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Assessment of perfluorocarboxylic acids in fluorinated high-density polyethylene containers and estimation of potential non-cancer risks associated with anticipated use scenarios

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ABSTRACT

High density polyethylene (HDPE) containers are fluorinated to impart barrier properties that prevent permeation of liquid products filled in the container. The process of fluorination may result in the unintentional formation of certain per- and polyfluoroalkyl substances (PFAS), specifically perfluoroalkyl carboxylic acids (PFCAs), as impurities. This study measured the amounts of PFCAs that may be present in the fluorinated HDPE containers, which could migrate into products stored in these containers. Migration studies were also conducted using water and mineral spirits to estimate the amount of PFCAs that might be found in the products stored in these containers. The migration results were used to conservatively model potential PFCA exposures from use of six product types: indoor-sprayed products, floor products, hand-applied products, manually-sprayed pesticides, hose-end sprayed products, and agricultural (industrial) pesticides. The potential that such uses could result in a non-cancer hazard was assessed by comparing the modeled exposures to both applicable human non-cancer toxicity values and environmental screening levels. Environmental releases were also compared to aquatic and terrestrial predicted no-effect concentrations (PNECs). The results of these analyses indicated no unreasonable non-cancer risk to humans, aquatic species, and terrestrial species from PFCAs in products stored in fluorinated HDPE containers.

1. Introduction

High-density polyethylene (HDPE) containers are used for a wide variety of consumer and industrial products, such as fuel tanks, household cleaners, pesticides, and other chemical storage. These containers may be fluorinated to impart barrier properties that prevent permeation of products stored in the container. The fluorination process has been commercially used since at least the 1980s as a method to comply with US Department of Transportation container permeability standards (USDOT, 1990). In addition, the US Environmental Protection Agency (USEPA) established pesticide container standards (USEPA, 2008) that incorporate the USDOT (1990) standards by reference. HDPE container fluorination is performed using a variety of technologies including in-mold fluorination, post-mold fluorination, and post-mold plasma fluorination (Vitale et al., 2022) using different methods according to the needs of the product manufacturer. If certain impurities, such as carboxylic acids, are present in the HDPE container, the fluorination process may unintentionally create other impurities on the fluorinated surface in the form of perfluoroalkyl carboxylic acids (PFCAs) which may migrate to the liquid product contents (Vitale et al., 2022). These per- and polyfluoroalkyl substance (PFAS) impurities do not impart barrier protection and are irrelevant to the functionality of the containers.

Sulfur may also be an impurity in HDPE since it may be in the petroleum feedstock material, although sulfur impurities are typically removed in the HDPE manufacturing process because they can interfere with the polymerization reactions (Platzer, 1983; Firor and Quimby, 2001). Therefore, perfluoroalkyl sulfonic acid (PFSA) impurities are not as likely to be formed during HDPE fluorination as are PFCAs. This observation is consistent with the findings of USEPA (2022c) and Vitale

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Table 1
PFCAs of interest.

Compound abbreviation	Compound name	CASRN	Number of carbons in chain
PFBA	Perfluorobutanoic Acid	375-22-4	4
PFPeA	Perfluoropentanoic Acid	2706-90-3	5
PFHxA	Perfluorohexanoic Acid	307-24-4	6
PFHpA	Perfluoroheptanoic Acid	375-85-9	7
PFOA	Perfluorooctanoic Acid	335-67-1	8
PFNA	Perfluorononanoic Acid	375-95-1	9
PFDA	Perfluorodecanoic Acid	335-76-2	10
PFUdA	Perfluoroundecanoic Acid	2058-94-8	11
PFDoA	Perfluorododecanoic Acid	307-55-1	12
PFTrDA	Perfluorotridecanoic Acid	72629-94-8	13
PFTeDA	Perfluorotetradecanoic Acid	376-06-7	14
PFHxDA	Perflurohexadecanoic Acid	67905-19-5	16
PFODA	Perfluorooctadecanoic Acid	16517-11-6	18

et al. (2022) where PFSAs were not detected during the migration testing of fluorinated HDPE containers.

In 2020–2021, a commercial mosquito control pesticide stored in fluorinated HPDE containers was found to contain PFCAs with carbon chain lengths of four to eleven, which were presumed to have migrated from the container into the pesticide product (USEPA, 2021a; 2022a,b). Subsequent USEPA testing indicated that certain PFAS compounds may migrate from fluorinated HDPE containers to other consumer products as well (USEPA, 2022c).

The goal of this study was to evaluate the presence of PFCAs in post-mold fluorinated HDPE containers for six product types, as well as to assess the potential risk to human and ecological receptors as a result of PFCAs migrating into the products stored in such containers or as a result of release in the environment. It should be noted that fluorinated HDPE containers evaluated in this study are never used for storage of drinking water; furthermore, drinking water containers do not typically require barrier protection to prevent water permeation (P. Iyer, personal communication, August 14, 2023). Conceptual exposure models included six container use scenarios representative of potential for exposure to people and the environment, namely:

- Indoor-sprayed products (products used for cleaning or degreasing surfaces inside the home, such as household trigger-spray bathroom and kitchen cleaners),
- Floor products (liquid concentrate or spray products used to seal, deodorize or degrease carpet, hardwood, and other types of indoor flooring),
- Products directly applied by hand (products that require direct hand contact with an applicator, such as single-use furniture wipes and furniture or countertop polish or color restorer applied with a cloth or mitt),
- Manually-sprayed pesticides (indoor and outdoor pesticide trigger spray products),
- Hose-end sprayed products (products applied at the end of a hose, such as pesticides and herbicides applied to lawns and gardens), and
- Agricultural (industrial) pesticides applied by aerial spraying or ground-level fogging.

The HDPE containers selected for this study were obtained from a company who fluorinates such containers and were subjected to post-mold fluorination at the higher end of the range of levels of fluorination used for commercial and industrial products in order to yield high-end estimates of potential exposures. Exposure estimates were based on measured PFAS migration from fluorinated HDPE containers into two types of solvents believed to be representative of the contents of six types of product containers: water and mineral spirits. Water migration tests were conducted to estimate exposures and hazards from aqueous products stored in the fluorinated HDPE containers. Mineral spirits migration tests were used to estimate exposures and hazards from products containing organic chemicals, such as agricultural pesticides. The potential non-cancer hazard associated with use of the six types of products was then assessed by comparing the exposure estimates for each PFCA to the applicable non-cancer toxicity value or screening level. To ensure that this assessment was health-protective, worst-case exposure assumptions and conservative modeling parameters were used in developing the exposure estimates.

