

Perfluoroethylcyclohexane Sulfonate (PFECCHS)

Current Knowledge of Physiochemical Properties, Environmental
Contamination and Toxicity

Whitepaper

Prepared by the Michigan PFAS Action Response Team (MPART) Human Health Workgroup (HHWG)
supported by and in conjunction with the Michigan Department of Health and Human Services (MDHHS)

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Executive Summary

The Michigan Department of Health and Human Services (MDHHS) and the Michigan PFAS Action Response Team (MPART) Human Health Work Group (HHWG) serve to protect the health of the residents in our state. One role of the HHWG is to develop and update characterizations of PFAS species, as information on them becomes available. To date, the HHWG has developed summary and screening level documents on PFOA, PFOS, PFHxS, PFNA, PFBS and with this document, a summary on PFECHS. Here, the current knowledge regarding physicochemical properties, commercial use, environmental contamination, and toxicity of PFECHS is characterized. The final section of this document outlines HHWG recommendations to MPART for addressing PFECHS in Michigan.

Table of Contents

| | |
|---|----|
| Introduction | 4 |
| PFECHS Summary | 5 |
| Physicochemical Properties | 5 |
| Similarities to PFOS. | 5 |
| Defining “PFAS” | 7 |
| Use | 7 |
| Environmental Contamination..... | 8 |
| Toxicity | 9 |
| Toxicodynamics..... | 9 |
| Toxicokinetics..... | 10 |
| Recommendations for MPART..... | 10 |
| Limitations | 10 |
| Appendix A: Published Physical and Chemical Properties of PFECHS..... | 11 |

Introduction

Perfluoroethylcyclohexane sulfonate (PFECHS) is an 8-carbon cyclic PFAS and is considered an analog of PFOS (meaning they share structural similarities). Commercially, it has been used as a replacement for PFOS in various formulations. PFECHS, similar to other long-chain PFAS, has been reported in environmental media around the world. Found in drinking water [1], wastewater [2], surface water [3-5], sediment [4], marine organisms [3, 4] and human blood [6], PFECHS is among the most widespread PFAS detected in the environment. There are persisting difficulties associated with the detection and quantification of PFECHS [7], possibly due to homologous and isomeric impurities that can result from the electrochemical fluorination (ECF) process by which PFECHS is derived, as discussed below.

Due to its flame-resistant and erosion-inhibiting properties, PFECHS found commercial use in aircraft hydraulic fluids beginning in the late 1940s. Multiple reports [3, 8, 9] have linked the use of PFECHS in aviation to environmental contamination. The 3M corporation began phasing out production of PFECHS in 2002, as part of an initiative to phase out PFOS and its analogs [10]. It remains unclear the degree to which the current use of PFECHS, its historical application, and/or the degradation of unidentified precursor products contributes to current environmental contamination.

Compelling evidence continues to accumulate indicating widespread presence of PFECHS in the environment, however, the toxicity of PFECHS is not yet well characterized. In addition to questions pertaining to health effects, many uncertainties remain about the ability to accurately quantify concentrations of PFECHS from environmental samples, its environmental fate and transport, and its ongoing presence in commercial products (e.g. as impurities associated with other PFAS). The following whitepaper summarizes what is currently known on these topic areas, including specific sections on:

- Physicochemical properties of PFECHS
- Prevalence in the environment
- Commercial/industrial sources of PFECHS
- Toxicity
- Recommendations for MPART

The existing literature on most of these topic areas is limited. ***Insufficient data exist at present to derive health-based comparison values for PFECHS.***

PFECHS Summary

Physicochemical Properties

The predicted physicochemical properties of PFECHS are tabulated in **Table 1** and **Appendix A1** of this document. **Figure 1** shows the chemical structure of PFECHS. PFECHS can be found with CAS Number 335-24-0 and CAS Number 646-83-3. CAS Number 335-24-0 is the potassium salt of CAS Number 646-83-3. Isomers of PFECHS have also been identified, including two potassium salts of PFECHS, with the CAS numbers: 67584-42-3 and 1135308-34-7. These are structural isomers of CAS number 335-24-0; note that the pentafluoroethyl group is in position 1 rather than position 4 found in CAS number 335-24-0.

