

Chemical Hazard Data Commons Working Paper¹

Finding Alternatives through Categorizing Functional Use

by Ann Blake

Originally published February 6, 2014

Revised February 27, 2014

Information about hazard will help industries identify chemicals to target for replacement, but finding the alternatives can be tricky. A Data Commons that links positively assessed chemicals to specific uses where they have proven effective could help product designers identify useful alternatives to hazardous ingredients. Functional use characterization schema to date have tended to be very industry specific and limited to one or two parameters. A highly flexible, multi-parameter system could support searches for potential alternatives across industries, accelerating innovation.

Previous sections describing the challenge and necessity of creating a Chemical Data Commons have detailed the data needs around unique chemical identification reliably tied to hazard information for chemicals in industrial use. As we continue to develop the practice of alternatives assessment, we discover that there is another layer of information required to support the selection of safer alternatives, and that is *functional use*. With a universe of tens of thousands of possible chemicals to assess, various players in the supply chain of a chemical, material or product need specific descriptive data about chemicals to differentiate those that have been successfully used for the same or related functions as a chemical of potential concern.

This section will provide an initial introduction to functional use, and describe current and planned work on developing a set of functional use parameters. These parameters will allow a variety of users throughout the life cycle of a chemical in a manufacturing process and final product to select safer alternatives that provide the desired performance characteristics.

Schifano and Tickner² describe the meanings of use and functional use as follows:

Three distinct meanings are embedded within the concept of “use.” First, *volumetric use* explores the question of how much is used, produced, or imported. Second, *applicative use* explores the 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). This definition provides information on the ways in which a target may be exposed to a chemical and the likelihood of exposure. Volumetric and applicative use represent the traditional ways in which use has been defined for the purposes of chemicals assessment and management and provide important concepts to support the rapid characterization of exposure, in combination with an understanding of the intrinsic hazard properties of a substance, such as persistence and biodegradation.

Functional use, on the other hand, explores the question of how a chemical is used and describes

¹ See Lent, Tom, et al, *Toward Safer Products: Accelerating Change with a Chemical Hazard Data Commons* for an overview of the Chemical Hazard Data Commons project at <https://commons.healthymaterials.net>

² Schifano, Jessica (OSHA) and Joel Tickner, University of Massachusetts at Lowell. *Functional Use: An underappreciated foundational concept in advancing safer chemistry* (January 2014, draft); to be submitted to Environmental Science & Technology at the invitation of the section editor.

the purpose of the substance in products or industrial processes.

Schifano and Tickner go on to detail three levels of functional use. At a *chemical* level, the most granular level of information, *functional use* refers to the structure and related physicochemical properties of a chemical. From an *end use* perspective, functional use describes the purpose that a chemical serves in a product or process (e.g., lubrication in an extrusion process). Finally, at the least granular level, *functional use* can describe at what performance attribute or *service* function a chemical provides in a material, product or process (e.g. flame retardancy, microbial resistance, flexibility, etc.) Different players in the ecosystem of chemical, material and product design, manufacture, use and disposal may require different subsets of functional use information depending on the problem they're trying to solve. Measurable attributes associated with each of these descriptive levels of *functional use* are further detailed below.

What users need from a functional use categorization schema

We are interested in establishing the likely users of information on chemical hazards and alternatives and investigating the specific information needs regarding *functional use* parameters that will enable decision-making. The main goal in defining these user groups was to examine whether different users in the supply chain/ ecosystem will have drastically different data needs that impact functional use categorizations. We have initially decided to profile three key anticipated data user groups; these profiles may require additional refinement as we proceed.

In order to define the functional use data users, we asked the question: What problem is each user group trying to solve, and therefore, what level of granularity of functional use data do they need in support of this task? The proposed user profiles consist of a subset of the potential users of the Data Commons described elsewhere in this document (see Data Commons at Work). The users profiled for functional use information purposes include: design chemists, supply chain players (formulators, product designers, manufacturing workers), regulatory scientists (government), and public health scientists (government or NGO). The initial categorization of users and their data needs are detailed below:

- Designers, developers and brand owners are increasingly changing their specifications and other purchasing practices in an effort to purchase products whose contents are disclosed and that avoid chemicals of concern.
- Supply chain players (the most varied group), including: formulators, design chemists, product designers, workers, and retailers, are increasingly examining their own products and processes for potential hazards and researching the viability of alternatives.
- Regulatory scientists, public health scientists and/or public/environmental health NGOs, are providing guidance on prioritization of chemicals for substitution.

Defining these initial user groups is the first step in establishing a framework of functional use parameters and building a data system that supports the decision-making of multiple users moving towards safer chemical and material choices. The next step will be to refine both the user group definitions and the functional use parameters proposed below.

***Data Commons Recommendation:* Vet the utility of proposed functional use parameters (see below) with representatives of the user profiles detailed above to identify the specific data needs for each user group's decision-making around safer alternatives.

Proposed functional use parameters for alternatives assessment

We propose the following functional use parameters as necessary to support the selection of safer alternatives. The goal would be that any given user, such as those described above, would have information about a chemical or material for which they are looking for an alternative that falls into a subset of these parameters. We are interested in refining which parameters and which levels of granularity are essential to supporting decisions about safer alternatives for each user group.

