



Effect of short-term sample storage and preparatory conditions on losses of 18 per- and polyfluoroalkyl substances (PFAS) to container materials

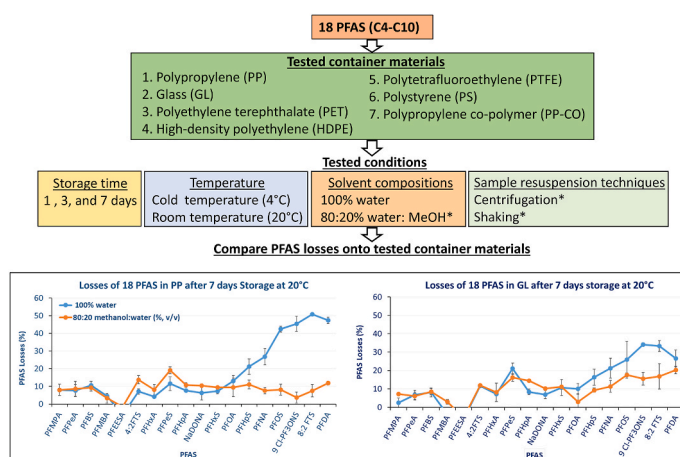
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HIGHLIGHTS

- Highest losses of long-chain PFAS in aqueous solution observed onto polypropylene.
- Sorption losses of long-chain PFAS decreased in 80:20 water:methanol (% v/v).
- Sorption losses of PFAS with temperature were dependent on the solvent composition.
- First study to report sorption losses of PFAS ether acids to 7 container materials.

GRAPHICAL ABSTRACT



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ABSTRACT

There is a lack of agreement on a suitable container material for per- and polyfluoroalkyl substances (PFAS) analysis, particularly at trace levels. In this study, the losses of 18 short- and long-chain (C4–C10) PFAS to commonly used labware materials (high-density polyethylene (HDPE), polypropylene (PP), polystyrene (PS), polypropylene co-polymer (PPCO), polyethylene terephthalate (PET), polytetrafluoroethylene (PTFE), and glass were investigated. The influence of sample storage and preparation conditions, i.e., storage time, solvent composition, storage temperatures (4 °C and 20 °C), and sample agitation techniques (shaking and centrifugation) on PFAS losses to the container materials were investigated. The results showed higher losses for most of the considered PFAS (up to 50.9%) in 100% aqueous solutions after storage for 7 days regardless of the storage temperature compared to those after 3 days. Overall, the order of losses to different materials varied for individual PFAS, with the highest losses of long-chain PFAS observed to PP and HDPE after 7-day storage at room temperature. The addition of methanol to aqueous PFAS solutions reduced the losses of long-chain PFAS to all tested materials. The use of sample centrifugation and shaking did not influence the extent of losses for most of the PFAS in 80:20 water:methanol (% v/v) to container materials except for 8:2 fluorotelomer sulfonic acid (8:2 FTS), 9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid (9Cl-PF3ONS), perfluorodecanoic acid (PFDA) and 4:2

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fluorotelomer sulfonic acid (4:2 FTS). This study demonstrates lower losses of both long- and short-chain PFAS to glass and PET. It also highlights the need for caution when deciding on sample preparatory steps and storage during the analysis of PFAS.

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are chemicals widely used in a broad range of consumer products and industrial applications due to their hydrophobic and oleophobic properties (Glüge et al., 2020). These properties also contribute to the persistent nature of PFAS in the environment and potential toxicity, leading to their recognition as legacy and new emerging contaminants (ECs) (Brase et al., 2021; Fry and Power, 2017). PFAS have been manufactured since the 1940s, and as early as 1970s perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) (legacy PFAS) were identified as pollutants (Klingelhöfer et al., 2024; Glüge et al., 2020). In the early 2000s, PFAS were detected in a variety of environmental matrices, and next generation (emerging) PFAS were designed and manufactured (ITRC, 2020). Consequently, several analytical methods have been developed to facilitate the analysis of legacy and emerging PFAS in various environmental compartments, including air, water, soil, and biota (Ahmadireskety et al., 2021; Folorunsho et al., 2023; Kourtchev et al., 2022; US EPA, 2024). These analytical methods help to determine PFAS occurrence, fate, and environmental transport. They also aid the assessment of PFAS risks and toxicity and provide strategies for their remediation in the environment (Nawaz and Sengupta, 2019; Selvaraj et al., 2021).

The analysis of PFAS in environmental matrices is generally a multistep process, which includes sample collection, storage, preparation and analysis. These steps have been reported to influence accurate measurements of PFAS (Shoemaker and Dan, 2020; Singh et al., 2022; Winchell et al., 2021), which is potentially due to the adsorption or/and desorption of these chemicals onto/from the surface of labware materials, and subsequently decreasing or increasing their analytical concentrations (Kumar et al., 2022; Winchell et al., 2021). A range of labware materials including glass (GL), polypropylene (PP), and high-density polyethylene (HDPE) has been used for the analysis of PFAS (Folorunsho et al., 2023; Ng et al., 2020; Sanan and Magnuson, 2020; US EPA, 2019; US EPA, 2024). The chemical and physical properties of these materials as well as those of PFAS, contribute to the rate of their adsorption losses via electrostatic and hydrophobic interactions with the labware material surface (Kumar et al., 2022; Lyu et al., 2022). Generally, electrostatic interaction takes place between the ionic functional group of PFAS molecules and those of the labware material surfaces such as the silanol group for GL surfaces, while hydrophobic (dispersion) interactions take place between nonpolar long-chain PFAS such as PFOS and nonpolar polymer chain of the container materials (Shafique et al., 2017; Zenobio et al., 2022).

