1 Introduction

This fact sheet addresses naming conventions of some of the most commonly reported PFAS based on historical use, current state of science research related to environmental occurrence, and available commercial analyses. For naming conventions related to additional PFAS, refer to Buck et al. (2011) and the USEPA’s CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard/chemical-lists/PFASMASTER). The definition of PFAS continues to evolve to reflect continued study of these compounds. Table 2-1 in the Guidance Document includes examples of PFAS definitions.

The PFAS family may be divided into two primary classes: polymer and nonpolymer as shown in Figure 1. Future updates to the family tree and nomenclature are expected with the evolving public knowledge of these compounds.

This fact sheet focuses primarily on nonpolymer PFAS most commonly detected in the environment. Additional information is available in Section 2.2 of the Guidance Document.

2 Nonpolymer PFAS

The class of nonpolymer PFAS encompasses two major subclasses: perfluoroalkyl substances and polyfluoroalkyl substances, which include many groups and subgroups of chemicals, examples of which are shown in Figure 1. Nonpolymer PFAS were selected as the focus of the Guidance Document because (1) they are included in most laboratory PFAS analyte lists; (2) they are the PFAS most commonly detected (to date) in humans, biota, and other
environmental media; (3) they appear to be relatively more abundant at PFAS investigation sites; (4) data may be available regarding potential human health and ecological effects from environmental exposure; and/or (5) state or federal guidance values may exist or be under development for some PFAS.

Perfluoralkyl Substances
Perfluoralkyl substances are fully fluorinated (perfluoro-) alkane (carbon-chain) molecules. Their basic chemical structure is a chain (or tail) of two or more carbon atoms with a charged functional group (or head) attached at one end. Common functional groups are carboxylates or sulfonates, but other forms are also detected in the environment. This structure, which is illustrated in Figure 2 for perfluorooctane sulfonate (PFOS) and perfluorooctane carboxylate, referred to as perfluorooctanoate (PFOA), can be written as:

\[ C_nF_{2n+1}R \]

where “\( C_nF_{2n+1} \)” defines the length of the perfluoralkyl chain tail, “\( n \)” is \( \geq 2 \), and “\( R \)” represents the attached functional group head. The functional group may contain 1 or more carbon atoms, which are included in the total number of carbons when naming the compound.

Perfluorooalkyl acids (PFAAs)
Perfluorooalkyl acids (PFAAs) are some of the least complex PFAS and currently are the class of PFAS most commonly tested for in the environment. Biotic and abiotic transformation of many polyfluoroalkyl substances may result in the formation of PFAAs. As a result, PFAAs are sometimes referred to as “terminal PFAS” or “terminal transformation products,” meaning no further transformation products will form from them under normal environmental conditions. Polyfluoroalkyl PFAS that transform to create terminal PFAAs are referred to as “precursors.” PFAAs are divided into two major subgroups:

- **Perfluorooalkyl carboxylic acids** (PFCAs), or perfluorooalkyl carboxylates, are terminal transformation products of select precursor polyfluoroalkyl substances, such as fluorotelomer alcohols (FTOHs). An example PFC is PFOA.
- **Perfluoroalkane sulfonic acids** (PFSA), or perfluoroalkane sulfonates, are also terminal transformation products of select precursor polyfluoroalkyl substances, such as perfluoroalkane sulfonamido ethanols (FASEs). An example PFSA is PFOS.

PFAAs are the majority of PFAS typically included in commercial laboratory target analyte lists and are the primary PFAS for which federal or state health-based guidance values have been established. As a result, PFAAs tend to drive site investigation and remediation decisions, and so it is helpful to understand the naming conventions for this class.

Table 1 illustrates how this naming structure works for select PFCAs and PFSA, which collectively are referred to as PFAAs. The full table is included in the Guidance Document.

