Aquatic Ecological Assessment for Shampoos: Sensitivity of the USETox Model to Parameter Uncertainty

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ABSTRACT SUMMARY

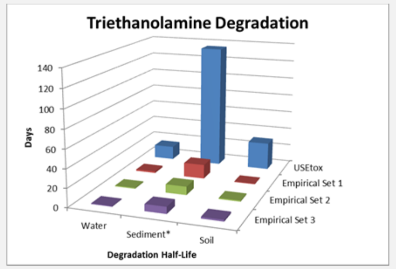
- The relative ranking of shampoos to elicit adverse aquatic effects is being evaluated under new product labeling rules in France using the USETox life cycle impact assessment model
- Model database contains few shampoo ingredients
- Model requires substantial data, including degradation rates in all media, partition coefficients, and all available aquatic effects data
- Government and/or industry need to develop a reliable dataset for shampoo ingredients before model's use to support decision-making is reliable
- Use of modeled input data and a lack of guidance on appropriate input data can lead to wide variations in model results, limiting utility of the current USEtox implementation for shampoo labeling

DEGRADATION RATES

- Model requires degradation rates in air, water, soil, and sediment.
- US EPA EPIWeb Fugacity Model default values, based on BIOWIN model are used in the model database.
- Low degree of distinction among substances' degradation rates because BIOWIN results are binned, not continuous – only eight distinct half-lives possible.
- Adequate empirical data unavailable for most substances – kinetics in air, water, soil, sediment.

Substitution of Empirical Data Alters Ingredient Rank

- Example – comparison of two shampoo ingredients in database
  - Triethanolamine – used for buffering, masking, emulsifying, surfactant
  - Sodium Citrate – used for buffering, chelating, masking



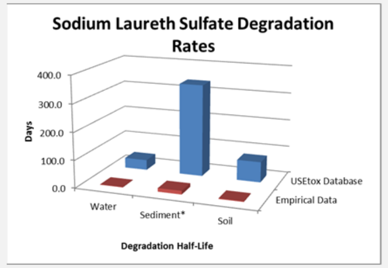
*Sediment half-life assumed to be nine times the water half-life in EPI Web; Equivalent assumption made for empirical data here. Empirical data from West and Gonsior, 1996.

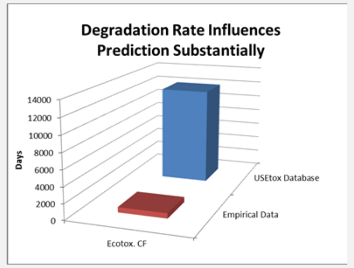
- Model result = Ecotoxicological Characterization Factor (CF) with units of Potentially Affected Fraction (of Species) · m³ · day · kg⁻¹

		CF	
Lower Potential Aquatic Impact	Triethanolamine	0.9 to 1.8	Empirical Biodegradation Data
	Sodium Citrate	2.6	USEtox Database
	Triethanolamine	14.1	USEtox Database

Substitution of Empirical Data Substantially Alters Prediction of Aquatic Effects

- Substantial shifting of CF occurs with key shampoo ingredients such as surfactants, which are not well represented in the model database
- Example – Sodium Laureth Sulfate – used for cleansing, emulsifying, foaming, surfactant
- Federle *et al.* (1997) measured surfactant degradation rates in river water and soil (values reported by HERA, 1994)



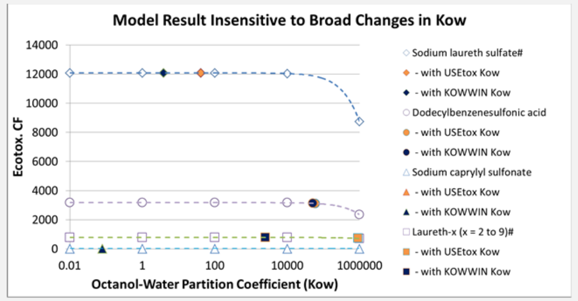


- USETox Database CF for Sodium Laureth Sulfate – ranks 1779 among 2498 substances – poorer than substances or mixtures widely recognized as having potent aquatic toxicity and/or persistence issues (Tetramethyl lead, Aroclor 1232, Arcoclor 1221, naphthalene, acenaphthene, fluorene, Silvex , Mirex)
- Use of empirical degradation data reduces CF 18-fold – new rank is 1017 of 2498 substances (re-ranked as lower impact than the substances listed above)
- Use of uncertain estimates and its influence on labeling may erroneously drive formulators to use ingredients that are less preferable from an aquatic toxicity standpoint.

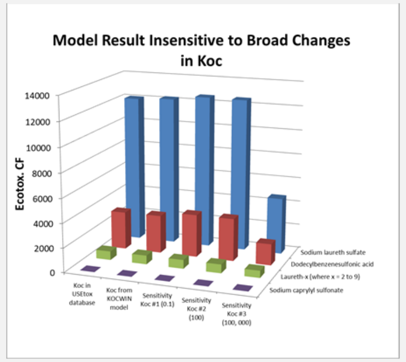
PARTITION COEFFICIENTS

- Surfactants are typically the most abundant non-water ingredients in shampoos.
- USEtox characterization factors for surfactants are classified as interim, and future focus is to use empirical, not modeled, partition coefficients. (Henderson *et al.*, 2011)
- USEtox relies on the octanol-water partition coefficient (Kow), and organic carbon-water partition coefficient (Koc), in part, to predict movement of chemicals in the environment.
- The octanol-water partition coefficient is not meaningful for surfactants, which accumulate at polar-non-polar interfaces.
- Numerous studies have shown that non-polar and cationic surfactants' sorption correlates to clay content as well as organic matter content at low surfactant concentrations – hence organic partition coefficients may not be predictive of real-world sorption.