Despite chemical stability of PFAS under environmental conditions, several factors such as solvent composition, sample storage time and temperature can influence PFAS adsorption onto the labware material surface. For instance, Point et al. (2019) reported greater adsorption of long-chain PFAS onto GL vials for a solution containing water and methanol at 75:25 (% v/v) compared to the same solvents with a composition of 25:75 (% v/v). The authors recommended using borosilicate GL because of its more inert crystalline solid state network when preparing PFAS with the latter solvent composition. Sample storage time has also been reported to be critical for PFAS adsorption losses. In this respect, Lenka et al. (2023) have shown that the increase in storage time influenced the rate of ultrashort-chain PFAS (i.e., perfluorobutanoic acid (PFBA) and perfluoropropionic acid (PFPrA)) adsorption onto GL and PP surfaces.

Therefore, the guidelines on the appropriate material for collecting and storing PFAS containing samples have been proposed by environmental agencies such as the United States Environmental Protection

Agency (US EPA) (Shoemaker and Dan, 2020). The US EPA recommends using PP and HDPE materials for sampling and analysis of PFAS (Shoemaker and Dan, 2020; US EPA, 2020). Moreover, the US EPA 533 and EPA 573.1 methods advise to avoid the use of containers made of GL for sample storage and preservation due to the adsorption of PFAS onto the sample container walls (Shoemaker and Dan, 2020; US EPA, 2019). As a result, numerous studies have adopted the use of PP for the sampling and storage of PFAS-containing samples (Chiaia-Hernandez et al., 2012; Lath et al., 2019; Mazzoni et al., 2015; Sanan and Magnuson, 2020; Valsecchi et al., 2015). The current recommendation by the US EPA 1633 method is to use HDPE only for sampling of PFAS in the environment (US EPA, 2024).

Meanwhile, more recent studies show that PP also adsorbs PFAS (Lath et al., 2019; Lenka et al., 2023; Söregård et al., 2020; Zenobio et al., 2022). For example, Lath et al. (2019), examined several filters and centrifuge tubes made from PP, polystyrene (PS), polycarbonate (PC) and GL materials for the loss of PFOA from aqueous solutions. Their results demonstrated that the lowest PFAS loss was for centrifuge tubes made of GL, while PP had the most significant adsorption loss. Another related study by Kleiner et al. (2021) evaluated adsorptive losses of various PFAS onto subsampling bottles made of silanised GL, PP and HDPE and showed no conclusive evidence to suggest an ideal bottle material for environmental sampling in terms of limiting PFAS adsorption. Moreover, Zenobio et al. (2022) examined the adsorption of a PFAS mixture containing six analytes including PFBA, PFOA, PFOS, hexafluoropropylene oxide dimer acid (HFPO-DA), perfluorobutanesulfonic acid (PFBS), and perfluorooctanesulfonamide (FOSA) onto container materials including PP, GL, PS, polyethylene (PET), and HDPE. In the latter study, similar to the results from Lath et al. (2019), a decrease in PFAS adsorption trend for tested container materials in the following order was reported: PP > HDPE > PET > GL > PS. These studies suggest that depending on the analyte of interest, labware from a specific material must be used to reduce uncertainties associated with PFAS losses during sample handling.

Environmental monitoring of PFAS generally involves the transport of samples from monitoring sites to a lab, and their storage, often at different temperatures and materials prior to analysis, which may influence the integrity of the samples and compromise the results of analysis (Kato et al., 2013). Considering insufficient and conflicting information on the suitability of the labware materials in the literature for PFAS analysis, the aims of this work were (1) to assess losses of an extensive number of PFAS (18 species) to labware made from commonly used materials, i.e., PP, GL, polytetrafluoroethylene (PTFE), PS, polypropylene co-polymer (PPCO), PET and HDPE, and (2) to assess several factors that might influence losses of organic analytes onto labware. These include examining the effect of sample storage temperature, sample solvent composition, storage time and sample agitation techniques (i.e., centrifugation and shaking) on PFAS adsorption to labware materials. Understanding the above factors are essential for ensuring data reliability, especially when evaluating quality assurance (QA), assessing and managing risks associated with PFAS pollution and exposure.

2. Materials and methods

2.1. Chemicals and materials

The following chemicals and reagents were used in this study: EPA-533PAR standard mixture containing 25 PFAS: PFBA; perfluoro-3-methoxypropanoic acid (PFMPA); perfluoropentanoic acid (PFPeA);

perfluoro-4-methoxybutanoic acid (PFMBA); perfluoro (2-ethoxyethane) sulfonic acid (PFEESA); perfluorohexanoic acid (PFHxA); perfluoroheptanoic acid (PFHpA); PFOA; perfluorononanoic acid (PFNA); perfluorodecanoic acid (PFDA); perfluoroundecanoic acid (PFUnDA); perfluorododecanoic acid (PFDoA); HFPO-DA; perfluorobutane sulfonic acid (L-PFBs); perfluoropentanesulfonate (L-PFPeS); perfluorohexane sulfonic acid (L-PFHxS); perfluoroheptanesulfonate (PFHpS); PFOS; 11-chloroicosafuoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS), perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid) (9Cl-PF3ONS); 4:2 fluorotelomer sulfonate (4:2 FTS); 6:2 fluorotelomer sulfonic acid (6:2 FTS); 8:2 fluorotelomer sulfonate (8:2 FTS), sodium dodecafluoro-3H-4, 8-dioxananoate (NaDONA) and perfluoro-3,6-dioxahexanoic acid (3,6-OPFHxA) at concentrations of 0.5 µg/mL, and EPA-533ES isotope dilution standard mixture containing 16 mass labelled (¹³C) PFAS: perfluorobutane sulfonic acid, ¹³C₃ (M3PFBS); perfluorohexane sulfonic acid, ¹³C₃ (M3PFHxS); perfluorooctane sulfonic acid, ¹³C₈ (M8PFOS); perfluorobutanoic acid, ¹³C₄ (M4PFBA); perfluoropentanoic acid, ¹³C₅ (M5PFPeA); perfluorohexanoic acid, ¹³C₅ (M5PFHxA); perfluoroheptanoic acid, ¹³C₄ (M4PFHpA); perfluorooctanoic acid, ¹³C₈ (M8PFOA); perfluorononanoic acid, ¹³C₉ (M9PFNA); perfluorodecanoic acid, ¹³C₆ (M6PFDA); perfluoroundecanoic acid, ¹³C₇ (M7PFUdA); perfluorododecanoic acid, ¹³C₂ (MPFDoA); 4:2 fluorotelomer sulfonate, ¹³C₂ (M2-4:2FTS); 6:2 fluorotelomer sulfonate, ¹³C₂ (M2-6:2FTS); 8:2 fluorotelomer sulfonate, ¹³C₂ (M2-8:2FTS) and hexafluoropropylene oxide, ¹³C₃ (M3HFPO) at the concentrations of 0.5–2.0 µg/mL (Wellington laboratories Inc.); Optima™ LC/MS grade water, Optima™ methanol, Optima™ ammonium acetate and Optima™ formic acid (99.0%) (Fischer Chemical); HiPerSlov CHROMANORM™ formic acid and HiPerSlov CHROMANORM™ methanol (VWR Chemicals). The specifications of the container materials used in this study are listed in Table 1, whereas the container dimensions, and container surface area to solution volume ratios are shown in Fig. S1 (of the Supplementary Data).

