Data Evaluation Criteria for Physical-Chemical and Fate Properties under TSCA

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Systematic Review Process

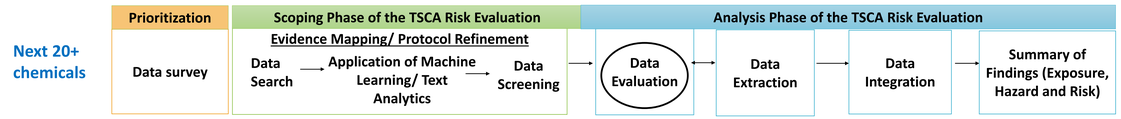
Systematic Review is a comprehensive, 'unbiased', transparent and reproducible way to identify relevant literature on a topic.

On June 22, 2016, the Frank R. Lautenberg Chemical Safety for the 21st Century Act was signed into law amending the Toxic Substance Control Act (TSCA), the Nation's primary chemicals management law. The U.S. EPA's Office of Pollution Prevention and Toxics (EPA/OPPT) intends to apply systematic review in developing risk evaluations under TSCA.

This involves implementing a structured process to identify, evaluate, and integrate evidence for the hazard and exposure assessments developed for risk evaluation. This poster describes the data evaluation process assessing the quality of multiple data types supporting the exposure assessment.

Data Evaluation Process within Systematic Review under TSCA

Key Stages of the Systematic Review Process in TSCA Risk Evaluations



Key Terms in Data Evaluation

Domain	Data evaluation is intended to assess the following four main study attributes or domains for Reliability, Representativeness, Accessibility/Clarity, and Variability/Uncertainty
Metric	Domains are assessed by evaluating sub-categories of study
Criteria	Specific criteria are developed for each metric, which express conditions of the confidence level assigned to the metric (high, medium, low, or unacceptable)
Data Quality Score	Quantitative score calculated following evaluation of discipline-specific and data type-specific data evaluation domains and metrics according to predefined scoring criteria and accounting for metric weighting factors.

Types of Data for Evaluation

Physical-Chemical Property	Fate Endpoints
Physical Form • Solid, liquid, gas	Bioconcentration Potential • Bioconcentration factor • Bioaccumulation factor • Trophic magnification factor • Biota-sediment accumulation factor
Physical Properties • Color • Scent	Sorption Information • Organic carbon-water partitioning (log K_{OC})
Melting Point	Biodegradation Rates • Aerobic biodegradation • Anaerobic biodegradation
Boiling Point	Abiotic Degradation Rates • Abiotic reduction • Hydrolysis • Incineration • Photolysis (aqueous, atmospheric) • Other abiotic processes
Water Solubility	Wastewater Treatment Removal
Octanol-Water Partition Coefficient (log K_{OW})	
Henry's Law Constant	
Density	
Viscosity	
Vapor Pressure	
Vapor Density	
Flash Point	
Autoflammability	
Refractive Index	
Dielectric Constant	

Physical-Chemical Properties: Experimental, Modeled Data

The physical-chemical property data quality metrics are designed to address experimental and modeling studies of physical-chemical properties as well as physical-chemical property information reported in databases, with a subset of physical-chemical property metrics applicable to each of these study types.

Fate: Experimental, Field Studies, Modeled, Monitoring Data

The fate data quality metrics are designed to address experimental, modeling, field, and monitoring studies which report information about biotic and abiotic transformation, partitioning, and transport processes, with a subset of fate metrics applicable to each of these study types.

Table 1. *Data quality domains and metrics for physical-chemical property studies*

Evaluation Domain	Evaluation Metric	Criteria
1. Substance	**1.Representativeness** (Chemical substance type)	Measured or estimated for chemical substance
		Measured or estimated for analogue
	2.Appropriateness (Relevant and consistent with known properties)	Measured and consistent with properties
		Measured analogue and consistent properties
		Measured and inconsistent properties
		Measured analogue and inconsistent properties
2. Test Reliability	**3. Reliability/Unbiased** (Method objectivity)	Answers specific question with clear objective
		No indication of bias towards a product or outcome
		Bias likely in methodology
		Severe bias in methodology
	4. Reliability/Analytical (Method reliability)	Standard analytical method or other standard method
		Non-standard method but appropriate **OR** method likely appropriate and included in peer-reviewed/recognized database/other secondary source
		Unreliable method used
		Method not appropriate
3. Other	**5. Databases** (QA/QC of data reports)	Recognized data repository that is peer-reviewed by SME and publicly available for review and use **OR** includes references to original source
		Known source, but missing elements for *high* designation (peer reviewed, available, references, etc.)
		Primary source without peer-review **OR** unknown secondary without peer review and original references
		Unknown source **OR** concerns with data source
	6. Models (Applicability and appropriateness)	Defined, unambiguous endpoint **AND** known performance and $r^2 > 0.7$, $q^2 > 0.5$, and SE < 0.3 (ECHA, 2016).
		Endpoint broad **AND/OR** lacks transparency, difficult-to-reproduce method used for (Q)SAR
		Algorithm not publicly available **AND/OR** external validation statistics are unavailable
		Performance unknown **OR** $r^2 < 0.7$, $q^2 < 0.5$ or SE > 0.3 (ECHA, 2016).

SME-subject matter expert; QA/QC-quality control/quality assurance

Evaluation of Metric Criteria

Some Flaws in Fate Data Sources

Serious flaws that render data sources unacceptable for use in TSCA risk evaluations have been identified for all fate metrics, as listed below. Serious flaws that make physical-chemical property data sources unacceptable have not been enumerated.