Kow, Koc Do Not Influence Model Result for Surfactants Over Wide Range of Values



For KOWWIN and KOCWIN models, C12 chain and 4 ethylene oxide (EO) units assumed



- Uncertainty in Kow and Koc is not influential on model result until projected coefficient is high (*i.e.*, log K ≈ 5)
- Given that sorption to clay can be important, when empirical Kd (distribution coefficient) is available, a pseudo-Koc can be entered into model to yield realistic Kd in interim model calculations for most realism

AQUATIC TOXICITY

- HC50 (hazard concentration for 50% of species – exposed to greater than the species EC50) used to characterize toxicity
- HC50 requires all valid aquatic toxicity data (not just sensitive organism data)
- Guidance on what types of studies to include is lacking
- Professional judgment plays a key role in data selection, so different assessors would come to different conclusions
- Example – Selection of data for Laureth-4 HC50

Species	N	Geomean L(E)C50 (mg/L)	Chronic Equivalent (mg/L)	Log (Chronic Equivalent)	Citations
Brachydanio rerio	2	2.1	1.1	0.0	Sasol 1996k, 1997j (in HERA, 2009)
Capitella capitata	2	1.6	0.8	-0.1	Stora, 1978
Carassius auratus	3	5.9	2.9	0.5	Kurata et al., 1977
Cyprinus carpio	1	1.2	0.6	-0.2	Sasol 1997k (in HERA, 2009)
Daphnia magna	5	1.4	0.7	-0.2	Solski and Erndt, 1987; Maki and Bishop, 1979, Wong et al., 1997, Sasol, 1993g, 1995e (in HERA, 2009)
Daphnia pulex	1	0.2	0.1	-1.0	Maki and Bishop, 1979 (in HERA, 2009)
Echinogammarus tibaldii	8	3.6	1.8	0.3	Pantani et al., 1995, 1997
Gammarus italicus	2	8.5	4.2	0.6	Pantani et al., 1990, 1997
Lemna minor	1	20	10	1.0	Solski and Erndt, 1987
Oryzias latipes	20	9.5	4.7	0.7	Kikuchi and Wakabayashi, 1984
Poecilia reticulata	1	8.6	4.3	0.6	Solski and Erndt, 1987
Salmo salar	3	2.4	1.2	0.1	Wildish, 1974
Scenedesmus quadricauda	1	3.3	1.7	0.2	Solski and Erndt, 1987
Scenedesmus subspicatus	6	1.3	0.6	-0.2	Cognis/Henkel 1997b, 1998e, Sasol 1993c, 1995b, 1997a (in HERA, 2009)
Scolelepis fulginosa	4	2.3	1.2	0.1	Stora, 1975, 1978

Aquatic Toxicity Data Selection Can Influence Model Result Substantially

Data Set	Description	HC50§	CF
Set 0	USEtox database value	0.467	716
Set 1	Full empirical database, all data considered acute	0.161	1450
Set 2	Set 1 but eliminate non-standard duration tests	0.030	1961
Set 3	Set 2 but use E_bC_{50} values for algae	0.014	2033
Set 4	Set 3 but eliminate branched homologs	-0.003	2112
Set 5	Set 4 but use standard species only	-0.336	4547
Set 6	Set 1 but consider algae and duckweed tests as chronic	0.221	1262

§ HC50 is the mean of the log (chronic equivalent L(E)C50) values from above

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The French Environment and Energy Management Agency (ADEME) is overseeing a new requirement for a comparative evaluation of the environmental performance of certain consumer products, including shampoos, to be provided to consumers. The USETox model was selected for this purpose. The aquatic environmental assessment in USETox is quantifed as a single value, a characterization factor (CF). The quality of the model results and sensitivity of the model to three critical factors are presented. First, USETox requires a significant number of input parameters , many of which are not widely available for the range of ingredients used in shampoos. Specifically, the biodegradation rate is important in the model, but adequate empirical data are often lacking for this parameter. Sensitivity of the model result to the use of empirical data vs. BIOWIN model results is examined. Second, surfactants are the are the most abundant non-water ingredient in shampoos, yet the environmental fate segment of the USETox model relies on a substance's octanol-water partition coeffiient (K_{ow}) – a parameter that is not meaningful for surfactants – to predict environmental partitioning. Two approaches for addressing the lack of a meaningful K_{ow} for surfactants are compared. Third, aquatic toxicity is quantified using a distribution approach rather than selecting a single study as the point of departure for determining a predicted no effects concentration. This approach requires more toxicity data than are available for many shampoo ingredients, and requires that all quality studies conducted for an ingredient be evaluated and incorporated into the CF determination. The use of modeled versus empirical data, as well as the influence of study selection versus rejection on the data distribution (and hence on the model results), are presented. The result of this evaluation shows that the model results are most sensitive to uncertainty around the effects factor, which can span orders of magnitude, compared to uncertainty around biodegradability and octanol-water partition coefficient for surfactants. This suggests that clear guidance around selection and use of effects data, which are applied consistently across ingredients, is critical to achieving quality results in aquatic assessments for shampoos in USETox.

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