2.2. PFAS adsorption studies

To determine the adsorption of PFAS onto PP, PPCO, PS, PTFE, PET, HDPE, and GL containers, batch experimental studies were performed in three replicates for each tested condition by varying the contact times, solvent composition, storage time, and temperatures.

2.2.1. The influence of solvent composition, storage time, and temperature

The experiments were conducted by preparing separate bulk PFAS solutions (at 7 ng/L) in 100% water (Optima™ LC/MS grade) and 80:20 water:methanol (% v/v). The tested solvent composition (80:20 water:methanol (% v/v)) was chosen to achieve retention of PFAS by the SPE polar endcapped C₁₈ stationary phase (Kourtchev et al., 2022). For all experiments, the transfer of PFAS from the neat into bulk solution was carried out using a pipette, after which the bulk solution was homogenised by swirling. Equal portions of PFAS solution (15 mL) were transferred directly into containers made of PP, HDPE, GL, PPCO, PS, PTFE

and PET materials and stored at two temperatures (4 °C and 20 °C) for 0 (control), 3 and 7 days. Due to the limited availability of the test materials, the influence of cold temperature (4 °C) on adsorption of PFAS was tested using four materials (PP, HDPE, GL and PET), while that of the room temperature (RT, 20 °C) was tested for all seven materials. Aliquots (5 mL) collected from each container material at days 0, 3 and 7 were transferred (using a pipette) into a 10 mL headspace (HS) glass vials (Chromacol 10-HSV) spiked with ¹³C PFAS internal standard (IS) to make 5 ng/L and analysed with online SPE LC-MS. Before conducting all experiments, the container materials, caps, vials and pipette tips were pre-washed with Optima™ LC/MS grade methanol (three times) and then rinsed with the Optima™ LC/MS grade water (three times). The tests were conducted in three replicates. The loss of PFAS to each container material (expressed as recovery) was calculated by comparing the chromatographic PFAS peak areas after storage (PA₁) with the PFAS peak area at day 0 (PA₀):

$$PFAS\ Recovery = \left(\frac{PA_1}{PA_0} \right) \times 100 \quad (1)$$

The peak areas for each PFAS were corrected with those from the corresponding IS ¹³C PFAS.

2.2.2. The influence of sample centrifugation and shaking

The influence of centrifugation and shaking on PFAS loss was conducted only on 80:20 water:methanol (% v/v) solution of PFAS at 5 ng/L. The PFAS solution (15 mL) was transferred directly from the bulk solution into a separate container made of PP, HDPE, GL, PPCO, PS, PTFE, and PET and centrifuged at 4000 rpm for 10 min. Separate tests were performed by shaking PFAS solution at 120 rpm for 1 h at RT. The study was conducted in three replicates for each tested material. Due to the limited availability of test materials, only four container materials (i. e., PP, HDPE, GL, and PET) were assessed for the influence of centrifugation while all seven container materials were tested for the influence of shaking. After sample centrifugation and shaking, the sample aliquots (5 mL) from each container material were transferred (using a pipette) into HS glass vials, spiked with ¹³C PFAS IS at 5 ng/L, and analysed with online SPE LC-MS. The PFAS loss onto each container material (expressed as recovery) was calculated by comparing PFAS peak areas after centrifugation/shaking (PA_{cs}) with those before centrifugation/shaking (PA_{cs0}). The peak areas for each analyte were corrected with corresponding IS.

$$PFAS\ Recovery = \left(\frac{PA_{cs}}{PA_{cs0}} \right) \times 100 \quad (2)$$

2.3. Analytical method

The samples were analysed using Liquid Chromatography (LC) Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer (MS) (Thermo Fisher, Bremen, Germany). An online SPE method based on Kourtchev et al. (2022) and Folorunsho et al. (2023) was used for the

Table 1
Specification of the tested container materials.

Container material	Material code	Container closure material	Capacity (mL)	Surface area to solution volume ratio	Supplier
Polypropylene	PP	Polypropylene	15	3.6	Fisherbrand™ (05-539-4)
Polypropylene co-polymer	PPCO	Polypropylene	30	3.0	Thermo Scientific™ Nalgene™(10757221)
Polystyrene	PS	Polypropylene	15	3.6	Appleton (LS020)
Polytetrafluoroethylene	PTFE	N/A	45	1.9	Fisherbrand™ (15913077)
Polyethylene Terephthalate	PET	Polypropylene	15	3.6	Coring™ (430055)
High-density polyethylene	HDPE	Polypropylene	30	3.0	Thermo Scientific™ Nalgene™ (2104-0001)
Glass	GL	Aluminium cap with a silicon liner	20	2.8	Fisherbrand™ (12971231)

analysis of PFAS.