2. Methods

2.1. Extraction and migration tests to determine PFCAs of interest

This study investigated the amount of PFCAs present in post-mold fluorinated HDPE container materials using a method similar to CEN/TS 15968:2010, an aggressive extraction methodology to ensure complete extraction of all PFCAs in the sample of the fluorinated HPDE container (chip method) (Table 1). Details of this extraction procedure are provided in the supplementary information. Briefly, an approximately 1 g sample was cut from each fluorinated HDPE container. Each sample was then immersed in a methanol solution and sonicated at 60 °C for 120 min. Following centrifugation, the supernatant was prepared via solid-phase extraction and analyzed on LC/MS-MS for extractable PFCA concentrations.

In addition to extraction of samples of the fluorinated containers to determine concentrations of PFCAs in the material itself, migration studies were also performed to measure the amounts of PFCAs that may migrate from the fluorinated HDPE container to two different types of liquids that are representative of container contents. Two solvents, namely, distilled water and mineral spirits (Sunnyside Corporation, Wheeling, Illinois, Product Number 803) were used to account for products with both aqueous and organic solvent bases.

Representative containers used for the migration study included 32-ounce and 1-gallon size fluorinated HDPE containers. Each container, which had not previously been used for any purpose, was fluorinated in duplicate. Each fluorinated container was filled with distilled water or mineral spirits to their respective fill capacities and stored at 50 °C for 28 days, which are standard USDOT permeation test conditions (49 Code of Federal Regulations § 173.24(e)(3)). Samples of the distilled water and mineral spirits were then collected and shipped to a commercial laboratory (Eurofins Lancaster Environment Testing, LLC, Lancaster, PA) under chain of custody for analysis to determine the PFCA concentration using USEPA Method 537.1 with isotope dilution. The values reported herein are the averages of the concentrations from each container size (each in duplicate) subjected to the highest fluorination level.

2.2. Applicable non-cancer toxicity values and screening levels for human and ecological receptors

Established regulatory non-cancer toxicity values and screening

Table 2
Indoor-sprayed product exposures and SLCRs.

Compound	Adult indoor spray product use				Drinking water protection from exposure to surface water contamination (down the drain pathway)			Aquatic animal protection from exposure to surface water contamination (down the drain pathway)		
	Estimated PFCA concentration in product (μg/L)	Total intake dose from spraying and rinsing (mg/kg bw-day)	RfD (mg/kg bw-day)	SLCR for adult indoor spray product use	Estimated maximum surface water concentration for human drinking water (μg/L)	Drinking water concentration screening level (μg/L)	SLCR for drinking water	Estimated maximum surface water concentration for aquatic animals (μg/L)	Aquatic animal PNEC (μg/L)	SLCR for aquatic animals
PFBA	3.7E+00	4.1E-08	1.0E-03[a]	**4.1E-05**	1.2E-04	1.8E+01[a]	**6.7E-06**	9.6E-04	6.2E+02	**3.0E-05**
PFPeA	1.1E+00	1.2E-08	5.0E-04[b]	**2.4E-05**	3.7E-05	1.2E+01[b]	**3.1E-06**	2.9E-04	3.2E+01	**3.6E-06**
PFHxA	3.1E-01	3.4E-09	5.0E-04[a]	**6.8E-06**	1.0E-05	9.9E+00[a]	**1.0E-06**	8.0E-05	8.0E+01	**1.0E-06**
PFHpA	7.9E-02	8.6E-08	2.3E-05[b]	**3.7E-03**	2.6E-06	5.6E-01[b]	**4.6E-06**	2.0E-05	2.5E+01	**8.2E-07**
PFOA	2.1E-02	2.3E-10	3.0E-06[a]	**7.6E-05**	6.7E-07	6.0E-02[a]	**1.1E-05**	5.4E-06	6.7E+00	**8.0E-07**
PFNA	5.5E-03	5.9E-11	3.0E-06[a]	**2.0E-05**	1.8E-07	5.9E-02[a]	**3.0E-06**	1.4E-06	6.7E+00[d]	**2.1E-07**
PFDA	1.4E-03	1.5E-11	1.5E-05[b]	**9.7E-07**	4.4E-08	3.7E-01[b]	**1.2E-07**	3.5E-07	6.7E+00[d]	**5.2E-08**
PFUdA	7.6E-04	8.2E-12	3.0E-04[a]	**2.7E-08**	2.5E-08	6.0E+00[a]	**4.1E-09**	2.0E-07	6.7E+00[d]	**2.9E-08**
PFDoA	4.0E-04	4.4E-12	5.0E-05[a]	**8.7E-08**	1.3E-08	1.0E+00[a]	**1.3E-08**	1.0E-07	6.7E+00[d]	**1.5E-08**
PFTrDA	3.9E-04	4.2E-12	1.2E-05[b]	**3.5E-07**	1.3E-08	2.9E-01[b]	**4.3E-08**	1.0E-07	6.7E+00[d]	**1.5E-08**
PFTeDA	2.3E-04	2.5E-12	1.0E-03[a]	**2.5E-09**	7.5E-09	2.0E+01[a]	**3.7E-10**	6.0E-08	6.7E+00[d]	**8.9E-09**
PFHxDA	4.6E-04	5.1E-12	1.0E-03[c]	**5.1E-09**	1.5E-08	2.0E+01[c]	**7.5E-10**	1.2E-07	6.7E+00[d]	**1.8E-08**
PFODA	4.6E-04	5.1E-12	4.0E-02[a]	**1.3E-10**	1.5E-08	8.0E+02[a]	**1.9E-11**	1.2E-07	6.7E+00[d]	**1.8E-08**

Values in **bold** were calculated from Equation 1.
[a] USEPA (2023a).
[b] TCEQ (2023).
[c] Used PFTeDA RfD and screening level from USEPA (2023a) as surrogate for PFHxDA.
[d] Used PFOA PNEC as a surrogate.

Table 3
Floor product exposures and SLCRs.

