

Chemical Categories

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**Progress Implementing Changes to the
New Chemicals Review Program under the Amended TSCA
Public Meeting**

December 6, 2017

Chemical Categories¹



- **A chemical category** is a group of chemicals whose physicochemical and human health and/or ecotoxicological properties and/or environmental fate properties are likely to be similar or follow a regular pattern, usually as a result of structural similarity.
- The similarities may be based on the following:
 - a common functional group (e.g. aldehyde, epoxide, ester, specific metal ion);
 - common constituents or chemical classes, similar carbon range numbers;
 - an incremental and constant change across the category (e.g. a chain-length category);
 - the likelihood of common precursors and/or breakdown products, via physical or biological processes, which result in structurally similar chemicals (e.g. the metabolic pathway approach of examining related chemicals such as acid/ester/salt).
- As a result of these similarities, data gap filling in a chemical category can be carried out by applying one or more of the following procedures: read-across, trend analysis, and (external) (Q)SARs.

¹From: Guidance on Grouping of Chemicals, Second Edition, Series on Testing and Assessment No. 194; ENV/JM/MOMO(2014)4

EPA/OPPT's Use of Chemical Categories: Existing Chemicals



- Existing Chemicals – EPA and OECD High Production Volume Programs
 - Closely related chemicals are considered as a group, or category, for (hazard) assessment; Not every chemical needs to be tested for every endpoint
 - Facilitates estimation of hazard for untested chemicals/endpoints via “Read Across”
 - Efficient way to reduce animal testing and costs of assessment
 - OECD **Guidance on Grouping of Chemicals**, is based on the guidance originally developed by EPA for the HPV Challenge Program

	Chemical 1	Chemical 2	Chemical 3	Chemical 4	
Structure	xxxxxxxx	xxxxxxxx	xxxxxxxx	xxxxxxxx	
Property 1	● → ○	○	● → ○	○	SAR/Read-across
Property 2	● → ○	○	○ ← ●	●	Interpolation
Property 3	○ ← ●	●	● → ○	○	Extrapolation
Activity 1	● → ○	○	● → ○	○	SAR/Read-across
Activity 2	● → ○	○	○ ← ●	●	Interpolation
Activity 3	○ ← ●	●	● → ○	○	Extrapolation

● Existing data point ○ Missing data point

EPA/OPPT's Use of Chemical Categories: New Chemicals



- Substances which fall into New Chemical Categories are ***not necessarily the chemical substances of greatest concern*** to EPA.
 - Category Chemicals may not be made up of the most hazardous chemicals, but rather they include chemicals for which sufficient history has been accumulated so that hazard concerns and testing recommendations vary little from chemical to chemical within the category
- Grouping chemicals with shared chemical and toxicological properties into categories, enables both PMN submitters and EPA reviewers to benefit from accumulated data and past decisional precedents
 - Streamline/focus EPA's **hazard (fate) review**
 - Expedite identification and provide consistency for **testing recommendations**, when a chemical **“may present unreasonable risk”** [and under amended TSCA when **“insufficient information for reasoned evaluation”**]
- Categories are not intended to be a comprehensive list of all substances that may be subject to further action in the New Chemicals Program;
 - Currently 56 NCP Chemical Categories: 31 Eco Only; 17 Eco + Health; 8 Health Only
 - Continual updating/development as resources allow
 - Some new categories developed due to new TSCA

Chemical Categories: Same Principles, Different Purposes



	Existing Chemicals (OECD & EPA HPV Programs)	TSCA New Chemicals
Category is based on similar physicochemical properties, fate properties and/or health or eco hazards	✓	✓
Category Boundaries	Category Justification (Narrative): Pchem, Fate, Hazard Data/Trends to support Read-Across	Pchem properties or 'cut-offs'/bands to quickly designate chemical "in" or not
Specific Chemicals Identified/Listed	✓	✗ (many/most CBI)
Data-Sharing/Extrapolation	Read-Across; group assessment	"Best" Analog with data for endpoint; sometimes multiple analogs to cover various endpoints
Testing Recommendations	✗	✓

NCP Chemical Category: Definition/Development



- Candidate categories are proposed by EPA's New Chemicals Program reviewers, based on experience reviewing PMNs on similar substances
- At proposal, the database supporting the category is evaluated for quality and for general applicability to other potential members of the category
- New Chemical Category:
 - **Definition:** describes the molecular structure a new chemical must have to be included in the category
 - **Hazard Concerns:** hazard concerns for the category are identified based on literature or data for other PMNs
 - **Boundaries:** conditions such as molecular weight, equivalent weight, the log of the octanol/water partition coefficient ($\log P$), or water solubility, that would determine inclusion in (or exclusion from) a category
 - **General Testing Strategy:** Identifies standard (e.g., OECD or OCSPP) hazard and fate tests to address concerns for the category