2.4. Quality assurance/quality control (QA/QC)

A number of measures were taken to reduce PFAS contamination during laboratory procedures. Prior to the analysis, the system was flushed continuously with mobile phases A:B (A-2 mM ammonium acetate in water with 10% methanol, and B-methanol) at 40:60% and a low flow rate (0.03 mL/min, overnight, respectively) to prevent accumulation of potential PFAS leachates from the system (Kourtchev et al., 2022). Container blanks (Optima™ LC/MS grade water without PFAS exposed to pre-washed and rinsed containers) were evaluated for background PFAS, and showed insignificant amounts (below limit of quantification (LOQ)). The use of blanks (Optima grade LC/MS water)

and quality control (QC) standards in every batch were adopted. At least 10 system (“zero volume”) and water blanks were injected before sample analysis, between samples, and at the end of the sequence resulting in insignificant amounts (below LOQ) of background PFAS. System suitability test was performed before the analysis of each experimental batch to ensure the adequate performance of the system. Considering that all final PFAS solutions (used in different materials exposure studies) were analysed from a 10 mL HS glass vial that is compatible with the instrument autosampler, these vials were assessed for the sorption of PFAS, taking into account the total time (holding time) required for the batch analysis. The sorption tests were conducted by filling a HS glass vial with 5 mL of 80:20 water:methanol (% v/v) solution and spiking with PFAS native standard mixture and IS at a concentration of 7.5 ng/L and 5 ng/L, respectively. The tests were

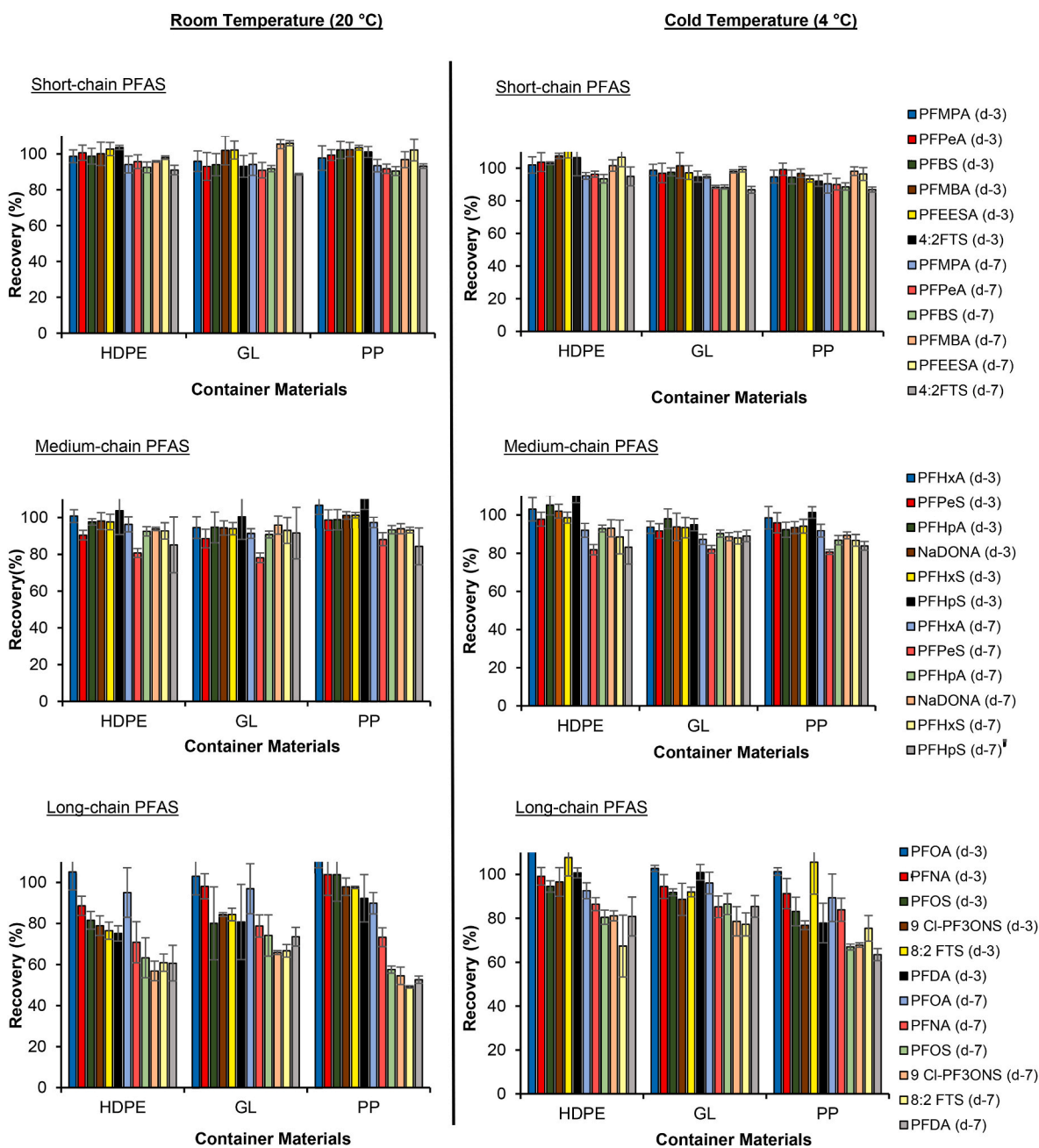


Fig. 1. Recoveries of PFAS in 100% water stored in HDPE, GL and PP container materials at RT (20 °C) and cold temperature (4 °C) for 3 and 7 days, labelled as “d-3” and “d-7”, respectively. HDPE = high-density polyethylene; GL = glass; PP = polypropylene. Error bars represent the standard deviation for experimental replicates (n = 3). Data for remaining materials are shown in Figs. S4-S7.

performed in three analytical replicates. PFAS solutions in HS glass vials were reinjected over 3 days showing minimal losses with recoveries ranging from 91.2% to 103.6% and 93.7%–102.8%, for all 18 target PFAS and corresponding ISs, respectively (as shown in Figs. S2 and S3). Statistical analysis was performed using Excel Version 2310 and IBM SPSS 28.0, and the results of data distribution, sample size and statistical difference are shown in Table S1–S2 and S4–S19. The Shapiro-Wilk test was used to determine whether the dataset follows a normal distribution. One-way analysis of variance ANOVA, Kruskal-Wallis one-way ANOVA and Dunn's post hoc tests, were then used to compare and determine the significant difference ($p < 0.05$) between the results from two or more tested conditions including the container materials.

