DTSC Green Ribbon Science Panel

November 12 and 13, 2015 Day 2

Topic 1: CPET Process and Lessons Learned

At the conclusion of its initial round of product and chemical research in 2014, DTSC's Chemical and Product Evaluation Team (CPET) organized a series of internal "lessons learned" meetings for staff. Key findings of these meetings were that we needed a better-defined process that included well-defined phases, consistent templates to capture our work, well-documented decisions, and realistic timeframes.

The team spent significant time redesigning its process; to help ensure its success, we developed a variety of templates for recording research findings, summarizing team recommendations, and documenting decisions. We also developed guidance documents for technical staff engaged in product and chemical research.

In recent months, DTSC has begun to put these newly-developed processes and tools into use to begin implementing the Priority Product Work Plan. We began by assigning each CPET member to a scoping team focused on one of the Work Plan's product categories. We assigned toxicologists to every team. Each person was asked to focus on one of the work plan's five policy priorities.

Tools, templates, and data sources developed for chemical/product scoping

After reassessing our first round of chemical/product scoping, the Safer Consumer Products (SCP) Program developed tools and templates to ensure consistent and methodical evaluation of scientific and other data related to products and chemicals. Our objective is to ensure thorough consideration of issues required by regulations and to clearly track what data we did and did not have on a chemical/product. We are also striving for consistency and rigor in our product and chemical evaluations.

Among the tools, templates and data sources identified or developed are:

- **Chemical Scoping Log (Template**)

Identifies broad questions for teams to research and to answer about Candidate Chemicals found in their assigned category and a place to document their findings and references. The log captures the basis for the Candidate Chemical's listing, key references regarding hazard traits and impacts, relevance of the chemical to DTSC policy priorities, exposure pathways, and other pertinent regulations.

Key benefits: consistency; helpful in explaining the basis for decisions.

- **Summary of Chemical Scoping Approach (Template**)

Describes scoping teams' approach to identifying an initial list of chemicals for their assigned product category and policy priority and their process for narrowing this list during scoping. Teams have the leeway to take different approaches to screening chemicals which is consistent with earlier GRSP advice.

Key benefits: documents approaches and rationales; helpful in explaining the basis for decisions.

- **Product Category Team Matrix (Template**)

Compiles and summarizes findings from the chemical scoping research done by the product category teams. Documents team recommendations and rationales.

Key benefits: consistency; better record-keeping; documents recommendations and their rationales; helpful in explaining the basis for decisions.

- **Initial Data Sources for Specific Policy Priorities (Reference)**

Lists key sources of data for each of the policy priorities identified in the Priority Product Work Plan. Includes a brief description of each data source, URLs, notes, and contact information for key people.

Key benefits: efficiency; consistency; supports a well-defined process.

- **Product Scoping Log (Template**)

Identifies broad questions for teams to research and to answer about a chemical used in a product subcategory or a specific product, including the chemical's function, exposure potential, and potential adverse impacts from exposure. Includes space for staff recommendations and a list of references.

Key benefits: consistency; supports a well-defined process; helpful in explaining the basis for decisions.

- **Regulatory Program Review Log (Template**)

Used to identify other relevant regulatory programs (international, federal, state, or other) that are either directly pertinent to the product-chemical combinations or to the possible exposure pathways for the product-chemical combination. Helpful in identifying regulatory gaps for chemical safety and for identifying products that contain a Candidate Chemical to comply a regulatory requirement unrelated to chemical safety (e.g., fire retardancy).

Key benefits: efficiency; consistency; supports policy decisions that have greater potential impacts.

- **Key Stakeholder List (Reference)**

Identifies key stakeholders from various sectors (industry, NGO, academic, government) for product categories, sectors, and chemicals.

Key benefits: efficiency; consistency; supports a well-defined process.

Initial Work Plan chemical scoping

Each scoping team was asked to identify key chemicals of interest that may cause impacts related to our policy priorities and therefore warrant further investigation. While we provided the scoping teams

with lists of initial resources to help them identify relevant chemicals, each person was free to employ various different approaches that made sense to him or her. This approach was consistent with earlier advice we received from the GRSP.

The early work from the scoping teams has been encouraging. While the scoping approaches taken by CPET's scientists and engineers were diverse (often due to the specifics of a person's assigned product category and policy priority or their professional expertise), in several cases scoping teams independently had similar findings. In all, team members researched several dozen Candidate Chemicals. Of these, the teams recommended that we continue to research about half.