Compound	Estimated PFCA concentration in product (μg/L)	RfD (mg/kg bw-day)	Adult floor product use		Child post-application exposure	
			Total intake dose (mg/kg bw-day)	SLCR for adult floor product use	Total intake dose (mg/kg bw-day)	SLCR for child post-application exposure
PFBA	3.7E+00	1.0E-03[a]	8.6E-07	**8.6E-04**	3.4E-06	**3.4E-03**
PFPeA	1.1E+00	5.0E-04[b]	1.1E-07	**2.2E-04**	1.0E-06	**2.0E-03**
PFHxA	3.1E-01	5.0E-04[a]	3.0E-08	**6.0E-05**	2.9E-07	**5.8E-04**
PFHpA	7.9E-02	2.3E-05[b]	3.5E-07	**1.5E-02**	7.3E-06	**3.2E-01**
PFOA	2.1E-02	3.0E-06[a]	1.0E-09	**3.3E-04**	1.9E-08	**6.3E-03**
PFNA	5.5E-03	3.0E-06[a]	2.2E-10	**7.3E-05**	5.0E-09	**1.7E-03**
PFDA	1.4E-03	1.5E-05[b]	5.5E-11	**3.7E-06**	1.3E-09	**8.7E-05**
PFUdA	7.6E-04	3.0E-04[a]	3.0E-11	**1.0E-07**	7.0E-10	**2.3E-06**
PFDoA	4.0E-04	5.0E-05[a]	1.6E-11	**3.2E-07**	3.7E-10	**7.4E-06**
PFTrDA	3.9E-04	1.2E-05[b]	1.6E-11	**1.3E-06**	3.6E-10	**3.0E-05**
PFTeDA	2.3E-04	1.0E-03[a]	9.3E-12	**9.3E-09**	2.1E-10	**2.1E-07**
PFHxDA	4.6E-04	1.0E-03[c]	1.9E-11	**1.9E-08**	4.3E-10	**4.3E-07**
PFODA	4.6E-04	4.0E-02[a]	1.9E-11	**4.8E-10**	4.3E-10	**1.1E-08**

Values in **bold** were calculated from Equation 1.
[a] USEPA (2023a).
[b] TCEQ (2023).
[c] Used PFTeDA RfD from USEPA (2023a) as a surrogate RfD for PFHxDA.

Table 4
Hand-applied product exposures and SLCRs.

Compound	Estimated PFCA concentration in product (μg/L)	RfD (mg/kg bw-day)	Total intake dose (mg/kg bw-day)	SLCR for adult product use
PFBA	3.7E+00	1.0E-03[a]	1.1E-06	**1.1E-03**
PFPeA	1.1E+00	5.0E-04[b]	2.8E-07	**5.6E-04**
PFHxA	3.1E-01	5.0E-04[a]	7.3E-08	**1.5E-04**
PFHpA	7.9E-02	2.3E-05[b]	5.1E-07	**2.2E-02**
PFOA	2.1E-02	3.0E-06[a]	2.3E-09	**7.6E-04**
PFNA	5.5E-03	3.0E-06[a]	4.1E-10	**1.4E-04**
PFDA	1.4E-03	1.5E-05[b]	1.1E-11	**7.2E-07**
PFUdA	7.6E-04	3.0E-04[a]	6.0E-12	**2.0E-08**
PFDoA	4.0E-04	5.0E-05[a]	3.2E-12	**6.4E-08**
PFTrDA	3.9E-04	1.2E-05[b]	3.2E-12	**2.7E-07**
PFTeDA	2.3E-04	1.0E-03[a]	1.8E-12	**1.8E-09**
PFHxDA	4.6E-04	1.0E-03[c]	3.6E-12	**3.6E-09**
PFODA	4.6E-04	4.0E-02[a]	3.6E-12	**9.0E-11**

Values in **bold** were calculated from Equation 1.
[a] USEPA (2023a).
[b] TCEQ (2023).
[c] Used PFTeDA RfD from USEPA (2023a) as a surrogate RfD for PFHxDA.

levels for PFCAs of interest were reviewed for use in the hazard assessment for humans and ecological receptors (Tables 2–7). USEPA has established residential soil, soil to protect groundwater, and drinking water regional screening levels (RSLs) for PFBA, PFHxA, PFOA, PFNA, PFUdA, PFDoA, PFTeDA, and PFODA (USEPA, 2023a). In accordance with the USEPA's hierarchy of human health toxicity values (USEPA, 2003), these screening levels were based on reference doses (RfDs) developed by the USEPA's Integrated Risk Information System (IRIS) program for PFBA and PFHxA, as well as minimum risk levels (MRLs) published by the Agency for Toxic Substances Disease Registry (ATSDR, 2021) for PFOA and PFNA. The USEPA has adopted RfDs from Wisconsin Department of Health Services (2020) in developing RSLs for PFUdA, PFDoDA, PFTeDA, and PFODA because the toxicity information was determined using methods similar to other accepted sources (USEPA, 2023a). In the absence of USEPA values for other PFCAs, screening levels developed by state agencies were reviewed. The Texas Commission on Environmental Quality (TCEQ, 2023) has established Protective Concentration Levels (screening levels similar to the USEPA RSLs) for residential soil, soil to protect groundwater, and drinking water for PFPeA, PFHpA, PFDA, and PFTrDA. Since established screening levels were not found for PFHxDA, the USEPA values for PFTeDA were conservatively used as surrogates to assess PFHxDA given the similarities in chemical structure. However, it is unknown whether PFHxDA elicits the same health effects as PFTeDA.

For ecological receptors, experimental predicted no-effect concentrations (PNECs) were derived from available data in the peer-reviewed literature for both aquatic (i.e., freshwater) and terrestrial (i.e., soil) organisms as described in Section 1 in the supplementary information. Consumer products such as those modeled in this risk assessment have a wide variety of use frequencies and durations. As such, chronic PNECs were conservatively used in the risk assessment to account for the upper range of potential exposure durations.

2.3. Conceptual exposure models

Each of the six product types considered in this study may be stored in a post-mold fluorinated HDPE container for consumer or industrial use. Figs. S1–S6 in the supplementary information illustrate the sources, pathways, and receptors considered in the selected conceptual exposure models for users of these products. Exposure estimation methods for each pathway and receptor are described below and in greater detail in Section 4 of the supplementary information.