3. Results and discussion

3.1. Influence of sample storage period on the PFAS losses onto different materials

It has been reported that the analyte to material contact time is crucial in any adsorption process, as it allows the adhesion of adsorbate molecules to take place (Kurniawati et al., 2021). The results of the losses (expressed as analyte recoveries) of PFAS (C4–C10) prepared in 100% water after storage for 3 and 7 days are shown in Fig. 1, while those prepared in 80:20 water:methanol (% v/v) are shown in Fig. S4. The recoveries of the PFAS from tested container materials ranged from $75.1 \pm 3.7\%$ to $112.1 \pm 4.9\%$ and from $49.1 \pm 0.6\%$ to $110.1 \pm 3.1\%$ for days 3 and 7, respectively. The results of one-way ANOVA (Tables S1–S2) showed significant difference ($p < 0.05$) between PFAS recoveries for days 3 and 7 for most of the tested analytes and materials. In general, long-chain PFAS (with carbon chain >8 for carboxylic PFAS, and carbon chain >7 for sulfonic PFAS) adsorbed to containers more than short-chain PFAS (with <6 carbon chain length) with increasing storage time. The most affected compounds were PFOS, 8:2FTS, and PFDA in PP and HDPE containers. For short-chain PFAS, there was a significant statistical difference between the analyte recoveries on days 3 and 7 for most of the materials except HDPE. Similarly, there was a significant statistical difference between days 3 and 7 losses for long-chain PFAS in GL, and other polymeric materials such as PP and PS. The observed behaviour may, in part, be attributed to the properties of the considered polymers such as surface area, diffusivity and crystallinity, which have been reported to influence the adsorption of organic compounds (Rochman et al., 2013; Shi et al., 2023). For instance, rubbery polymers such as PP, PS, and HDPE are expected to provide greater diffusion of organic compounds within the material matrix compared to those from glassy (more crystalline) polymers such as PET or GL (Rochman et al., 2013), which may explain the observations in our work. Moreover, sorption patterns are compound specific e.g., the increasing affinity to materials with greater hydrophobicity and varying functional groups, potentially explaining the losses of long-chain PFAS to tested container materials in this study.

Table S3 presents a summary of existing studies on the adsorption of PFAS in aqueous matrices including water, organic solvents and blood onto different container materials. Our results are consistent with those from Lath et al. (2019) and Zenobio et al. (2022) which reported an increase in the adsorption of PFOA and PFOS, among others, onto PP, PET, PS, and HDPE within 7 and 10 days. However, in contrast to our results, Wang et al. (2016) reported no loss for short- and medium-chain PFAS, including PFOA and PFHxS, whereas losses of 5–16% were observed for long-chain PFAS, PFOS, PFNA, and PFDA onto the surface of HDPE bottles after 2-week sample storage. The higher PFAS losses (19.1–39.3%) to HDPE observed in our study are likely due to the lower concentration of analytes in our study (7 ng/L) compared to that (100 ng/L) used in Wang et al. (2016). In this respect, the PFAS losses due to adsorption are shown to increase at low concentrations (Weed et al., 2022). Moreover, Lath et al. (2019) reported a proportional loss of PFOA onto PP, PC, and GL container walls with a decrease of PFOA

concentration.

To the best of the author's knowledge, our study is the first to report the influence of contact time on the losses of long- and short-chain per- and polyfluoroalkyl ether acids such as PFMPA, PFMBA, PFEESA, NaDONA, and 9Cl-PF3ONS onto seven container materials including PTFE.

3.2. Influence of solvent composition on the PFAS loss to tested materials

The effect of solvent composition on the losses of PFAS to PP, GL, HDPE and PET materials is shown in Fig. 2, while for PPCO, PS and PTFE is shown in Fig. S8. The losses of 18 PFAS in 100% water for the tested materials were up to $50.9 \pm 0.6\%$ while in 80:20 water:methanol (% v/v), up to $24.8 \pm 11.4\%$. Our results show higher losses of long-chain PFAS in 100% aqueous solutions compared to those in 80:20 (% v/v) water: methanol to all tested materials. The highest losses of PFAS were observed for 8:2 FTS, PFDA, 9Cl-9PF3ONS and PFOS onto PP (50.9%, 47.8%, 46.5% and 42.8%, respectively). Overall, the effect of solvent composition on the losses of considered PFAS varied with the container materials. Irrespective of the tested solvent composition, there was no significant difference between the PFAS recoveries (for both short- and medium-chain) from the tested container materials except for PFMPA ($p = 0.040$), whose trend of losses to container materials was as follows: HDPE $>$ PP $>$ PET $>$ PPCO $>$ PTFE $>$ GL (Tables S4–S7). Meanwhile, in 100% water, all considered long-chain PFAS, except 9Cl-PF3ONS ($p = 0.079$), showed a significant difference between recoveries in different container materials (Tables S8–S14). Moreover, the highest losses for all the considered long-chain PFAS in 100% water were observed onto PP and HDPE after 7 days of storage at RT.

It has been reported that PFAS solubility in water decreases with an increase in carbon chain length (Du et al., 2014; Point et al., 2019; Söregård et al., 2020), which can potentially explain the more pronounced losses of long-chain PFAS in 100% aqueous solutions observed in our study. Our results are in agreement with previous studies showing higher adsorption of longer-chain PFAS in 100% water to PP and GL (Berger et al., 2011; Mancini et al., 2023; Söregård et al., 2020). Kourtchev et al. (2022) reported higher extraction efficiencies of long-chain PFAS (PFNA, PFOS, 8:2 FTS, PFDA, and PFUDa), than the short-chain ones with increased methanol content. Recently, Lenka et al. (2023) also reported lower losses of PFPrA, PFBA, and PFBS in PP containers with 1:1 methanol:water (v/v) than in 100% water. Moreover, an earlier PFAS adsorption study by Holm et al. (2004) reported a 25% loss of PFOS onto GL in acetonitrile:water (5:95, % v/v). Meanwhile, Zhang et al. (2022) reported a substantial decrease in the losses of tested perfluoroalkyl ether carboxylic acids (PFCEA) with increasing water content (0–20%) in protic solvents including acetonitrile, acetone and dimethyl sulfoxide (DMSO).