Ongoing challenges

As outlined above, DTSC has learned from its experiences in the first round of product and chemical research. We have refined our process and developed useful tools that are already proving their value. Nevertheless, we continue to face certain challenges as we endeavor to identify products and chemicals for which identifying safer alternatives will have a meaningful impact. These include:

1. Time and resource constraints. In some cases, scoping teams lack the time or expertise to understand broad or complex chemical classes and prioritize specific members for further investigation. We continue to look for approaches for screening chemicals at the class level. For example, the azo and benzidine dyes and perfluoroalkyl and polyfluoroalkyl substances are two quite complex classes that would require significant time to adequately research and assess in order to identify potential chemicals of concern.

2. Data gaps for hazard traits. CPET has been exploring various external tools for addressing data gaps, such as EPA's Sustainable Futures tools.

3. Limitations of the Candidate Chemical (CC) list. Each of the authoritative lists were made for a specific purpose which may or may not align with our regulatory needs. In some instances, DTSC's CC list includes only a subset of members of a chemical class. The missing chemicals are sometimes newer and more commonly used.

4. Unavailable or frequently out-of-date product ingredient data. (We relied on, e.g., CPCat[1] and Household Products Database.[2])

5. Evaluating low dose chronic exposure to chemicals in the product categories.

6. Balancing the need for both breadth and depth of expertise in chemical and product categories. Staff need to master both a breadth of knowledge of chemicals and product categories in the early scoping of products (e.g. broad swath of chemicals in personal care

[1] EPA's Chemical and Product Categories database (CPCat) maps >43,000 chemicals to a set of terms categorizing their usage or function. The data come from a variety of sources including the Substances in Preparation in Nordic Countries (SPIN) database, EPA, and FDA.

[2] The National Library of Medicine's Household Products Database identifies chemical ingredients in over 7,000 consumer brands based on data compiled in Material Safety Data Sheets (MSDS)

products) and then as research proceeds, a considerable depth of knowledge in a specific chemical category or product area.

Questions for GRSP discussion

1. Do you believe that the tools we have described will meet the stated objectives for which they were adopted?
2. Can you suggest ways (tools, approaches) of addressing these challenges – especially for Challenges #2-4 – data gaps for hazard traits, limitations of the CC list, and product ingredient data?
3. How can we best use the GRSP to facilitate investigations that require depth of expertise beyond current staff capability?

Topic 2: Structural and Functional Chemical Taxonomies

At its last meeting, the Green Ribbon Science Panel (GRSP) asked the Safer Consumer Products (SCP) Program to consider using various chemical classification schemes in its chemical and product research, including chemical structural approaches and functional approaches. The panel pointed out that both approaches can be useful at various stages of SCP implementation including chemical screening, identifying chemical/product combinations and for assessing alternatives. The line between structural and functional taxonomy schemes can be blurry because members of a structural class may also have functionally similarities. DTSC has evaluated both types of chemical groupings and has found that each perspective has advantages.

Chemical groupings allow DTSC to ask questions and learn at a more general level without specifying a particular individual chemical or product. We identify both structural and functional groupings of chemicals in the 2015–2017 Priority Product Work Plan, which has already led to discussions with stakeholders about azo and benzidine dyes, diisocyanates, and fragrances. This is in line with one of the goals of the Work Plan: to facilitate discussion with industry and other stakeholders – and tap into their expertise – in advance of naming specific Priority Products.

Grouping structurally-related chemicals

Structural groupings can be useful to the SCP Program when a structural feature shared by members of a group is related to a hazard trait. For example, diisocyanates as a class are asthmagens and sensitizers and are potential substitutes for one another for making polyurethane products. Similarly, a CPET team researching furnishings might look at brominated flame retardants as a class because of their common structural properties and related hazard traits.

In some cases, an authoritative body may identify a group of structurally-related chemicals on one of the lists that make up DTSC's Candidate Chemicals List. When this happens, the group itself is a Candidate Chemical. However, extrapolating data from one member of a structural class to another, or from the class as a whole to a specific member, has pitfalls. Hazard traits may differ significantly between members of a structurally-related class, due to, e.g., the orientation of the common structural feature or differences in physicochemical properties. Unless the listing body has provided hazard trait data that is specific to the group member, DTSC would have to independently document the potential adverse impacts of the individual chemical.