Indoor-sprayed products were modeled using a bathroom spray cleaner scenario as the higher surface area and smaller room volume resulted in more conservative exposures than other product uses. Adult indoor-sprayed user exposure pathways included solvent-mediated dermal absorption, direct contact from post-application rubbing off, or incidental ingestion.

Floor products were modeled using a floor sealant based on the high mass of product used over a floor's surface area compared to other floor products. Adult floor product user exposure pathways included solvent-mediated dermal absorption, direct contact from post-application rubbing off, or incidental ingestion. Exposures to children from PFCAs in floor product surface residue were also modeled as children may have a greater proportion of their skin in contact with floors.

Products directly applied by hand were similarly modeled using a furniture polish based on the high mass of product used indoors compared to other hand-applied products. Exposure pathways for adults applying furniture polish by hand included solvent-mediated dermal absorption, direct contact from post-application rubbing off, and incidental ingestion.

Exposure pathways for adults from both manually-sprayed and hose-end sprayed pesticides included solvent-mediated dermal absorption and aerosol inhalation. Post-application pesticide exposure pathways to children included inhalation as well as hand-to-mouth and object-to-mouth incidental ingestion. In addition, risks to humans (from residential soil, groundwater, and vegetable consumption) and terrestrial animals were estimated for PFCAs in pesticides applied to soil by both manual sprayer and hose-end sprayer. While a complete exposure assessment was conducted, only the greatest modeled vegetable consumption exposures are reported here, which were to children 1–2 years old from the hose-end sprayed pesticide scenario.

Exposure pathways to adults handling agricultural pesticides applied aerially or by ground-fogger included solvent-mediated dermal absorption, aerosol inhalation, and incidental ingestion. This risk assessment also considered conservative agricultural and hose-end sprayed pesticide applications to soil, which may result in PFCA exposures to humans directly from soil and groundwater leachate. Vegetable consumption following hose-end sprayed pesticide applications to soil were also modeled. However, the vegetable consumption exposures from agricultural pesticides were not modeled as the hose-end sprayed applications to soil were greater, and thus more conservative.

2.4. Exposure models

Exposures for each product use scenario were modeled as described below. All assumptions, equations, and default inputs are described in Section 4 of the supplementary information, along with the model documentation (RIVM, 2022; USEPA, 2012; 2014, 2021b).

2.4.1. Indoor household products

For indoor household products, the RIVM Consumer Exposure (ConsExpo) model was used to estimate consumer exposures to PFCAs in non-pesticide products, including spray cleaner, floor sealant, and furniture polish for adult users of the products and children who may contact product residue post-application. ConsExpo (RIVM, 2021) is a web-based tool that has been approved and validated for use in consumer product exposure assessments intended for chemical risk characterizations by numerous international regulatory agencies. ConsExpo was used to model dermal, inhalation, and oral exposures to PFCAs for adult users of products, as well as dermal and oral exposure to children who may contact product residue.

The USEPA's Standard Operating Procedures (SOPs) for Residential Exposure Assessments ("Residential SOPs") provide guidance for estimating aggregate non-dietary exposures to ingredients in pesticide products in residential settings (USEPA, 2012). The Residential SOPs estimate (1) inhalation and dermal exposures for adult handlers during mixing, loading, and application, and (2) adult and child post-application exposures, which may include inhalation, dermal, and incidental ingestion pathways. The Residential SOP was used to estimate

Table 5
Manually-sprayed pesticide exposures and SLCRs.

Compound	Esti-mated PFCA concen-tration in product (μg/L)	RfD (mg/kg bw-day)	Adult handler pesticide use		Child post-application exposure		Est. PFCA concen-tration in soil (mg/kg dw soil)	Human protection from soil exposure		Groundwater protection from soil		Terrestrial animal protection from soil exposure	
			Total intake dose (mg/kg bw-day)	SLCR for adult handlers	Total intake dose (mg/kg bw-day)	SLCR for children post-application		Resident soil screen-ing level (mg/kg dw soil)	SLCR for resident soil	Soil to protect ground-water screening level (mg/kg dw soil)	SLCR for soil to protect ground-water	Terres-trial animal PNEC (mg/kg dw soil)	SLCR for terres-trial animals
PFBA	3.7E+00	1.0E-03[a]	9.5E-09	**9.5E-06**	1.1E-04	**1.1E-01**	7.6E-04	7.8E+01[a]	**9.8E-06**	6.5E-03[a]	**1.2E-01**	6.4E-01	**1.2E-03**
PFPeA	1.1E+00	5.0E-04[b]	2.9E-09	**5.8E-06**	3.3E-05	**6.5E-02**	2.3E-04	3.3E+01[b]	**7.0E-06**	4.2E-02[b]	**5.5E-03**	5.6E-01	**4.1E-04**
PFHxA	3.1E-01	5.0E-04[a]	7.9E-10	**1.6E-06**	8.9E-06	**1.8E-02**	6.3E-05	3.2E+01[a]	**2.0E-06**	2.4E-03[a]	**2.6E-02**	8.1E-01	**7.8E-05**
PFHpA	7.9E-02	2.3E-05[b]	2.0E-10	**8.8E-06**	2.3E-06	**9.9E-02**	1.6E-05	1.5E+00[b]	**1.1E-05**	4.6E-03[b]	**3.5E-03**	1.0E-03	**1.6E-02**
PFOA	2.1E-02	3.0E-06[a]	5.3E-11	**1.8E-05**	6.0E-07	**2.0E-01**	4.2E-06	1.9E-01[a]	**2.2E-05**	9.1E-04[a]	**4.7E-03**	5.2E-01	**8.2E-06**
PFNA	5.5E-03	3.0E-06[a]	1.4E-11	**4.6E-06**	1.5E-07	**4.9E-02**	1.1E-06	1.9E-01[a]	**5.9E-06**	2.5E-04[a]	**4.5E-03**	5.2E-01[d]	**2.2E-06**
PFDA	1.4E-03	1.5E-05[b]	3.5E-12	**2.3E-07**	3.3E-08	**2.2E-03**	2.8E-07	9.9E-01[b]	**2.8E-07**	2.2E-02[b]	**1.3E-05**	5.2E-01[d]	**5.3E-07**
PFUdA	7.6E-04	3.0E-04[a]	1.9E-12	**6.4E-09**	1.8E-08	**6.0E-05**	1.5E-07	1.9E+01[a]	**8.1E-09**	4.5E-02[a]	**3.4E-06**	5.2E-01[d]	**3.0E-07**
PFDoA	4.0E-04	5.0E-05[a]	1.0E-12	**2.0E-08**	9.4E-09	**1.9E-04**	8.1E-08	3.2E+00[a]	**2.5E-08**	1.7E-01[a]	**4.8E-07**	5.2E-01[d]	**1.6E-07**
PFTrDA	3.9E-04	1.2E-05[b]	9.9E-13	**8.2E-08**	9.3E-09	**7.8E-04**	7.9E-08	6.1E-01[b]	**1.3E-07**	6.1E-02[b]	**1.3E-06**	5.2E-01[d]	**1.5E-07**
PFTeDA	2.3E-04	1.0E-03[a]	5.9E-13	**5.9E-10**	5.6E-09	**5.6E-06**	4.7E-08	6.3E+01[a]	**7.5E-10**	9.4E+00[a]	**5.0E-09**	5.2E-01[d]	**9.1E-08**
PFHxDA	4.6E-04	1.0E-03[c]	1.2E-12	**1.2E-09**	1.1E-08	**1.1E-05**	9.4E-08	6.3E+01[c]	**1.5E-09**	9.4E+00[c]	**1.0E-08**	5.2E-01[d]	**1.8E-07**
PFODA	4.6E-04	4.0E-02[a]	1.2E-12	**2.9E-11**	1.2E-08	**3.0E-07**	9.4E-08	2.5E+03[a]	**3.8E-11**	2.2E+02[a]	**4.3E-10**	5.2E-01[d]	**1.8E-07**

