

# **Functional Substitution: Advancing Safer Alternatives Through Use- Based Thinking**

Joel Tickner, ScD

UMASS Lowell

Jessica Schifano, JD, MPH

US Occupational Safety and Health Administration

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[joel\\_tickner@uml.edu](mailto:joel_tickner@uml.edu)

# Overview

- Challenges of current chemical-by-chemical risk-based approaches to chemicals management
- Opportunities use-based thinking opens up for thinking about substitution
- Functional substitution as a way to reframe chemical problems
- Needs and opportunities

# Bottom Line

- Functional substitution - applying use as a lens to identify, evaluate, and select safer alternatives for achieving a particular function, end use, or service – can ultimately promote the development of and transition to safer alternatives

# Challenges of the current chemical-by-chemical approach

- Slow, resource intensive approach to chemicals management – focus on whether the chemical is an “unacceptable” risk
- Chemicals of concern often used for specific function, performance, cost, but sometimes less clear rationale
- Restrictions can lead to regrettable substitutions
- Does not focus on innovation or green chemistry solutions

# Example TCE

- Twenty years of toxicity and risk assessments, mostly focused on carcinogenicity and pharmacokinetic model
- As certain regulations and restrictions increase, substitution to alternative (less regulated) solvents
- Trade-offs for worker health and safety
- Alternative approach: focus on function (degreasing) and explore options for achieving that function

# Defining use

- Use is the discrete application of a substance in a material, product, process, or technology.
- Three distinct meanings
  - *Volumetric use* - *how much* is used, produced, or imported.
  - *Applicative use* - *way in which* the chemical is used or incorporated into a product or industrial process (e.g. closed system, consumer product use, dispersive use, applied to surface, incorporated into the matrix).
  - *Functional use* - *why and how* a chemical is used – its purpose
- Conventionally used as a surrogate for exposure.

# How use-based information has been applied to date

- In the context of exposure evaluation and risk assessment
  - EPA ChemUSES, Chemical Data Reporting
  - REACH – Use Descriptor System
- In the context of pollution prevention and design for environment
  - EPA Use Cluster Scoring; Design for Environment
  - MA Toxics Use Reduction Program Five Chemical Assessment

# Examples of Use-Based information in Pollution Prevention

- MA Five Chemicals Assessment
  - Review of alternatives for five chemicals of concern
  - Identified major uses of each chemical
  - Selected Massachusetts priority uses for alternatives assessment
  - Conducted alternatives assessments for 16 different use categories of the five chemicals evaluating environment/health, economic, technical feasibility