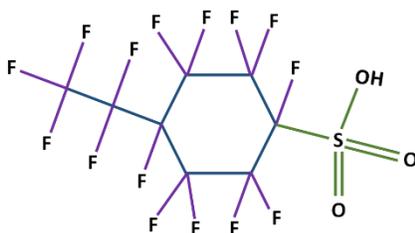


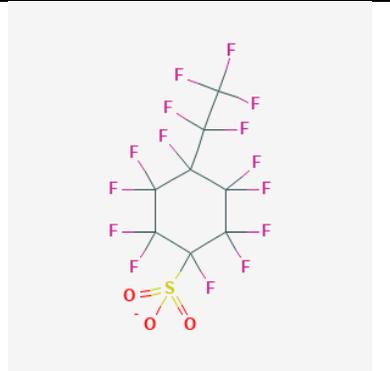
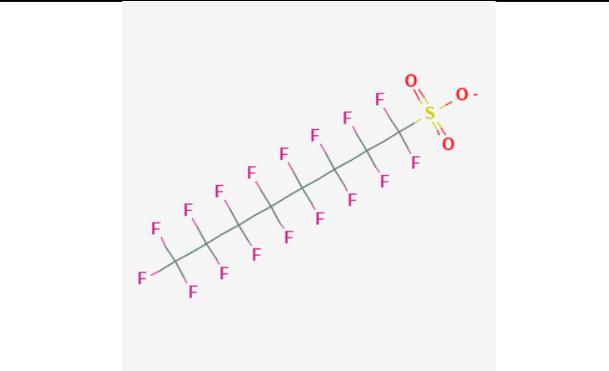
Figure 1. Structure of the neutral form of PFECHS. Adapted from "Emerging poly- and perfluoroalkyl substances in the aquatic environment: A review of current literature," by Xiao F. 2017, *Water Res*, 124: p. 482-495.

Additional characteristics of PFECHS can be predicted based on its known or estimated physicochemical properties. For instance, log albumin/water partition coefficients for PFAS are known to increase with longer chain lengths and sorption to albumin is generally stronger for the perfluorinated sulfonates (like PFECHS) than for the carboxylates [11]. Similarly, long-chain PFAS (≥ 8), like PFECHS, are thought to have a higher log dissociation constant (Kd) compared to shorter chain PFAS, which is supported by empirical evidence showing PFECHS has a high average log Kd in a water-sediment system [12]. Cyclic PFAS such as PFECHS also show less sediment sorption compared to linear and branched PFAS. Cyclic PFAS likely have higher hydrophobicity compared to linear PFAS [13]. PFECHS has also been characterized as potentially bioaccumulative and persistent [2, 3, 7].

Similarities to PFOS. PFECHS is an 8-carbon cyclic analog of the linear PFOS. PFECHS has similar physicochemical properties as PFOS and, accordingly, is thought to have similar persistence in the environment and kinetics in humans and animals [12, 14]. Of note, there is evidence that the albumin/water partition coefficient for PFECHS is within the range associated with PFOS [15]. Additional similarities between environmentally relevant forms (i.e. anionic) of PFECHS and PFOS are listed in **Table 1** below.

Table 1. Comparison of predicted physicochemical properties of anionic forms of PFECHS and PFOS

| Physico-chemical properties | PFECHS (CAS# 80988-54-1) | PFOS (CAS# 45298-90-6) |
|-----------------------------|-----------------------------|---------------------------|
| | | |