Values in **bold** were calculated from Equation 1.

[a] USEPA (2023a).

[b] TCEQ (2023).

[c] Used PFTeDA RfD and screening levels from USEPA (2023a) as surrogates for PFHxDA.

[d] Used PFOA PNEC as a surrogate.

Table 6
Hose-end sprayed product exposures and SLCRs.

Compound	Esti-mated PFCA concen-tration in product (µg/L)	RfD (mg/kg bw-day)	Adult handler use		Child post-application exposure		Est. PFCA concen-tration in soil (mg/kg dw soil)	Application to soil				
			Total intake dose (mg/kg bw-day)	SLCR for adult handlers	Total intake dose (mg/kg bw-day)	SLCR for children post-application		SLCR for resident soil[d]	SLCR for soil to protect ground-water[e]	SLCR for terrestrial animals[f]	Total dose from vegetable consumption (mg/kg-day)	SLCR for vegetable consumption[g]
PFBA	3.7E+00	1.0E-03[a]	3.2E-09	**3.2E-06**	7.2E-08	**7.2E-05**	2.5E-07	**3.2E-09**	**3.9E-05**	**3.9E-07**	2.6E-07	**2.6E-04**
PFPeA	1.1E+00	5.0E-04[b]	9.8E-10	**2.0E-06**	2.2E-08	**4.4E-05**	7.7E-08	**2.3E-09**	**1.8E-06**	**1.4E-07**	1.3E-08	**2.5E-05**
PFHxA	3.1E-01	5.0E-04[a]	2.7E-10	**5.4E-07**	6.0E-09	**1.2E-05**	2.1E-08	**6.5E-10**	**8.7E-06**	**2.6E-08**	5.2E-09	**1.0E-05**
PFHpA	7.9E-02	2.3E-05[b]	6.9E-11	**3.0E-06**	1.5E-09	**6.7E-05**	5.4E-09	**3.6E-09**	**1.2E-06**	**5.4E-06**	1.8E-08	**7.9E-04**
PFOA	2.1E-02	3.0E-06[a]	1.8E-11	**6.0E-06**	4.0E-10	**1.3E-04**	1.4E-09	**7.4E-09**	**1.5E-06**	**2.7E-09**	1.0E-10	**3.4E-05**
PFNA	5.5E-03	3.0E-06[a]	4.7E-12	**1.6E-06**	1.1E-10	**3.5E-05**	3.7E-10	**1.9E-09**	**1.5E-06**	**7.1E-10**	1.2E-10	**4.0E-05**
PFDA	1.4E-03	1.5E-05[b]	1.2E-12	**7.9E-08**	2.6E-11	**1.8E-06**	9.2E-11	**9.3E-11**	**4.2E-09**	**1.8E-10**	1.3E-12	**8.8E-08**
PFUdA	7.6E-04	3.0E-04[a]	6.6E-13	**2.2E-09**	1.5E-11	**4.9E-08**	5.1E-11	**2.7E-12**	**1.1E-09**	**9.8E-11**	5.9E-13	**2.0E-09**
PFDoA	4.0E-04	5.0E-05[a]	3.5E-13	**6.9E-09**	7.7E-12	**1.5E-07**	2.7E-11	**8.4E-12**	**1.6E-10**	**5.2E-11**	4.6E-12	**9.2E-08**
PFTrDA	3.9E-04	1.2E-05[b]	3.4E-13	**2.8E-08**	7.6E-12	**6.3E-07**	2.6E-11	**4.3E-11**	**4.3E-10**	**5.1E-11**	3.2E-12	**2.7E-07**
PFTeDA	2.3E-04	1.0E-03[a]	2.0E-13	**2.0E-10**	4.5E-12	**4.5E-09**	1.6E-11	**2.5E-13**	**1.7E-12**	**3.0E-11**	3.3E-14	**3.3E-11**
PFHxDA	4.6E-04	1.0E-03[c]	4.0E-13	**4.0E-10**	9.0E-12	**9.0E-09**	3.1E-11	**5.0E-13**	**3.3E-12**	**6.0E-11**	7.2E-13	**7.2E-10**
PFODA	4.6E-04	4.0E-02[a]	4.0E-13	**1.0E-11**	9.0E-12	**2.2E-10**	3.1E-11	**1.2E-14**	**1.4E-13**	**6.0E-11**	8.2E-13	**2.0E-11**

Values in **bold** were calculated from Equation 1.