NCP Chemical Category: Use in Evaluation



- When a new substance is identified as being a member of a category, the chemical is evaluated in the context of the potential health or environmental concerns associated with that category
- Identification of a chemical as belonging in a NCP Chemical Category happens early, typically at SAT and hence, streamlines/focuses hazard assessment
- NCP Categories include Testing Strategies; hence, if testing is deemed necessary,
 - Identification of tests is expedited
 - Consistency in testing requests may be realized

Chemical Categories - New



- **4 Lung Effects Categories:** Polycationic Substances (Cationic Binding); General Surfactants; Waterproofing Agents; Insoluble Polymer Lung Overload
 - Need for definitive finding prompted search for more/quantitative data
 - Tiered testing strategy; includes in vitro (non-animal) testing approaches
 - Status: Working with submitters that 'suspended' PMN review to scope testing
- **Photo-Acid Generators (PAG) Category:**
 - 8(e) Data Submissions challenged previous assumptions
 - Tiered testing strategy; includes in vitro (non-animal) testing approaches
 - Status: Working with submitters that 'suspended' PMN review to scope testing
- **Tracer Chemicals:**
 - Received PMNs for over 100 structurally similar chemicals with same use
 - Strategically identified which chemicals to test and developed testing strategy
 - Status: strategic testing agreed; candidate for formal development of category
- **Perfluorinated Chemicals**
 - Approximately **400** chemicals in several structural categories (e.g., ethers, sulfonamides, sulfonic acids, phosphonic acids) compiled; Data (health tox, eco tox, fate) for **< half**
 - Next Steps: Data review; integrate with Agency-wide PFAS hazard characterization effort
 - Status: candidate for formal development of category

Chemical Categories - Future



- To date, new chemical category development has been based on:
 - Accrual of experience and desire to streamline reviews – first NCP Categories
 - Resource availability (NCP Categories updated periodically, as allowed)
 - Necessity – e.g., amendments to TSCA/definitive finding; new data challenging assumptions; large number of similar PMN submissions
- EPA is soliciting input/ideas on if/how to develop additional/update existing Chemical Categories; Docket:
EPA-HQ-OPPT-2017-0585 at <http://www.regulations.gov>

Sustainable Futures

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Sustainable Futures: Background



- New Chemical Reviews are mandated to be conducted in 90 days (absent extension)
- Most new chemical notices that EPA reviews lack test data needed to fully estimate potential risks
- Lacking experimental data, EPA has relied on screening methods to review and evaluate new chemicals under TSCA to help identify chemicals that could pose unreasonable risk
- Grew out of the Pollution Prevention Framework and Eastman Kodak Project XL and PPG Industries Project XL
 - Project XL (eXcellence and Leadership) was a voluntary program in which EPA offered regulatory flexibility to encourage companies, communities and others to develop/test cleaner, cheaper, smarter alternatives that could produce superior environmental results beyond those that would have been achieved under current regulations and policies.
- The methods, which EPA created, are the basis of the ***Sustainable Futures*** program and are available to the chemical industry and other stakeholders at no cost

Sustainable Futures: Goals



- To provide chemical developers the same risk-screening models that EPA uses to evaluate new chemicals before they enter the market
- To provide EPA's computer-based models and training in their use to help companies develop safer chemicals quickly and cost-effectively

<https://www.epa.gov/tsca-screening-tools>

- To provide companies that take the training and graduate from Sustainable Futures an expedited EPA premanufacture review

Sustainable Futures / P2 Framework Manual

**U.S. Environmental Protection Agency
Office of Chemical Safety and Pollution Prevention**

EPA-748-B12-001

2012



Sustainable Futures: Graduates



- BASF
- Cabot Corporation
- Cargill Incorporated
- Chevron Phillips Chemical Company
- Clariant Corporation
- Cytec Industries, Inc.
- Eastman Kodak, Inc.
- Givaudan Fragrances Corporation
- PPG Industries
- International Flavors and Fragrances, Inc.
- NALCO Champion, An Ecolab Company
- 3M

Sustainable Futures: Moving Forward



- Continue/Discontinue/Re-invent Program
- Increase/Decrease Training Workshops
 - EPA has conducted approximately 2-4 per year
 - Requires sponsors (industry, academia, other interested parties)
- Update on-line Sustainable Futures / P2 Framework Manual to reflect new TSCA
 - **Minimal technical changes;** Manual is largely step-by-step instruction/demonstration of the technical analysis EPA conducts using predictive models, which has not changed significantly under amended TSCA;
 - Reporting formats/transparency has increased
- Overlap with Points-to-Consider: PtC is 'short version' of SF/P2 Framework without chemical/specific examples or detailed information on predictive tools

Sustainable Futures: Moving Forward



Other Ideas/Input?

Docket EPA-HQ-OPPT-2017-0585 at
<http://www.regulations.gov>