Bridging Life Cycle and Exposure Ontologies to Enable Rapid Exposure Estimation and Comparative Exposure Assessment

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Safer Products

• Informed chemical use in modern society should consider (NAS, 2014)...
  – Function/performance,
  – Impacts to environment and health
  – Societal costs/benefits
• Decisions about chemicals and alternatives are not purely technical, but rather value-driven or context-dependent (NAS, 2014).
• Chemical activity is modulated by environmental and biological context
A Framework to Guide Selection of Chemical Alternatives. NAS, 2014

Context-The Actionable Heart
Goal

- Fit-for-purpose decision making to maximize benefits and minimize adverse impacts
- Efficient, holistic (i.e., product-based) chemical evaluation
- Rapid exposure estimation for risk-based chemical evaluation
Approach

• Leverage science, methods, and information developed to support chemical risk assessment (RA) and product lifecycle assessment (LCA).

• Enable access to disparate data across the product lifecycle to estimate exposures.

• Develop tools and workflows to support context-driven evaluation of alternatives (and drive development of information to fill gaps).
While the individual pieces had an intimate scale, they became monumental when viewed holistically within the combined environment of the assemblage.
Central Concepts in Ontologies

_exo_

“stressor interacts with a receptor via an exposure event resulting in an outcome”

_LCAmin_

“agent interacts with a flow via an activity resulting in a product”
A Minimal Ontology Pattern for Life Cycle Assessment Data. Janowicz et al., 2015
Proposed Bridged Ontology Architecture

- Essential linkages specified within LcaEpa
  - lcaMin:Activity owl:EquivalentTo cdr:Activity
  - frs:Facility rdfs:subclassOf lcaMin:Agent

EPA LCA Schemes
- LcaMin
- LcaHt
- LcaComp

Bridges to External Schemes
- OlcaMap
- EcoMap

Data Source RDF
- Nei
- Ghgrp

Data Source RDF from 3 Round Stones
- Frs
- Srs
- Cdr
- Tri
- Rcra
Relational View of Selected ExO Domains

https://bioportal.bioontology.org/ontologies/EXO

Providing the Missing Link: the Exposure Science Ontology ExO

High level schematic of ExO integration within a broader biological context

Chemical (e.g., MeSH) ➔ Exposure Stressor (e.g., ExO) ➔ Exposure Receptor (e.g., ExO) ➔ Exposure Event (e.g., ExO, ExpoCastDB)

Is a

Interacts with (e.g., CTD)

Gene Products ➔ Gene ➔ Genes

Interact via

Pathways, Networks, Reactions (e.g., KEGG, Reactome)

Occur within

Biological System (e.g., Functional model of anatomy)

Assessed by

Exposure Phenotype Outcome (e.g., OMIM, MeSH)

Encode

Annotated with

Biological Process, Molecular Function, Cellular Component (e.g., Gene Ontology)

Results in an

Is a

Interacts with (e.g., CTD)
High level schematic of integration of ExO and LCAmin
Some Closing Thoughts

• Leverage data and models from New Approach Methodologies (NAMs) being developed to accelerate the pace of risk assessment.

• Leverage life-cycle thinking and data resources.

• Apply, extend, and bridge ontologies to access data streams developed for RA and LCA and enable rapid, comparative exposure evaluation.

• Develop context driven and fit-for-purpose work flows and metrics to support AA and inform decisions.