[a] USEPA (2023a).

[b] TCEQ (2023).

[c] Used PFTeDA RfD and screening levels from USEPA (2023a) as surrogates for PFHxDA.

[d] Resident soil screening levels listed in Tables 5 and 7.

[e] Soil to protect groundwater screening levels listed in Tables 5 and 7.

[f] Terrestrial animal PNECs listed in Tables 5 and 7.

[g] RfDs used in vegetable consumption SLCRs.

Table 7
Agricultural aerial/ground fogger pesticide exposures and SLCRs.

Compound	Esti-mated PFCA concen-tration in product (μg/L)	RfD (mg/kg bw-day)	Adult handler pesticide use		Est. PFCA concen-tration in soil (mg/kg dw soil)	Human protection from soil exposure		Groundwater protection from soil		Terrestrial animal protection from soil exposure	
			Total intake dose (mg/kg bw-day)	SLCR for adult handlers		Resident soil screen-ing level (mg/kg dw soil)	SLCR for resident soil	Soil to protect ground-water screening level (mg/kg dw soil)	SLCR for soil to protect ground-water	Terrestrial animal PNEC (mg/kg dw soil)	SLCR for terrestrial animals
PFBA	1.56E-01	1.0E-03[a]	2.2E-10	**2.2E-07**	2.4E-11	7.8E+01[a]	**3.0E-13**	6.5E-03[a]	**3.6E-09**	6.4E-01	**3.7E-11**
PFPeA	3.9E-02	5.0E-04[b]	5.4E-11	**1.1E-07**	5.9E-12	3.3E+01[b]	**1.8E-13**	4.2E-02[b]	**1.4E-10**	5.6E-01	**1.1E-11**
PFHxA	3.9E-02	5.0E-04[a]	5.4E-11	**1.1E-07**	5.9E-12	3.2E+01[a]	**1.8E-13**	2.4E-03[a]	**2.5E-09**	8.1E-01	**7.3E-12**
PFHpA	3.9E-02	2.3E-05[b]	5.4E-11	**2.3E-06**	5.9E-12	1.5E+00[b]	**3.9E-12**	4.6E-03[b]	**1.3E-09**	1.0E-03	**5.9E-09**
PFOA	3.9E-02	3.0E-06[a]	5.4E-11	**1.8E-05**	5.9E-12	1.9E-01[a]	**3.1E-11**	9.1E-04[a]	**6.5E-09**	5.2E-01	**1.1E-11**
PFNA	3.9E-02	3.0E-06[a]	5.4E-11	**1.8E-05**	5.9E-12	1.9E-01[a]	**3.1E-11**	2.5E-04[a]	**2.4E-08**	5.2E-01[d]	**1.1E-11**
PFDA	3.9E-02	1.5E-05[b]	5.4E-11	**3.6E-06**	5.9E-12	9.9E-01[b]	**5.9E-12**	2.2E-02[b]	**2.7E-10**	5.2E-01[d]	**1.1E-11**
PFUdA	3.9E-02	3.0E-04[a]	5.4E-11	**1.8E-07**	5.9E-12	1.9E+01[a]	**3.1E-13**	4.5E-02[a]	**1.3E-10**	5.2E-01[d]	**1.1E-11**
PFDoA	3.9E-02	5.0E-05[a]	5.4E-11	**1.1E-06**	5.9E-12	3.2E+00[a]	**1.8E-12**	1.7E-01[a]	**3.5E-11**	5.2E-01[d]	**1.1E-11**
PFTrDA	3.9E-02	1.2E-05[b]	5.4E-11	**4.5E-06**	5.9E-12	6.1E-01[b]	**9.7E-12**	6.1E-02[b]	**9.7E-11**	5.2E-01[d]	**1.1E-11**
PFTeDA	3.9E-02	1.0E-03[a]	5.4E-11	**5.4E-08**	5.9E-12	6.3E+01[a]	**9.3E-14**	9.4E+00[a]	**6.3E-13**	5.2E-01[d]	**1.1E-11**
PFHxDA	3.9E-02	1.0E-03[c]	5.4E-11	**5.4E-08**	5.9E-12	6.3E+01[c]	**9.3E-14**	9.4E+00[c]	**6.3E-13**	5.2E-01[d]	**1.1E-11**
PFODA	3.9E-02	4.0E-02[a]	5.4E-11	**1.4E-09**	5.9E-12	2.5E+03[a]	**2.4E-15**	2.2E+02[a]	**2.7E-14**	5.2E-01[d]	**1.1E-11**

Values in **bold** were calculated from Equation 1.
[a] USEPA (2023a).
[b] TCEQ (2023).
[c] Used PFTeDA RfD and screening levels from USEPA (2023a) as surrogates for PFHxDA.
[d] Used PFOA PNEC as a surrogate.

exposure to adult handlers applying a ready-to-use trigger-spray pesticide product used in an indoor environment for perimeter/spot/bedbug treatment (coarse application), as well as to estimate exposure to adults and children who may contact post-application product residue.

2.4.2. Outdoor household products

Potential consumer PFCA exposures to outdoor household pesticide products applied with a hose-end sprayer were conservatively modeled using the USEPA Residential SOPs for both liquid concentrate and ready-to-use hose-end sprayer products applied to gardens/trees and lawns/turfs, totaling four separate scenarios. Applications to lawns/turfs yielded the greatest estimated exposures and are presented below. Exposure estimates were developed for adult handlers, as well as adults and children who may contact product residue outdoors post-application.

2.4.3. Agricultural pesticide products

Workers mixing, loading, and applying agricultural (industrial) pesticide products outdoors may potentially be exposed to PFCAs that have migrated from the post-mold fluorinated HDPE container to the product. Similar to the Residential SOPs, the USEPA Standard Operating Procedures for Occupational Pesticide Exposure ("Occupational SOPs") are based on the worker activity (e.g., mixing/loading and applicator), formulation type, application method, and application type. Occupational exposures to outdoor pesticides mixed/loaded and applied via aerial spraying or ground-level truck-mounted fogging were modeled using the Occupational SOPs.