Another challenge is that some members of a structural class are on DTSC's Candidate Chemicals List while others are not; the non-CC members may or may not exhibit a hazard trait.[3]

[3] Specified in OEHHA's regulations: California Code of Regulations, title 22, chapter 54

Examples of structurally-related classes

- Aromatic amines
- Diisocyanates– chemical structure feature, structural and functional
- Brominated flame retardants
    - Polybrominated biphenyls (PBBs)
    - Polybrominated diphenylethers (PDBEs)
- Perfluoroalkyl and polyfluoroalkyl substances (PFAS) – some more data rich than others

Grouping chemicals into functional classes

Functional use taxonomies are also very relevant to DTSC's SCP program. Chemicals with drastically different physicochemical properties and hazard traits may serve the same function in consumer products and may become replacements or alternatives. When we identify potential Priority Products with Chemicals of Concern, it is important to be aware of existing alternatives in the same functional use category, what hazard traits they may exhibit, and whether they are on the Candidate Chemicals List. Understanding a chemical's functional use class can also help us anticipate alternative chemicals that a responsible entity may evaluate in its Alternatives Analysis (AA). However, as with structural groupings, grouping chemicals by their functional use category also has challenges and pitfalls and, as noted earlier, functional categories often overlap with structural categories. Further, our Candidate Chemical list may not encompass all the chemicals in a functional class, limiting our ability to identify the chemical in a chemical/product combination. Also, the same chemical may have more than one function, depending on the product, and may fall into multiple functional use categories.

Examples of functionally-related classes

- Paint stripping: Both methylene chloride (an organohalogen solvent; acutely toxic and carcinogenic) and sodium hydroxide (a strong base; caustic) are used to strip paint.
- Surfactants: This encompasses a wide category of chemicals some of which are on our Candidate Chemical list and some of which are not.
- Lubricants: as with surfactants, this is a broad functional class of chemicals that may have a wide range of hazard traits.

The importance to AA

Both functional and structural groupings have value during the Alternatives Analysis process. Evaluating chemical alternatives from a functional use perspective encourages decision-makers to look beyond groups of structurally similar substitutes–an approach that often results in a "regrettable substitution." Understanding structural similarities within a chemical group can help with the management of data gaps during the screening and evaluation phase of AA process. For example, "read-across" techniques, trend analyses, and specifically qualitative or quantitative Structure-Activity Relationship (Q)(SAR) models, have all been extensively used to extrapolate between chemicals within

a structural class to address specific data gaps. However, these existing tools have limitations and were often designed for a different purpose. Therefore, practitioners must be mindful of their limitations and uncertainties when using them as the basis for decisions.

Questions for GRSP discussion

For today's GRSP discussion, we want your feedback as to whether our assessment of benefits and challenges of using functional and structural groupings of chemicals in implementing the SCP regulations are on target and whether there are other factors we haven't considered.

1. When is applying chemical groupings/classes most valuable relative to the SCP regulations (chemical screening, product research, alternatives analysis)? When is using a structural class approach most appropriate? When is a functional use class appropriate?
2. Can you provide relevant examples from your work or experience that illuminate the strengths and weaknesses to using chemical groupings to inform decisions? What has proved valuable?
3. Would a functional use perspective add anything to the conclusions we draw based on a structural approach? How can the two types of chemical taxonomy build on, or be used to complement, each other? What are the implications if one approach supports or, in contrast, in any way confounds earlier conclusions from the other approach?
4. Can you suggest a tool or tools that would help us more efficiently screen members of complex classes?
5. What precautions would the panel give staff about working within a given chemical class framework?
6. Are there other strengths and limitations of using structural and functional use groupings?
7. Are there other chemical taxonomies that may be helpful in DTSC's selection of priority products or evaluation of alternatives?

Questions related to AA:

8. What uncertainties should an AA practitioner consider when applying structural grouping methods to addressing data gaps? How should uncertainty be taken into account to inform decisions, both from responsible entity's and Department's perspectives?
9. Based on your working experience, please list examples/resources for using a structurally related chemical grouping approach from AA application's perspective? Please discuss any strengths and limitations you have encountered for this approach.