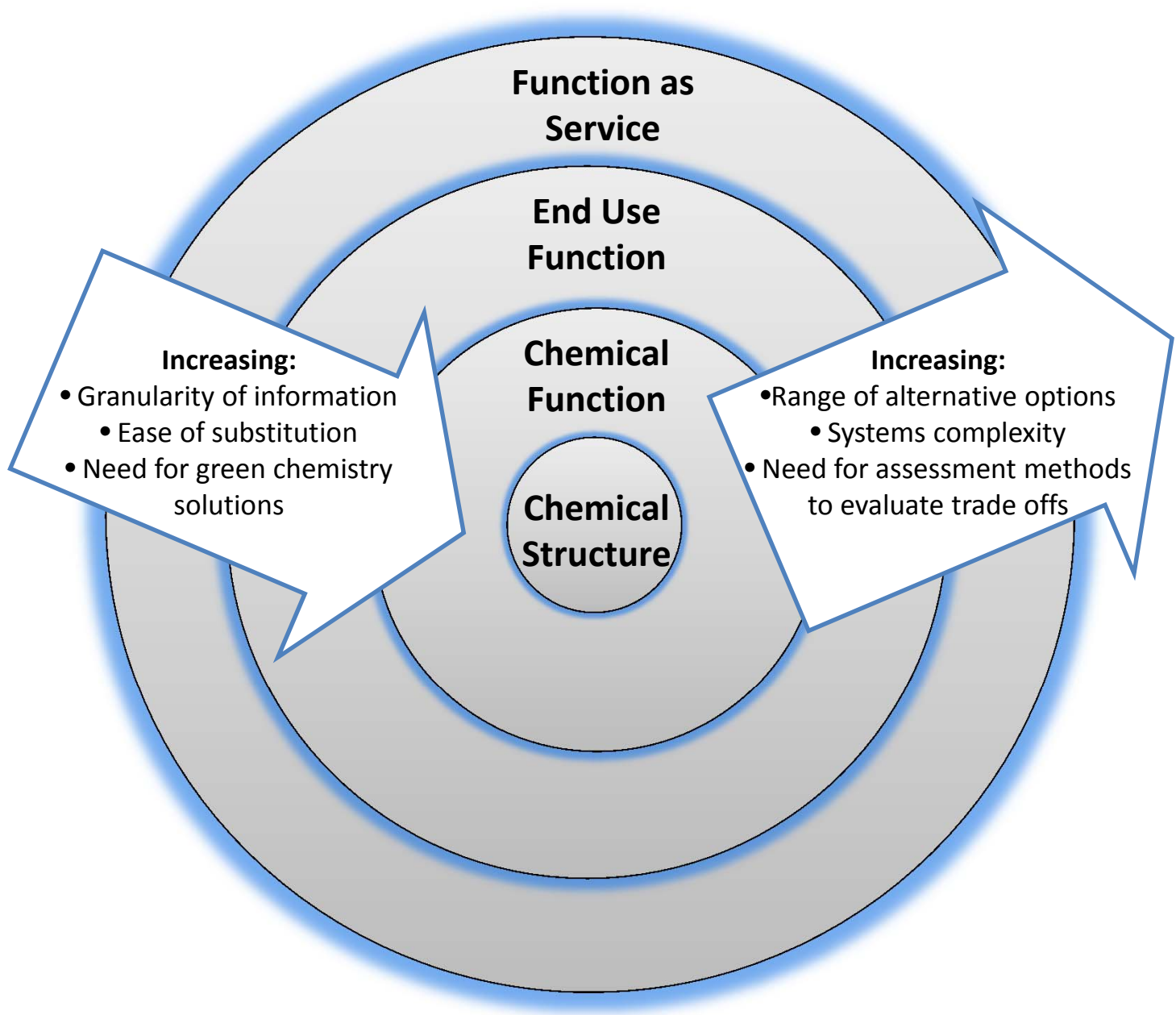


# Examples of Use-Based Information in Pollution Prevention

- EPA Use Clusters Scoring
  - Creation of use clusters – competing chemicals and technologies for a functional use in a particular industry (e.g. rubber chemical production with nine clusters)
  - Information on hazard, exposure, pollution prevention opportunities and regulatory interest used to rank chemicals within clusters and to identify high priority clusters

# Defining Functional Substitution

- The application of information on function to identify, evaluate, and select safer alternatives that achieve a particular result.
- Three conceptual levels
  - Chemical Function
  - End use function
  - Function as service



Functional Substitution Level	Chemical in Product BPA in Thermal Paper	Chemical in Process Methylene chloride in Metal Part Degreasing
<b>Chemical Function (Chemical Change)</b>	<p>Is there a functionally equivalent chemical substitute (i.e. chemical developer)?</p> <p><b>Result: Drop-in chemical replacement (e.g. BPS)</b></p>	<p>Is there a functionally equivalent chemical substitute (i.e. chlorinated solvent degreaser)?</p> <p><b>Result: Drop-in chemical replacement (e.g. n-PB, TCE)</b></p>
<b>End Use Function (Material, Product, Process Change)</b>	<p>Is there another means to achieve the function of the chemical in the product (i.e. creation of printed image)?</p> <p><b>Result: Redesign of thermal paper, material changes</b></p>	<p>Is there another means to achieve the function of the process (i.e. degreasing)?</p> <p><b>Result: Redesign of the process (e.g. ultrasonic, aqueous)</b></p>
<b>Function As Service (System Change)</b>	<p>Are cash register receipts necessary? Are there non-chemical alternatives that could achieve the same purpose (i.e. providing a record of sale to a consumer)?</p> <p><b>Result: Alternative printing systems (e.g. electronic receipts)</b></p>	<p>Is degreasing metal parts necessary? Are there other alternatives that could achieve the same purpose (i.e. providing metal parts free of contaminants for other end uses)?</p> <p><b>Result: Alternative metal cutting methods</b></p>

# Benefits of a functional substitution approach

- Provides a greater ability to more efficiently screen through a broader range of chemical and design alternatives in a comparative manner
- Helps avoid regrettable substitutions
- Provides a way to make data more useable and sortable to different users
- Creates a cooperative environment for development and application of safer alternatives

# Needs for advancing use-based thinking approaches

- A system for consistent definitions, classification and characterization of functions
- More comprehensive and actionable chemical hazard data
- Scientific tools to compare chemical and design alternatives for particular functions
- Models for translating a functional substitution approach into existing policy frameworks

# Opportunities for the CompTox community

- Improved structural models for toxicity prediction
- High throughput data streams that can provide early signals of potential problems from chemical alternatives
- More effective characterization and understanding of how chemical properties and structure affect toxicity that can be translated into design criteria for chemists.
- Tools to integrate data types into a hazard “classification”

# Conclusions

- Use-based thinking through functional substitution provides an opportunity to reframe chemicals problems around possible solutions
- Rather than focus on assessing the risks of thousands of chemicals, it is possible to compare alternatives for hundreds of uses and identify where development of green chemistry alternatives is needed
- The focus on functional substitution does not obviate the need for evaluating risk but can narrow down options to those that may be safest for a particular need.



# Future papers

- Data categorization options on function and application
- Case studies on how companies self-identify function and application
- Policy options to advance a use-based thinking approach
- Using use information to rapidly characterize potential exposure (qualitative risk assessment)

# Collaborators

- Ann Blake – Environmental and Public Health Consulting
- Marty Mulvihill – UC Berkeley, Center for Green Chemistry
- Cathy Rudisill – SRC Inc.
- Cal Baier-Anderson and Charles Bevington – US EPA