2.4.4. Exposure from contaminated product release to soil

PFCAs remaining in soil after outdoor product use could potentially be incidentally ingested by people or terrestrial organisms that contact the soil. These compounds may also potentially migrate to groundwater that is used for human drinking water supply. Conservative estimates were developed for PFCAs in soil following outdoor application of hose-end and manual spray products as well as outdoor agricultural pesticide use. This exposure model was based on mass balance principles of a release in a non-site-specific location.

This assessment included a conservative estimate of PFCA exposure through ingestion of home-grown vegetables following release to soil. The estimates reported herein were based on the scenario resulting in the most highly exposed group, children 1–2 years old. The example product used for this scenario was a hose-end spray product applied to a home-grown garden as it also resulted in the greatest modeled exposures.

2.4.5. Exposure from contaminated product release to surface water via wastewater treatment effluent

If PFCAs are present in some indoor consumer products, such as bathroom spray cleaners, they may be transported down the drain to a wastewater treatment plant (WWTP) and into the effluent where they may be available for intake by humans or uptake by aquatic species downstream of the discharge point. The USEPA's Exposure and Fate Assessment Screening Tool (E-FAST) (USEPA, 2014) was used to conservatively estimate potential exposures resulting from these down-the-drain releases.

2.5. Assessment of non-cancer hazard

The potential for any exposures to pose an unacceptable non-cancer

hazard was assessed by calculating the ratio of the estimated concentration or dose to established non-cancer toxicity values or screening levels according to Equation (1). This ratio was given the term "screening level comparison ratio" or SLCR. SLCRs less than or equal to 1 indicated no unreasonable risk for the given exposure scenario.

$$\text{SLCR} = \frac{\text{Estimated concentration or dose}}{\text{Human or ecological toxicity value or screening level}} \quad \text{Equation 1}$$

3. Results and discussion

3.1. Results from extraction of fluorinated HDPE container

The extraction (chip method) results are provided in Table S1 in the supplementary information. Only PFBA, PFPeA, PFHxA, PFHpA, and PFOA were detected in the methanolic extracts. However, only PFBA and PFPeA were found above the limit of quantitation, and 62% of the results were below the detection limit.

3.2. Results from migration studies

Table S2 in the supplementary information provides the PFCA concentrations measured in the migration tests with distilled water. The concentrations from the fluorination level yielding the greatest PFCA concentrations were used for this risk assessment. Several PFCA species were non-detect in the distilled water samples (<62% detected). In the case of mineral spirit samples, all PFCA species were non-detect. To model exposures, all non-detected PFCAs were conservatively assumed to be present at a concentration equal to one half of the analytical detection limit for the purposes of this risk assessment. The supplementary information (Section 2) provides additional details about the migration test results.

There were some samples with detections of PFNA, PFDA, PFUdA, PFDoA, and PFTrDA in the water migration tests, but none of these particular PFCAs were detected in the HDPE extraction studies. These contradictions in analytical results may be attributed to the differences between sample matrices and laboratory analytical methods. In fact, the detection limits for the methanol extracts ranged from 0.11 to 1.8 μg/kg (ppb) plastic, whereas the detection limit for the water samples ranged from 0.00044 to 0.00097 μg/kg water (0.44–0.97 ng/L, ppt). PFAS analytical detection limits for clean water are generally more sensitive than for other matrices. For example, USEPA (2021c) explained that matrix interference is expected when analyzing PFAS in mineral spirits. Nevertheless, Table S3 demonstrates that the mass of PFCAs in the methanol extracts exceeded the mass of PFCAs in the water migration tests, even when assuming a concentration of half the detection limit for all non-detect results. These results were consistent with those reported by Vitale et al. (2022) for methanol extraction test results for PFCAs from post-mold fluorinated containers (Set 3 in the study), where all of the concentrations were reported with a data qualifier of some type; most were given a 'J' flag indicating the chemical was detected at a concentration between the limit of detection and limit of quantification, or were non-detected, or the detection was uncertain. These results were also generally consistent with Whitehead and Peaslee (2023) who reported maximum methanolic extraction test results of 23 μg/kg plastic for PFBA, which were within an order of magnitude as those reported in this study, as well as decreasing concentrations for PFCAs as the chain length increased.

The detection limits for the mineral spirits samples (0.10–0.40 μg/kg) were similar to those of the methanol extracts. However, every sample in the mineral spirits migration tests was below the detection limit, indicating the lower affinity for PFCAs to migrate from the fluorinated HDPE material to the mineral spirits.

3.3. Estimated exposures and SLCRs

Tables 2–7 summarize the conservatively estimated exposures and SLCRs for each of the product use scenarios. In every exposure scenario, even with the use of worst-case assumptions and inputs and imputing half the detection limit for all non-detected results, the SLCRs were <1.0, and many of them were far less than 1.0 demonstrating that there are no unacceptable non-cancer hazards. This result is expected given that PFCAs are generated only from trace impurities in the HDPE materials, rather than intentionally added to the containers. In addition, many PFCAs, especially the longer-chain compounds (Table S2 in the supplementary information), were not detected in the water migration tests.

These findings agree with other assessments of PFAS in consumer products using risk ratio approaches. An early study by Washburn et al. (2005) estimated PFOA margins of exposure ranging from 10^4 to 10^{11} for consumer use of textiles, carpets, and thread seal tape, indicating no unreasonable risk to sensitive populations. Another risk assessment on use of cosmetics (body lotion, foundation, and concealer) containing certain PFCAs resulted in margins of exposure of 34 to 1.1 million, even when assuming 70% dermal absorption of PFCAs (Danish Environmental Protection Agency, 2018). Massarsky et al. (2022) similarly concluded that the presence of perfluorooctanesulfonic acid and PFBA in dental night guards were unlikely to pose a health concern and constituted a negligible contribution to environmental PFAS.

The risk assessment presented herein focused on the non-cancer effects of PFCAs. The carcinogenic potential of PFAS in humans, especially PFOA, has been subject to controversy within the scientific community, as significant limitations and inconsistencies have been identified in the body of evidence for epidemiological studies. For example, Steenland and Winquist (2021) concluded "the evidence for an association between cancer and PFAS remains sparse" and that "epidemiologic studies of PFAS have been informative, but not entirely conclusive." Specifically, the authors noted several limitations and flaws in the design and methods of these epidemiological studies, which in some instances, can "lead to questionable associations" (Steenland and Winquist, 2021). An independent assessment of the epidemiological evidence base is currently underway to evaluate the overall strength of the evidence concerning PFOA exposures and cancer in humans. In addition, certain cancer endpoints in rodent models have been shown to have limited to no relevance to humans, including liver tumors and Leydig cell testicular tumors reported in rats following chronic exposure to PFOA (Klaunig et al., 2012; Corton et al., 2018; Steinbach et al., 2015). The animal evidence base for PFOA and cancer will also be reviewed and assessed for relevance to human health risk assessment. These weight of evidence assessments for cancer and PFOA exposure will be the subject of a separate publication.