| | | |
|---|--|--|
| Structure |  |  |
| Molecular Weight | 461.13 g/mol | 499.12 g/mol |
| Boiling Point | 221 °C | 219 °C |
| Melting Point | 74.1 °C | 71.0 °C |
| Henry's Law Constant (K_h) | 2.80e-8 atm·m ³ /mole | 1.85e-11 atm·m ³ /mole |
| Octanol/Air Partition Coefficient ($\text{Log}K_{oa}$) | 4.92 | 4.75 |
| Octanol/Water Partition Coefficient ($\text{Log}P$ or K_{ow}) | 3.8 | 4.9 |
| Vapor Pressure | 1.59e-2 mmHg | 1.49e-2 mmHg |
| Water Solubility | 1.35e-3 mol/L | 1.07e-3 mol/L |
| References | https://comptox.epa.gov/dashboard/DTXSID20892328 https://pubchem.ncbi.nlm.nih.gov/compound/23504419 | https://comptox.epa.gov/dashboard/DTXSID80108992 https://pubchem.ncbi.nlm.nih.gov/compound/Perfluorooctanesulfonate |

Cheminformatics tools also support significant structural similarity between PFOS and PFECFS through the calculation of a Tanimoto coefficient¹. This is a scientifically recognized measure of molecular similarity that has been used across multiple sectors, including regulatory and industry². This assumes structurally analogous compounds display similar physicochemical properties and adverse human health effects. ChemIDplus³ is a web-based chemical database provided by the United States National Library of Medicine. It provides a structural similarity search function quantifying the level of structural features shared between two chemical compounds. Results from a structural similarity search conducted with ChemIDplus at a cut-off level of 70% identified PFOS as a surrogate exhibiting 81.4534% structural

¹ Utilizing parent form of PFECFS

² https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4456712/pdf/13321_2015_Article_69.pdf

³ <https://chem.nlm.nih.gov/chemidplus/>

similarity to PFECHS. The conventional cut-off values range from 70-80%. Therefore, at >81%, significant structural similarity is indicated between PFOS and PFECHS.

Correspondingly, a Tanimoto coefficient supporting significant structural similarity between PFOS and PFECHS was also calculated through ChemMine⁴. This is a web-based platform supported by grants from the National Science Foundation and National Institutes of Health's National Institute on Aging⁵. A Tanimoto coefficient of 0.63⁶ was calculated between PFOS and PFECHS⁷. A conventional Tanimoto coefficient cut-off value of >0.6 signifies a significant level of structural similarity between two compounds⁸. Both ChemIDplus and ChemMine demonstrate evidence in support of significant structural similarity between PFOS and PFECHS. Therefore, PFECHS displays significant structural similarity to PFOS, a characteristic member of the PFAS family of compounds.

Defining "PFAS"

As a fully-fluorinated cyclic compound, PFECHS resides outside some common definitions of "PFAS", which do not include cyclic compounds, as described in Buck et al. (2011):

"...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} ."

As part of the evolving definition of "PFAS", however, the Organization for Economic Co-operation and Development [17] stated:

"the definition of a perfluoroalkyl moiety has been expanded from " (C_nF_{2n+1}) " in Buck et al. (2011) to " $-C_nF_{2n}-$ " so as to include PFASs with both ends of the perfluoroalkyl moiety connected to a functional group (e.g., perfluoroalkyl dicarboxylic acids, $HOOC-C_nF_{2n}-COOH$), including cyclic analogues of linear PFASs (e.g., $C_6F_{11}SO_3K$, CAS No. 3107-18-4)."

The Interstate Technology and Regulatory Council (ITRC) has a national workgroup titled, "History, Use and Naming" that will continue to delve into this issue throughout 2020 and has indicated plans to address the issue of cyclic compounds.

Use

PFECHS was marketed for use as an erosion inhibitor in aircraft hydraulic fluids. Production of PFECHS has been phased out in the United States, beginning in 2002, via 3M's phased-out of perfluorooctanesulfonyl fluoride (POSF)-based materials. However, the use of these chemicals in aircraft hydraulic fluids is still permitted in Canada and the United States.