Our observations are also in line with those from Zenobio et al. (2022) and Berger et al. (2011), which suggested that PP may not be a suitable material for long-chain PFAS storage. Moreover, Point et al. (2019) indicated that the chemical structure of PP enhances the material's interaction with the hydrophobic tail of PFAS via van der Waals molecular interactions. Hence, the addition of organic solvent (e.g., methanol) to aqueous environmental samples can effectively reduce the long-chain PFAS losses to container materials (Lenka et al., 2023).

3.3. Influence of temperature on PFAS loss to tested materials

The effect of two storage temperatures i.e., RT, (20 °C) and cold (4 °C) on the losses of 18 PFAS to PP, HDPE, GL and PET after 7 days is summarised in Fig. 2. The tested temperatures are most typically used to store and handle aqueous samples for PFAS analysis (Winchell et al., 2021). The influence of temperature on the loss of PFAS showed a strong dependency on the solvent composition.

For PFAS stored in 100% water, higher losses were observed at RT (up to $50.9 \pm 0.6\%$) compared to cold temperature (up to $39.7 \pm 5.8\%$).

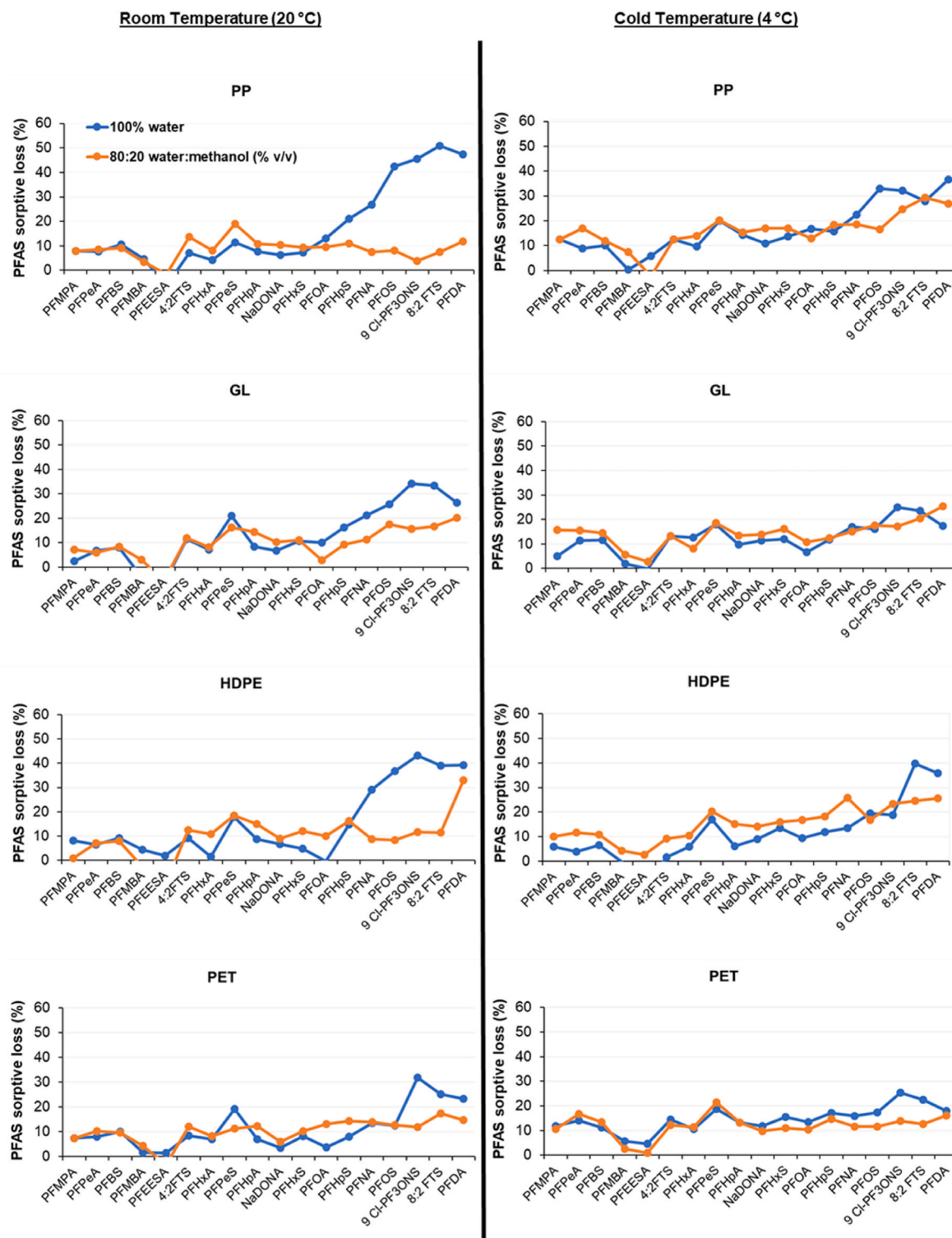


Fig. 2. Loss of PFAS in 100% water and 80:20 water:methanol (% v/v) to PP, GL, HDPE and PET materials after storage for 7 days at RT (20 °C) and cold temperature (4 °C). Data for remaining materials are shown in Fig. S8.

Meanwhile, for PFAS stored in 80:20 water:methanol (% v/v), the influence of temperature was minimal (large variability, as per large standard error), with losses of PFAS up to $37.8 \pm 11.4\%$ and $29.3 \pm 1.7\%$ for RT and cold temperature, respectively. As shown in Table S15, a significant statistical difference was observed between the recoveries of long- and short-chain PFAS at 4 °C and 20 °C to tested materials except for PET. However, no significant statistical difference was observed between the recoveries of medium-chain PFAS (with carbon

chain length of 6–8, e.g., PFHxA, PFHxS, PFHpA) at 4 °C and 20 °C to tested materials except for PET. Overall, the effect of temperature on the losses of short- and medium-chain PFAS onto tested container materials was minimal, while the losses of long-chain PFAS (ranging from 0.2 to 50.9%) slightly increased with higher temperature for most of the tested materials. Moreover, large variability (as per large standard error, see Fig. 1) was observed for the long-chain PFAS stored at RT compared to that at cold temperature.