3.4. Study limitations

Uncertainties are inherent in all risk assessments and, as is standard practice for screening level assessments, worst-case assumptions and input parameters were used to ensure that non-cancer hazard was not underestimated. The toxicity values used in this assessment were extrapolated from studies using conservative approaches. Additionally, as there were no toxicity values available for PFHxDA, we used USEPA's RfD and RSLs for PFTeDA as surrogates. Likewise, the ecological toxicity literature for compounds with carbon chain lengths greater than that of PFOA was sparse. Therefore, the ecological toxicity levels for PFOA were conservatively used for those longer-chain compounds, which also introduced uncertainty in the risk assessment.

The exposure estimates were based on the migration testing data for the highest fluorination level. This, coupled with the conservative, simplifying assumptions used in the exposure modeling, may have resulted in overestimations of potential exposure. Information regarding the potential dermal absorption of PFOA from a liquid product is sparse,

and the assumption of 50% absorption is likely to overestimate exposure potential. In fact, Abraham and Monien (2022) reported PFOA dermal absorption of only 1.6%. Another example of conservative assumptions used in this risk assessment are the conservative default parameters embedded in the PFCA soil to protect groundwater screening levels (RSLs). In particular, these screening levels assume that the contamination source is infinite, contaminants are uniformly distributed throughout the zone of contamination, and the contamination extends from the surface to the water table (USEPA, 2023c). However, these highly conservative assumptions are not likely to be typical of the scenarios considered herein that release PFCAs to soil. This risk assessment also assumed that a WWTP would not remove PFCAs, and the PFCAs in WWTP effluent released into surface waters remain in the aqueous phase. However, as with soil, PFCA interactions with environmental waters are complex and depend on several factors, such as hydrophobic interactions, electrostatic forces, pH, steric constraints, solution ionic composition, PFAS molar volumes, and co-contaminants. Hydrophilic short-chain PFAS tend to remain in surface waters, whereas hydrophobic PFCAs tend to accumulate in sediments (Bai and Son, 2021). Higher concentrations of PFCAs in sediments are likely because of the higher hydrophobicity and sorption affinity to organic matter. Nevertheless, given the very low concentrations in these media predicted by worst-case modeling, these complexities in soil, water, and sediment interactions are not expected to significantly affect the conclusions reached in this assessment.

PFCAs in hose-end sprayer products applied to soil in a household vegetable garden were modeled for uptake by vegetables using the method given by USEPA (2005). This method requires use of PFCA bioconcentration factors (BCFs). For PFCAs that did not have empirical BCFs available, BCFs were estimated according to log K_{OW} values. However, this approach has been reported as inappropriate for PFAS compounds, which have been observed to bind to proteins, rather than to partition to lipids or water (EFSA CONTAM Panel, 2020; Rayne and Forest, 2009). PFAS can possess both hydrophilic and hydrophobic properties, which make K_{OW} a problematic indicator of true partitioning behavior (Chelcea et al., 2020). In addition, because many PFAS are acids, they are in their ionic form in water, making them unsuitable for physicochemical property models meant for application to neutral species (Chelcea et al., 2020; USEPA, 2016). Nevertheless, the modeled vegetable uptake for all LCPFACs with both empirical and predicted BCFs resulted in SLCRs well below 1.0 for human vegetable consumption.

USEPA (2023b) has proposed an RfD of 3×10^{-8} mg/kg-day for PFOA as part of its draft maximum contaminant level (MCL) drinking water regulation. This proposed value is lower than the current RfD used in this assessment (3×10^{-6} mg/kg-day) by a factor of 100. If the proposed RfD were to be used for this risk assessment, the related PFOA RSLs for humans would likewise be reduced by a factor of 100 assuming that other factors used in deriving screening levels would remain unchanged. In all but one scenario, using the proposed PFOA RfD would also yield SLCRs below 1.0; the single scenario that would result in an SLCR greater than 1.0 is for children with direct contact to 0.5-gallon of pesticides manually sprayed indoors immediately following application (SLCR = 20). However, there is inherent uncertainty in the proposed RfD, which includes an assessment factor of 10 to account for human variability. Furthermore, this risk assessment included highly conservative exposure assumptions, including a 50% dermal absorption factor, although Abraham and Monien (2022) reported PFOA dermal absorption of only 1.6% as noted above. Considering the low likelihood of this scenario, the uncertainty in the proposed RfD, and the understanding that this risk assessment used a conservative screening-level approach, this relatively elevated SLCR would not necessarily indicate an unreasonable risk given the highly conservative underlying assumptions.

4. Conclusions

This study indicates that consumers may potentially be exposed to PFCAs that may migrate into liquid products stored in fluorinated HDPE containers. However, importantly, the SLCRs for all use scenarios and products are well below 1.0, demonstrating that such products and uses do not pose an unacceptable non-cancer hazard even with all of the many worst-case assumptions and inputs used in this assessment. Similarly, worst-case modeling indicates that PFCA concentrations potentially released to the environment from fluorinated HDPE container product use do not pose an unacceptable non-cancer hazard to humans, aquatic species, or terrestrial animals.

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CRediT authorship contribution statement

LeeAnn Racz: Conceptualization, Investigation, Methodology, Writing – original draft. **Alison Gauthier:** Data curation, Formal analysis, Validation. **Jennifer Bare:** Data curation, Formal analysis, Validation. **Melissa Heintz:** Investigation, Validation. **David Feifarek:** Investigation. **Stephanie Kennedy:** Investigation. **Julie Panko:** Conceptualization, Investigation, Methodology, Supervision, Writing – review & editing.

Declaration of competing interest

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Data availability

Data will be made available on request.

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Appendix A. Supplementary data

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