PFAS - Selected Definitions

Toxics Use Reduction Institute, March 2020

The following resources may be useful in considering ways to describe and define the broad chemical category of PFAS.

1. OECD. 2018 Toward a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFAS)[i]

This document describes how OECD has created a database of PFAS. The following points describe the way in which OECD defined the scope of the database. The scope of the database is a focus on alkyl substances with three or more carbons (≥ C3) and ethers with two or more carbons (≥ C2).

- The database focuses on those PFASs that contain a perfluoroalkyl moiety with three or more carbons (i.e. $–C_nF_{2n}–$, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. $–C_nF_{2n}OC_mF_{2m}–$, n and $m \geq 1$). (note: includes perfluorocarbons)
- The database does NOT include:
  - C1 and C2 chain lengths unless ether moiety is present
  - Methodology notes: *Some PFASs with shorter-chain perfluoroalkyl(ether) moieties have also been present in products as intended ingredients (e.g., lithium bis(trifluoromethylsulfonyl)imide (CAS number 90076-65-6,) [C1] as electrolytes in the manufacture of batteries for electric vehicles or stationary applications; ECHA, 2018) or as impurities (e.g., Barzen-Hanson and Field, 2015), and/or in the environment (e.g., Barzen-Hanson and Field, 2015); however, they are not within the scope of this study.*

2. Buck, et al. 2011. "Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins."

This seminal paper provided a definition of PFAS, drawing from industry, government and academic expertise. It defines PFAS as fluorinated alkyl chains with one or more carbon (≥ C1) ending in CF_3.

- A subset of fluorinated substances is the highly fluorinated aliphatic substances that contain 1 or more C atoms on which all the H substituents (present in the nonfluorinated analogues from which they are notionally derived) have been replaced by F atoms, in such a manner that they contain the perfluoroalkyl moiety $C_nF_{2n+1}–$. *[i.e., must at least contain CF_3-]* These compounds are hereafter referred to as ''perfluoroalkyl and polyfluoroalkyl substances'' and denoted by the acronym PFASs.

3. EPA approach to PFAS terminology

EPA has not adopted a definition of PFAS. PFAS are defined in the recent National Defense Authorization Act. In addition, EPA has made some efforts to clarify some terminology related to PFAS.

- From the NDAA which adds substances to TRI[ii], the term ''PFAS'' means perfluoroalkyl and polyfluoroalkyl substances that are man-made chemicals with at least one fully

fluorinated carbon atom. The term ‘‘fully fluorinated carbon atom’’ means a carbon atom on which all the hydrogen substituents have been replaced by fluorine.

- EPA distinguishes between the term perfluorocarbons (PFCs) and the term per- and poly-fluoroalkyl substances (PFAS). EPA notes that the key concerns associated with PFCs are different from the concerns associated with many other PFAS. PFCs are potent greenhouse gases, whereas other PFAS pose a range of other health and environmental concerns.
- EPA has created a research list of several hundred PFAS. These are chemicals that have been identified as particular priorities for investigation by EPA. EPA's updated research list of 199 substances (EPAPFASRL) and the 2 prioritized lists of 75 include, in addition to typically recognized PFAS:
  - Ethers, incl perfluoroethers (fully fluorinated w ether linkage)
  - C2 (e.g., trifluoroacetic acid) and C3 substances
  - cyclic rings
  - PFAS with chlorine and iodine substituents
  - HFEs (hydrofluoroethers)
  - Substances without CF_3 end group

Additional detail from the TRI listing under NDAA

- TRI listing under NDAA of certain long chain PFAS and GenX lists specific chemicals as well as any substance that is included in the definition of long chain perfluoroalkyl carboxylate and phosphonic/phosphinic chemical substances in the SNUR for carpet (40 CFR 721.10536)[iii]:
  - (1) The chemical substances identified below, where $5 < n < 21$ or $6 < m < 21$, are subject to reporting under this section for the significant new uses described in paragraph (b)(2) of this section.

    (i) $CF_3(CF_2)_n$-COO-M where M = H − or any other group where a formal dissociation can be made;
    (ii) $CF_3(CF_2)_n$-CH = CH2;
    (iii)$CF_3(CF_2)_n$-C(= O)-X where X is any chemical moiety;
    (iv)$CF_3(CF_2)_m$-CH2-X where X is any chemical moiety; and
    (v) $CF_3(CF_2)_m$-Y-X where Y = non-S, non-N heteroatom and where X is any chemical moiety.

[i] *TOWARD A NEW COMPREHENSIVE GLOBAL DATABASE OF PER-AND POLYFLUOROALKYL SUBSTANCES (PFASs)*. 4MAY2018. OECD Series on Risk Management No. 39. https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/

[ii] National Defense Authorization Act of 2020 section 332(c), (2) and (3), https://www.congress.gov/116/crpt/hrpt333/CRPT-116hrpt333.pdf

[iii] 40 CFR § 721.10536 - Long-chain perfluoroalkyl carboxylate chemical substances https://www.law.cornell.edu/cfr/text/40/721.10536