<table>
<thead>
<tr>
<th>( X )</th>
<th>( Y )</th>
<th>Acronym</th>
<th>Name</th>
<th>Formula</th>
<th>CAS No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>B = buta (4 carbon)</td>
<td>A = Carboxylate or carboxylic acid</td>
<td>PFBA</td>
<td>Perfluorobutanoate</td>
<td>( C_7F_7CO^+ )</td>
<td>45048-62-2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Perfluorobutanoic acid</td>
<td>( C_7F_7COOH )</td>
<td>375-22-4</td>
</tr>
<tr>
<td></td>
<td>S = Sulfonate or sulfonic acid</td>
<td>PFBS</td>
<td>Perfluorobutane sulfonate</td>
<td>( C_7F_7SO^+ )</td>
<td>45187-15-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Perfluorobutane sulfonic acid</td>
<td>( C_7F_7SOH )</td>
<td>375-73-5</td>
</tr>
<tr>
<td>A = Carboxylate or carboxylic acid</td>
<td>PFOA</td>
<td>Perfluorooctanoate</td>
<td>( C_7F_{15}CO^+ )</td>
<td>45285-51-6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Perfluorooctanoic acid</td>
<td>( C_7F_{15}COOH )</td>
<td>335-67-1</td>
</tr>
</tbody>
</table>

Many of the commonly detected PFAAs are denoted using the following structural shorthand acronym:

\[ \text{PFXY} \]

where:

\[ P = \text{perfluoro} \]

\[ X = \text{the carbon chain length using the same naming conventions as hydrocarbons based on the number of carbons (for example, B for butane or 4 carbons, Pe for pentane or 5 carbons)} \]

\[ Y = \text{the functional group (for example, A = carboxylate or carboxylic acid and S = sulfonate or sulfonic acid)} \]
Naming Conventions for Per- and Polyfluoroalkyl Substances (PFAS)  

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Acronym</th>
<th>Name</th>
<th>Formula</th>
<th>CAS No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O = octa (8 carbon)</td>
<td>S = Sulfonate or sulfonic acid</td>
<td>PFOS</td>
<td>Perfluorooctane sulfonate</td>
<td>C₈F₁₇SO₃⁻</td>
<td>45298-90-6</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Perfluorooctane sulfonic acid</td>
<td>C₈F₁₇SO₃H</td>
<td>1763-23-1</td>
</tr>
</tbody>
</table>

Long-Chain versus Short-Chain Distinction

PFAs are sometimes described as long-chain and short-chain to group PFCAs and PFSAs that may behave similarly in the environment. Table 2 illustrates the differences in the short-chain and long-chain PFCAs and PFSAs.

<table>
<thead>
<tr>
<th>Number of Carbons</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>PFCAs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Short-chain PFCAs</td>
<td>PFBA</td>
<td>PFFeA</td>
<td>PFHxA</td>
<td>PFHpA</td>
<td>PFOA</td>
<td>PFNA</td>
<td>PFDA</td>
<td>PFUnA</td>
<td>PFDa</td>
</tr>
<tr>
<td>Long-chain PFCAs</td>
<td></td>
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<td></td>
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<td></td>
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<td></td>
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</tr>
<tr>
<td>PFSAs</td>
<td>PFBS</td>
<td>PFFeS</td>
<td>PFHxS</td>
<td>PFHpS</td>
<td>PFOS</td>
<td>PFNS</td>
<td>PFDS</td>
<td>PFUnS</td>
<td>PFDa</td>
</tr>
<tr>
<td>Short-chain PFSAs</td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Long-chain PFSAs</td>
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</tbody>
</table>

Anion versus Acid Form

As noted above, the names for the anionic and acid forms of PFAs are often used interchangeably. However, it is critical to know which form is being discussed because of differences in their physical and chemical properties and behavior in the environment. Some important things to keep in mind regarding the anionic vs. acid forms are:

- Most PFAs are present in environmental and human matrices in their anionic form. For example, PFOS is present in the environment in the anionic form, perfluorooctane sulfonate.
- Although laboratories may be reporting PFOA or PFOS using the acid form of their name, they are actually measuring the anionic form (for example, perfluorooctanoate or perfluorooctane sulfonate), as this is the form that exists in the environment.
- The acid form and their associated cationic salts have CAS numbers, while the anionic forms may not. For example, PFOS can exist as different salts (cationic), including sodium, lithium, potassium, or ammonium. Each of these salts will have a different CAS number:
- When the salt or acid exists in water or other liquids, it will dissociate (lose its hydrogen or associated ion) and the salt or acid will break off and form the anion (for example, COO⁻).