A summary of the previous studies reporting influence of temperature on PFAS adsorption onto container materials is presented in Table S3. Our observations are comparable to those from Zhang et al. (2022) which reported no measurable loss of medium-chain PFAS, PFHxA and PFHxS after storage at RT (20.2 °C). The results of PFOS losses to the containers at higher temperature are also consistent with studies of sorption to the sample matrix, e.g., humic acid (Jia et al., 2010). The latter study indicated that PFOS sorption is spontaneous (Gibbs Free energy change <0) and endothermic (enthalpy change of sorption >0). Hence, increased distribution coefficient (the ratio of analyte concentration in solid to liquid phase) is expected at higher temperatures for longer chain PFAS (Nguyen et al., 2020). Woudneh et al. (2019) reported a decrease in the concentration of long-chain PFAS, e.g., 8:2 FTS with increasing temperature from -20 °C to 20 °C in the studied matrices (spiked bottled water, surface water, and effluent water). Moreover, Zenobio et al. (2022) reported lower adsorption of PFAS to

PP, PET and HDPE at 4 °C than at 20 °C. Similarly, Shafique et al. (2017) reported an increase in the adsorption of PFOA onto silica with increasing temperatures from 20 to 45 °C. As suggested by Karthikeyan et al. (2005), the enhanced adsorption at higher temperatures observed in this study is likely due to an increased rate of intraparticle diffusion of adsorbates (PFAS) into the pores of the adsorbent (container material surface) at higher temperatures. Meanwhile, Kato et al. (2013) reported an insignificant loss of PFHxS, PFOA, PFOS and PFNA in serum after 10 days storage at 20 °C in PP. As discussed earlier (in section 3.2), this is likely due to the PFAS solvent or matrix composition, which has been reported to influence PFAS losses to materials. To the authors' knowledge, this is the first study reporting the influence of temperature on the losses of 18 PFAS to other than GL and PP container materials.

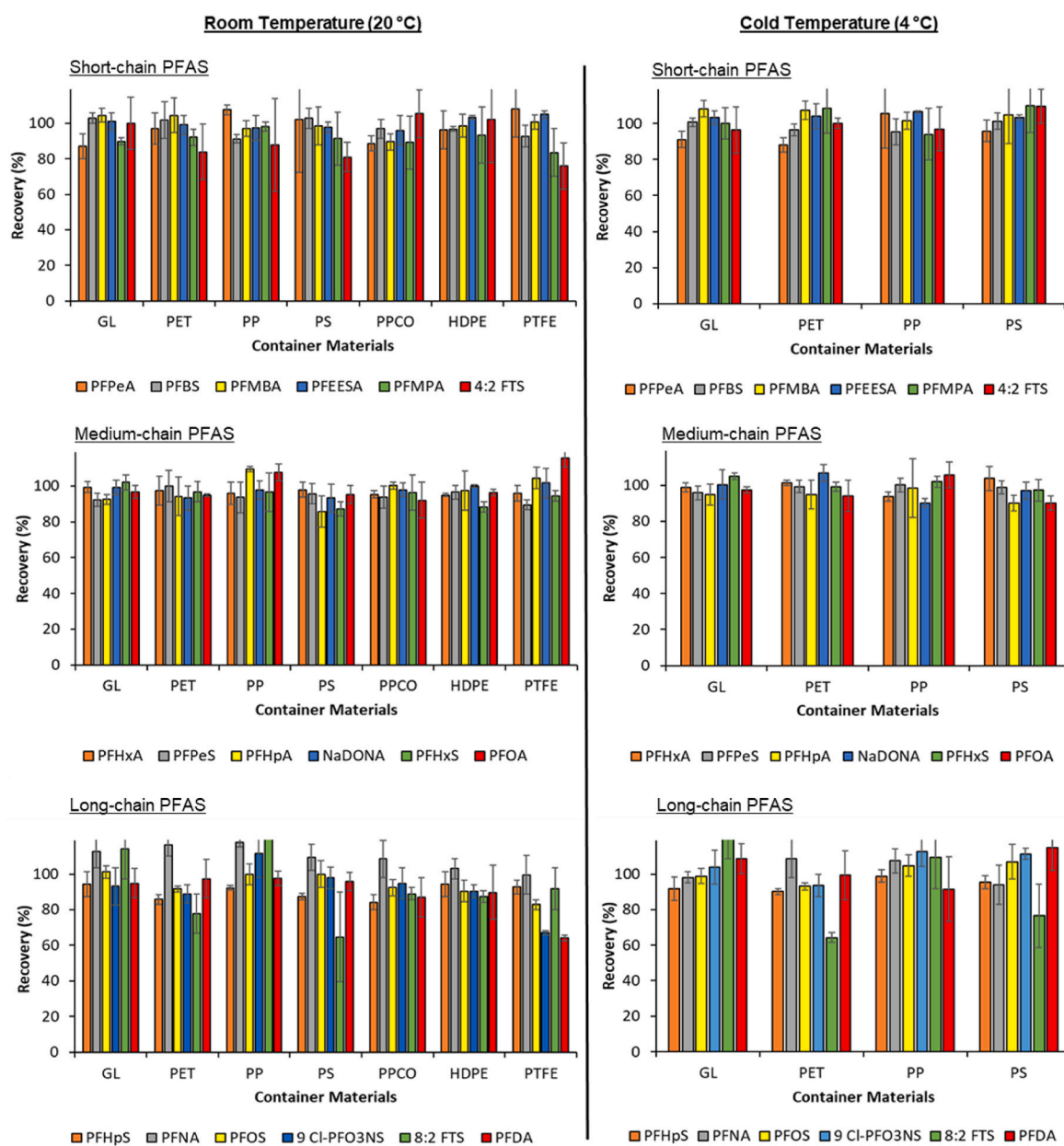


Fig. 3. Recoveries of PFAS after centrifugation at 4000 rpm for 10 min and shaking at 120 rpm for 1 h using HDPE, GL, PET, PP, PS, PPCO, PTFE. The studies were conducted in four container materials for centrifugation and seven materials for shaking due to limited material availability. Error bars represent the standard deviation for replicates (n = 3).