⁴ <http://chemmine.ucr.edu/>

⁵ <https://chemminetools.ucr.edu/about/>

⁶ Utilizing maximum common substructure metric

<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2718661/pdf/btn186.pdf>

⁷ ChemMine provided both AP and MCS Tanimoto coefficients. As MCS-based similarity measures have been shown to be more effective than AP-based methods at searching chemical databases, MCS Tanimoto coefficients are considered (<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2718661/>)

⁸ <https://chemminetools.ucr.edu/help/>

Perfluorocycloalkyl sulfonates are available commercially under the tradenames FC-95 and FC-98, from 3M, Minneapolis, MN. FC-95 and FC-98 are proprietary marks of the 3M Company and may contain between 0.01 to 0.15% wt, based on the total hydraulic fluid composition, of a perfluoroalkyl or perfluorocycloalkyl sulfonic acid, or a metal salt of the same, or mixture of these sulfonic acids and metal salts, where the alkyl groups encompass 1 to 10 carbon atoms and the cycloalkyl groups from 3 to 10 carbon atoms (U.S. Patents). According to their respective material safety data sheets (MSDS) [18] FC-98, but not FC-95, contains the cyclic perfluoroalkyls like PFECHS: 3M's FC-98 MSDS lists 66–70% PFECHS, 18–22% perfluoro-4-methylcyclohexanesulfonate (PF4MeCHS), 9–13% of a perfluoro-dimethylcyclohexanesulfonate (PF4diMeCHS), 1–3% perfluorocyclohexanesulfonate (PFCHS), and 0.1–0.5% of other “residual organic fluorochemicals”.

Stefanac et al. (2018) quantified PFECHS in various commercial samples from industrial manufacturers and identified *cis*- and *trans*- PFECHS as constituting a significant percentage of the fluorinated products detected, as did linear and branched PFOS. The complex mixture of fluorinated products and their isomers contained in these commercial erosion-inhibiting products may complicate the ability to accurately report the concentrations of PFECHS from environmental samples [19].

An OECD (2005) report⁹ mentions the manufacture/use of PFECHS in at least 3 countries (Italy, Norway, and Sweden); marketed use was described as hydraulic fluid or was not disclosed. Information such as the amount of PFECHS manufactured during the 2003 calendar year was only disclosed for Italy. It was either unknown or kept confidential for the other 2 countries. The report mentions there are up to three Swedish companies that marketed products containing PFECHS.

An additional, less recognized, use is the potential for perfluorocyclohexyl sulfonate salts to be used as components of printer inks (see patent from Wei-Ping, 2002). A Xerox patent for ink jet [20] references the possibility of C1 to C30 cyclic alkyls with either hydrogen or fluorine atoms in its composition. Limited supporting information is currently available for this use and the degree to which cyclic PFAS like PFECHS may be present in printer ink is not known.

Environmental Contamination

PFECHS has been found in surface water (ranging from 0.16–5.7 ng/L) and top predator fish (ranging from <MDL to 3.7 ng/g wet weight in whole body homogenate) from the Great Lakes [3]. Detections of perfluoromethylcyclohexane sulfonate (PFMeCHS), an impurity associated with a commercial PFECHS formulation, were also reported in the dissolved phase [3]. Herring gull eggs from the Great Lakes have also been shown to have detectable concentrations of PFECHS [21, 22]. Detectable concentrations of PFECHS have been reported in other freshwater bodies [5, 21], the Baltic Sea [13], samples of drinking water [1], and the Arctic ice cap [9].

Detectable concentrations of PFECHS have been reported in waters and/or amphipods near airports [7, 8, 21], with declining concentrations detected in amphipods the further the collection point was from the airport [8]. Wastewater treatment plants have also been associated with detections of PFECHS, both in nearby fish [23] and in effluent from the plant [2]. PFECHS has also been detected in multiple media

⁹[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono\(2005\)1&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2005)1&doclanguage=en)

from the high Arctic [9, 21, 24] with evidence suggesting proximity to an airport or atmospheric deposition as a relevant source.

PFECHS has also been detected in pooled serum samples from Swedish women [6], where the authors report serum concentration of PFECHS were highest during the 1990s through the early 2000s. **Table 2** summarizes the extent to which PFECHS has been detected in environmental media or in biological matrices.

