ICE-based SSDs using *M. bahia* as the surrogate species were in agreement with those derived from empirical SSDs under constant or spiked exposures



## Discussion

- ❖ This study provides petroleum-specific toxicity estimation (ICE) models that can be applied to a broad range of aquatic species using a SSD-based approach
- ❖ The predicted-observed differences of toxicity values were within the fold difference found across inter-laboratory comparisons
- ❖ ICE-based SSDs produced HC5 values similar to those of empirical SSDs, adding reliability to the use of ICE models to augment toxicity data
- ❖ Additional toxicity data could help improve existing ICE models
- ❖ ICE models can provide information when the costs of toxicity testing are prohibitive, or when species-specific toxicity testing is restricted or not feasible

## References

- [1] Bejarano, et al., 2014. Development and application of DTox: A quantitative database of the toxicological effects of dispersants and chemically dispersed oil. IOOSC, Savannah, GA, USA
- [2] Bejarano and Barron, 2014. Development and Practical Application of Petroleum and Dispersant Interspecies Correlation Models for Aquatic Species. ES&T 48(8): 4564-4572.
- [3] Barron et al., 2013. Development of aquatic toxicity benchmarks for oil products using species sensitivity distributions. IEAM 9(4): 610-615.

## Acknowledgements

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