3.4. Influence of agitation technique on the loss of PFAS to tested materials

Due to the high adsorption losses of long-chain PFAS in 100% water (as shown in section 3.2) the sample agitation tests were performed only in 80:20 water:methanol (% v/v) solvent composition. The influence of sample shaking and centrifugation on the adsorption losses of PFAS to different container materials is summarised in Fig. 3. For most of the tested PFAS in different containers, minor losses were observed when using both agitation techniques. However, lower recoveries of PFDA ($64.1 \pm 1.6\%$) and 9Cl-PF3ONS ($64.1 \pm 1.3\%$), were observed from PTFE materials after shaking. Moreover, low recoveries of 8:2 FTS were observed after shaking ($64.3 \pm 2.8\%$) and centrifugation ($64.7 \pm 25.1\%$) when using PET and PS, respectively (Fig. 3). There was no statistical difference ($p > 0.05$) between the recoveries of most of the tested PFAS from either agitation technique, except for 4:2 FTS in PS ($p = 0.043$), PFHpS in PP ($p = 0.036$) and PS ($p = 0.026$), and 9Cl-PF3ONS in PS ($p = 0.026$), as shown in Table S16.

The insignificant loss of most of the tested PFAS, except for 8:2 FTS, PFDA, and 9Cl-PF3ONS, observed after using either of the agitation techniques, is likely a result of the good solubility of PFAS in 80:20 water:methanol (% v/v), as indicated in the previous tests shown in section 3.2. Agitation could influence diffusion kinetics at the solution boundary layer by increasing mass transfer coefficients Wang and Guo (2022). The insignificant losses of tested PFAS, especially the short- and medium-chain PFAS, to containers after agitation indicate that most of these compounds may not exhibit diffusion at the solution boundary layer. Our results also indicate limited diffusion of short- and medium-chain PFAS at the water-container interface due to small surface-to-solvent volume ratios (Table 1) in the sorption experiment. However, the high losses of 8:2 FTS to PET and PS after agitation indicate the potential diffusion of long-chain fluorotelomer PFAS to these polymer materials after agitation.

The number of studies in the literature reporting the influence of these agitation techniques on PFAS losses is very limited and has been summarised in Table S17. Our results are comparable with those by Zhang et al. (2021) which reported negligible losses of PFOS and PFOA in pH adjusted solution after shaking. Folorunsho et al. (2023) also reported negligible losses of PFAS in 80:20 water:methanol (% v/v) after centrifugation in GL containers. To our knowledge, this is the first study reporting a direct comparison between agitation techniques commonly used in PFAS analysis and also their influence on the loss of 18 PFAS.

4. Conclusion

In this study, we investigated potential adsorption losses of an extensive number of (C4–C10) PFAS to commonly used labware materials, i.e., HDPE, PP, PS, PPCO, PET, PTFE and GL. Analytical aspects such as sample storage time and agitation techniques that are commonly used during the analysis of PFAS have been investigated and discussed. The extent of PFAS losses has been shown to vary between the tested materials depending on the properties of the analyte (i.e., chain length and functionalities). Our results indicate that longer sample storage time (7 days) enhances losses of tested PFAS to container materials which depend on the solvent composition and sample storage temperature. The more pronounced PFAS losses were observed in 100% aqueous solutions, particularly for long-chain PFAS (C9–C10 for carboxylic groups and C8–C10 for sulphonic groups). Sample storage temperature has shown to directly affect PFAS losses to container walls. This effect was more pronounced in 100% aqueous solutions stored at RT compared to those at cold temperature (4 °C), especially for the long-chain PFAS. Therefore, the storage of PFAS samples (containing long-chain PFAS) in containers for a period longer than 3 days at RT, is discouraged. However, in line with the recent studies (e.g., Kourtchev et al., 2022; Folorunsho et al., 2023; Lenka et al., 2023), the addition of polar solvent such as methanol has shown to reduce losses of long-chain PFAS to a

sample storage container. Both tested sample agitation techniques showed negligible losses of most PFAS in 80:20 water:methanol (% v/v) solution except for PFDA and 9Cl-PF3ONS in PTFE and 8:2 FTS in PS and PET. Overall, the order of losses to different materials varied between considered PFAS. The highest losses of the long-chain PFAS were observed in PP and HDPE. Our results indicate that while PP may not be the best container material for handling long-chain PFAS for more than 3-day period, other materials such as GL and PET may be used as an alternative.

It should be noted that the mass balance of PFAS losses to the containers was not considered. Such information could be useful for understanding a type or a mechanism of adsorption. Our study emphasises the need to account for the losses of PFAS to common laboratory materials in sampling and experimental protocols. Other factors such as an environmental matrix which are reported to influence the extent and a rate of PFAS adsorption (Lath et al., 2019; Scott et al., 2021; Woudneh et al., 2019; Wu et al., 2020) should be considered. To our knowledge, this is the first study that reports the losses of long- and short-chain PFAS (18 PFAS) to an extensive list of commonly used container materials, and at trace level concentrations. Identification of the appropriate sample storage containers and storage conditions are essential for ensuring data reliability, especially when assessing and managing risks associated with PFAS pollution and exposure.

CRedit authorship contribution statement

Omotola Folorunsho: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Jishnu Pandamkulangara Kizhakkethil:** Investigation, Formal analysis. **Anna Bogush:** Writing – review & editing, Supervision, Conceptualization. **Ivan Kourtchev:** Writing – review & editing, Writing – original draft, Supervision, Resources, Project administration, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.chemosphere.2024.142814>.

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