These proposed parameters constitute a description of granularity of information intended to fit within the framework described by Schifano and Tickner. The tiers of granularity and attributes are detailed below:

Granularity Level	Attribute	Parameter	Examples
A	Independent characteristics of the substance	Chemical structure, chemical class	Organic/ inorganic, halogenated, diphenyl ether, phenols; chemical moieties that contribute to toxicological impacts
		Physicochemical properties	Flame retardancy, boiling point, thermal resistance, viscosity)
B	Relationship of the substance to a partner substance or parent material (as additive) or product	Performance Function (in the product)	Adhesion, insulation, stabilization, crosslinking, structural support
		Parent/partner material	PVC, polyurethane, isocyanate, epoxy
		Product type	Paint, caulk, shoe, electrical cable, cosmetic, seat covering
		Substrate (what the material works on or between)	Metals, rubber, wood, concrete, also may be substrate combinations, e.g., "metal to wood"
C	Relationship of the parent product to the environment	Process	Painting, carpet installation, traffic surface cleaning, anodizing, circuit board cleaning
		Environment (context)	Industrial, commercial, residential, health care, caustic chemicals, building envelope, building finishes, Automobile electronics manufacture,

Examination of Current Schema for Potential Functional Use Parameters

We examined sixteen existing systems for functional use categorization from government, industry and other stakeholders including labor and independent research institutions. These included US EPA's Chemical Data Reporting, US EPA Design for Environment, the Consumer Specialty Products Association (CSPA) ingredient dictionary, the Substances in Products in Nordic Countries (SPIN) database, the European Trade Union's RiscTOX database, SubSPORT, the National Library of Medicine's HazMap database for occupational exposures, and three industry trade directories, Innovadex, McCutcheon's and the Global Product Categorization (GPC) for the Global Data Synchronization Network (GDSN.)

Our goal in examining these systems was to explore what could be learned from existing systems of categorization in terms of broad versus narrow definitions of functional use. In addition we wished to further refine the data needs of stakeholders in the effort to find safer alternatives for industrial chemical uses. Our research investigated whether any current system of functional use categorization provides functional use definitions that meet the needs of key users in selecting safer alternatives. If not, what gaps exist in current functional use categorization systems, and how can they be completed in a set of functional use parameters to support safer selections of chemicals, materials and products?

The systems under examination were designed for purposes as varied as chemical data reporting across industrial sectors, tracking of chemicals in a subset of consumer products, and the B2B sale of industrial products in the supply chain. The current analysis focused on parsing out the various levels of functional use parameters operating in each system. While the analysis is still in process, the initial assessment shows that in existing categorization systems, generally only a subset of the functional use parameters we describe are included in any one system. In addition, multiple levels of granularity of functional use parameters are operating in the same system simultaneously, making the system sub-optimal for the purposes of supporting decisions on safer alternatives.

****Data Commons Recommendation** Complete a cross-mapping of proposed Chemical Data Commons functional use parameters with existing functional use characterization systems.

Proposal to create a comprehensive functional use framework to support alternatives assessment across industries

The next steps in the creation of a more comprehensive functional use framework to support cross industry alternatives assessment are outlined below.

First, the functional use parameters proposed above should be vetted a) in conversation with representatives of user groups likely to utilize these parameters in selecting safer alternatives, b) against functional use parameters embedded in existing systems for reporting chemicals in products, and c) against the existing alternatives assessment/ substitution case study literature. This analysis will help to inform the Chemical Data Commons about the level of functional use granularity necessary for effective substitution.

Once the set of functional use parameters has been vetted as described, a data system can be designed around these parameters. Components of relatively new systems designed for chemical disclosure such as the Health Product Declaration can also be incorporated into the Chemical Data Commons comprehensive functional use framework. The framework could then be tested using the small subsets of existing chemical hazard and alternatives data.

Issues Raised For Further Discussion/ Next Steps

- Do a better job of linking the broader framework of functional use descriptors with the parameter system outlined above.
 - Discussions with Joel Tickner, Jessica Schifano and others specifically focused on clarifying shared definitions of functional use will continue in the next 1-2 months
- Develop a product “use pattern” classification, at a minimum to tag existing reports and alternatives assessments. Further develop the “C” level data, relationship to the environment in a more pragmatic fashion.
 - Discussion with Data Commons community members with more expertise in this area will continue over the next 1-2 months
- Additional work on defining users, and coordinate with other descriptions of data users in the community
 - Discussion with IC2 and other community members who have experience in this area will continue
- Complete assessment of what parameters are actually used in the available literature on alternatives assessments and substitution; use this to inform the design of the functional use component of the broader Data Commons platform.
- Functional use in the more complex cases where a chemical can perform multiple functions, or when one is comparing materials rather than individual chemicals.
 - BizNGO/ Clean Production Action are preparing to release the next iteration of the Plastics Scorecard in April 2014, a tool designed to evaluate hazard for a class of materials
 - Suggestions welcome on how to continue conversation in these areas

Additional Comments Welcome

Please submit to Ann Blake (ann@annblake.com) and Tom Lent (tlent@healthybuilding.net)