Broadly, fate data sources with one or more of these serious flaws are considered unacceptable:

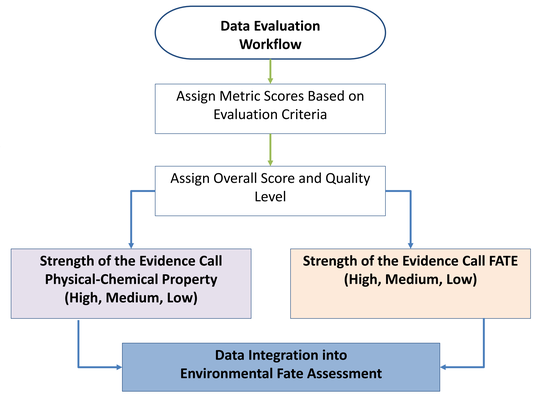
- Critical study details are not reported which prevents meaningful results interpretation, e.g.,
- Study results may have been unduly influenced by the nature or quantity of impurities or carrier, solvents, or test substance stability or storage conditions
- Test method, test conditions, or analytical method were not reported, not suitable to the test substance, or not suitable to the outcome being assessed
- Necessary control groups were not reported or included
- Sampling or data assessment methods are not suitable to the outcome(s) of interest
- Other sources of variability or uncertainty may have influenced the results
- Statistical methods or calculations likely produced biased results
- Results were completely inconsistent with existing information about the test substance

Table 2. *Data quality domains and metrics for fate endpoint studies, weighting factor 2*

Domain	Critical Metrics with Weighting Factor of 2	Rationale
Test Substance	**1. Test Substance Identity** Identified and characterized to ensure study relevancy	Identified definitively and specific form characterized
		Identified by trade name or other internal designation
		Identified but lacks specific characteristics **OR** uncertainties/conflicts in identification that substantially impacted study results
		Test substance cannot be identified
Test Conditions	**6. Testing Conditions** Defined without ambiguity for valid comparison across studies	Monitored, reported, and appropriate for the method.
		Deviations or omissions in testing conditions, but not likely to have a substantial impact on study results
		Inappropriate test conditions for the study method and deviations likely substantial impact on study results
		Test conditions not reported, data insufficient **OR** testing conditions were not appropriate for the method
Test Organisms	**9. Test Organism – Degradation** Report must enable assessment of suitability and organism differences within or between studies	Organism, species or inoculum reported **AND** are appropriate and routinely used for similar studies types
		Organism, species or inoculum reported, but not routinely used and deviation not likely to have impacted study results
		Organism, species or inoculum reported, but not routinely used or appropriate **OR** pre-adapted inoculum **AND** no justification provided which is likely to have a substantial impact on study
		Organism, species, or inoculum source were not reported
	10. Test Organism – Partitioning Report must enable assessment of suitability and organism differences within or between studies	Test organism reported **OR** obtained from reliable source **AND** routinely used for simila study types
		Test organism from reliable source OR routinely used for similar study types, but one or more characteristics not reported; omissions not likely to have a substantial impact on study results
		Test organism not from reliable source OR not routinely used/inappropriate for study types, and no justification for selection provided; deviations likely to have a substantial impact on study results
Data Presentation and Analysis	**15. Data Presentation** Detailed reports showing valid study conclusions	Target chemical and study related **QC** parameters reported **AND** analytical method suitable for detection and quantification of target and transformation
		Target chemical and study related QC parameters not reported but omissions not likely to have a substantial impact on study results
		Insufficient evidence presented **AND** omissions likely to have a substantial impact on study results Method used not suitable for detection of the test substance

Table 3. *Data quality domains and metrics for fate endpoint studies, weighting factor 1*

Domain Number/ Description	Metric Number/Description
1. Test Substance	2. Test Substance Purity
2. Test Design	4. Test Substance Stability
3. Test Conditions	5. Test Method Suitability
	7. Testing Consistency
	8. System Type and Design
5. Outcome Assessment	11. Outcome Assessment Methodology
	12. Sampling Methods
6. Confounding/ Variable Control	13. Confounding Variables
	14. Outcomes Unrelated to Exposure
7. Data Presentation and Analysis	16. Statistical Methods & Kinetic Calculations
8. Other	17. Verification or Plausibility of Results
	18. QSAR Models



Weighted Scoring System

Within each metric are descriptions of High (metric score=1), Medium (2), Low (3), or, for some metrics, Unacceptable qualities. Fate metrics of greater importance to data quality evaluation were assigned a weighting factor of 2 (Table 3), while all other fate metrics and all physical-chemical property metrics are assigned a weighting factor of 1.

Overall Study Score = ∑ (Metric Score × Weighting Factor)/∑ (Weighting Factors)

For studies with no serious flaws that would render them unacceptable for use, the overall study scores range from 1 to 3 and are interpreted to an overall data quality rating:

In summary

The outcome of the data quality evaluation is a qualitative assessment of confidence in a study or data set. The numerical scoring system is applied to ascertain a qualitative rating for consistency and transparency, and overall data quality ratings are used during evidence integration to evaluate the weight of the evidence. Expert judgment is required to assess studies against the metrics. The guidance for each metric is written to generally apply to applicable physical-chemical or fate studies

Reference

U.S. EPA. 2018. Application of Systematic Review in TSCA Evaluations. EPA Document# 740-P1-8001