Table 2. Environmental media or biological matrices in which PFECHS has been detected.

| Matrix/Media | Reference |
|--------------------------------------|---|
| Fresh water | De Silva et al., 2011; Lescord et al., 2015; Houde et al., 2016 |
| Brackish water (Baltic Sea) | Joeress et al., 2019 |
| Drinking water | Kabore et al., 2018 |
| Wastewater effluent | Howard & Muir, 2010 |
| Ice Cap | MacInnis et al., 2017 |
| Sediment | Lescord et al., 2015; MacInnis et al., 2019 |
| Dust Samples | De Silva et al., 2012 |
| Predator fish: whole body | De Silva et al., 2011; Lescord et al., 2015 |
| Predator fish: muscle, liver, plasma | Houde et al., 2013 |
| Benthic invertebrates | Lescord et al., 2015 |
| Amphipods | de Solla et al., 2012 |
| Egg (herring gull and bald eagle) | Letcher et al., 2015; Su et al., 2017; Wu et al. 2020 |
| Serum (human) | Miaz et al., 2020 |

Toxicity

Limited data are available characterizing the toxicity of PFECHS and no data are currently available on biological effects in mammalian species. The evidence that is available to date is summarized below.

Toxicodynamics

Toxicodynamic effects in two model species have been described in the literature: microalgae and plankton. In microalgae (*Chlorella species*), 14-day exposure to PFECHS (at 10, 100 and 1000 ng/L) significantly reduced growth and inhibited catalase activity (highest concentration only) and increased superoxide dismutase and peroxidase activities, which could be indicative of oxidative stress [25]. In plankton (*Daphnia magna*), 12-day exposure to PFECHS (0.06 and 6 mg/L) resulted in the under-regulation of vitellogenin-related genes (VTG1), which could be indicative of endocrine disruption [5]. PFECHS exposure also resulted in some up-regulation of genes related to the cuticle; however, no overt signs of toxicity were elicited (e.g. on survival, reproduction) at those concentrations [5].

Of note, the administration of a commercially available PFECHS product has been described under experimental conditions (e.g. Houde et al., 2016). As discussed above, such products almost certainly contain a complex mixture of PFECHS isomers or other closely related compounds, making it more challenging to identify, with precision, the effects attributable to PFECHS alone. However, considering the high likelihood that these same commercial products are the source of environmental contamination, the results of such experimental milieu are likely applicable to questions of environmental contamination.

Toxicokinetics

PFECHS has been shown to accumulate in kidney, liver, bladder, blood, muscle, and plasma of fish, in bird eggs, and in human serum [6, 7, 21-23, 26]. PFECHS likely shares similar biological mechanisms for uptake and distribution as branched and linear PFOS [7]. One notable exception is that the median liver/blood ratio for PFECHS in fish may be significantly higher than for PFOS (both branched and linear) [7].

Two reports have estimated a mean log bioaccumulation factor (BAF) for PFECHS in fish: 2.7 [7] and 2.8 [3]. These BAFs rank below other long-chain PFAS, including PFOS, from these studies. As generally discussed in De Silva et al. (2011) and Wang et al. (2016), PFECHS would likely not be considered highly bioaccumulative based on these BAFs alone, however, considering what is known about the bioaccumulation of other similar PFAS, more information is needed to conclusively categorize the bioaccumulative potential of PFECHS. Moreover, considering the persistent nature of PFECHS in the environment, bioaccumulation remains a relevant topic for future research.

Recommendations for MPART

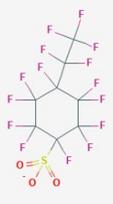
Based on the limited, currently available data, it is our recommendation that MPART and the Human Health Workgroup continue efforts to synthesize new information related to PFECHS, particularly toxicological data, as it becomes available. Only once key information related to the toxicity and environmental behavior of PFECHS become available can reliable recommendations be made to the public concerning environmental contamination by PFECHS. However, considering that some physicochemical properties are shared among PFECHS and PFOS, a compound for which robust toxicological information is available, the Human Health Workgroup recommends that MPART supports MPART agencies in their inclusion of PFECHS for future analyses of environmental media. To this end, we also recommend that MPART considers cyclic compounds, like PFECHS, as included structures when defining "PFAS". This will permit MPART agencies to characterize the extent and concentrations of PFECHS in Michigan. Equipped with that information, the eventual emergence of reliable toxicological data will leave MPART agencies well-positioned to develop screening and health-based criteria for PFECHS.