Linear and Branched Isomers of PFAs

Many PFAs may be present as mixtures of linear and branched isomers (chemicals with the same chemical formula, but different molecular structures) depending on the manufacturing process that was used. These structural differences are important because they may affect how the compounds behave in the environment. The presence of linear and branched isomers may be useful in understanding sources of PFAs and the age of the source, since the production of isomers varies by manufacturing processes. For example, the fluorotelomerization process produces primarily linear PFAAs, whereas the ECF process produces a mixture of linear and branched PFAA isomers. The presence of linear and branched isomers may also have implications for partitioning, transport, and bioaccumulation.

Polyfluoroalkyl Substances

Polyfluoroalkyl substances and some side-chain fluorinated polymers are increasingly being identified as important to understanding the fate and transport of PFAs at release sites and in the environment (OECD 2013; Butt, Muir, and Mabury 2014; Liu and Mejia-Avendaño 2013; Wang et al. 2011; Mejia-Avendaño et al. 2020). Figure 1 highlights the polyfluoroalkyl substances that, to date, have most commonly been detected at PFAS sites (Barzen-Hanson et al. 2017; OECD 2018).

Polyfluoroalkyl substances are distinguished from perfluoroalkyl substances by not being fully fluorinated. Instead, they are aliphatic substances for which all hydrogen atoms attached to at least one (but not all) carbon atom have been replaced by fluorine atoms, in such a manner that they contain the perfluoroalkyl moiety CₙF₂ₙ₊₁ (Buck et al. 2011). More information is included in Section 2.2.4 of the Guidance Document. Figure 3 shows an example of a polyfluoroalkyl substance where two of the carbons in the tail are not fully fluorinated, while the remaining carbons are. This also illustrates the “n:x” naming convention for fluorotelomer substances where “n” is the number of fully fluorinated carbons (in this case, 8) and “x” is the number of carbons that are not fully fluorinated (in this case, 2).
Naming Conventions for Per- and Polyfluoroalkyl Substances (PFAS) continued

The carbon-hydrogen (or other non-fluorinated) bond in polyfluoroalkyl molecules creates a “weak” point in the carbon chain that is susceptible to biotic or abiotic transformation. As a result, many polyfluoroalkyl substances that contain a perfluoroalkyl \( C_nF_{2n+1} \) moiety are potential precursor compounds that have the potential to be transformed into PFAAs.

Fluorotelomer Substances
Fluorotelomer substances are polyfluoroalkyl substances produced by the fluorotelomerization process. The transformation of fluorotelomer-based substances is a potential source of PFCAs in the environment, but not PFSAs (Buck et al. 2011). The following fluorotelomer substances are those most commonly detected in the environment to date:

- Fluorotelomer alcohols (FTOHs): The n:2 fluorotelomer alcohols (n:2 FTOHs) are key raw materials in the production of n:2 fluorotelomer acrylates and n:2 fluorotelomer methacrylates (Buck et al. 2011).
- Fluorotelomer sulfonic acids (FTSs): The n:2 fluorotelomer sulfonic acids (n:2 FTSs) have been detected in environmental matrices at sites where aqueous film forming foam (AFFF) has been used, and also in wastewater treatment plant effluents and landfill leachate. FTSs are precursor compounds and can undergo aerobic biotransformation to form PFCAs (Buck et al. 2011).
- Fluorotelomer carboxylic acids (FTCAs): These compounds form through the biotransformation of FTOHs (Buck et al. 2011; Mejia Avendaño et al. 2016) and have been detected in landfill leachate.

3 Polymer PFAS
Polymers are large molecules formed by combining many identical smaller molecules (or monomers) in a repeating pattern. Subclasses in the polymer class include fluoropolymers, polymeric perfluoropolyethers (PFPE), and side-chain fluorinated polymers. Some polymer PFAS are currently believed to pose less immediate human health and ecological risk relative to some nonpolymer PFAS. As stated previously, most compounds of interest at environmental release sites are nonpolymers.

4 References and Acronyms
The references cited in this fact sheet and further references can be found at https://pfas-1.itrcweb.org/references/. Reference numbers are included in this fact sheet for non-unique citations in the Guidance Document reference list.

The acronyms used in this fact sheet and in the Guidance Document can be found at https://pfas-1.itrcweb.org/acronyms/.