Limitations

The limitations of the conclusions drawn here are a direct reflection of the limitations currently inherent in the published literature on PFECHS. Very few published studies are available and fewer still contain the information required to draw conclusions about the risks associated with exposure. As more information becomes available, the conclusions and recommendations made here can be updated.

There are additional limitations due to the analytical measurement of PFECHS. EPA Methods 533 and 537.1 do not include PFECHS as an analyte. The EGLE Drinking Water Laboratory currently runs EPA Method 537.1. The MDHHS Analytical Chemistry Laboratory runs an isotope dilution method for over 20 PFAS, but does not currently include PFECHS as an analyte.

Appendix A: Published Physical and Chemical Properties of PFECHS

| | Various forms of PFECHS | | |
|--|--|---|--|
| | Parent Compound (Neutral or Acid Form) | Anionic Form ^[1] | Potassium Salt of PFECHS ^[2] |
| Structure |  |  |  |
| Molecular Formula | C ₈ HF ₁₅ O ₃ S | C ₈ F ₁₅ O ₃ S ⁻ | C ₈ F ₁₅ KO ₃ S |
| IUPAC Name | 1,2,2,3,3,4,5,5,6,6-decafluoro-4-(1,1,2,2,2-pentafluoroethyl) cyclohexane-1-sulfonic acid | 1,2,2,3,3,4,5,5,6,6-decafluoro-4-(1,1,2,2,2-pentafluoroethyl) cyclohexane-1-sulfonate | potassium;1,2,2,3,3,4,5,5,6,6-decafluoro-4-(1,1,2,2,2-pentafluoroethyl) cyclohexane-1-sulfonate |
| CAS Number | 646-83-3 | 80988-54-1 | 335-24-0 |
| Molecular Weight | 462.13 g/mol | 461.12 g/mol | 500.22 g/mol |
| Exact Mass | 461.940688 g/mol | 460.93341 g/mol | 499.896569 g/mol |
| Density | 1.87 to 1.93 g/cm ³ | | |
| Melting Point | 41.5 to 90.5 °C | 74.1 °C | 74.1 °C |
| Boiling Point | 221 to 256 °C | 221 °C | 221 °C |
| Solubility | 9.68e-6 to 1.35e-3 mol/L | 1.35e-3 mol/L | 1.35e-3 mol/L |
| Vapor Pressure | 9.38e-5 to 1.59e-2 mmHg | 1.59e-2 mmHg | 1.59e-2 mmHg |
| Henry's Law Constant (K _h) | 2.80e-8 atm-m ³ /mole | 2.80e-8 atm-m ³ /mole | 2.80e-8 atm-m ³ /mole |
| Octanol/Water Partition Coefficient (LogP or K _{ow}) | 3.19 to 5.92 | 5.92 | 5.92 |
| References | https://pubchem.ncbi.nlm.nih.gov/compound/101650 https://comptox.e | https://pubchem.ncbi.nlm.nih.gov/compound/23504419 | https://pubchem.ncbi.nlm.nih.gov/compound/23668548 https://comptox.e |

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|--|---|--|---|
| | pa.gov/dashboard/DTXSID70275965 | https://comptox.e pa.gov/dashboard/DTXSID20892328 | pa.gov/dashboard/DTXSID50880117 |
|--|---|--|---|

Data Source: National Center for Biotechnology Information. PubChem Database; U.S. Environmental Protection Agency. Chemistry Dashboard.

Note, these values are all computed using Quantitative Structure Activity Relationships (QSARs) and EPA's CompTox Chemicals Dashboard mentions the Data Quality of this record as "Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers".

[1](#) Form of PFECHS most likely to be found in the environment

[2](#) Form of PFECHS that is commercially available on the market

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