




TECHNICAL NOTE

Effects of a variable air–water interface on injection of PFAS—Lessons learned from column tests with porous media

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Assigned to Associate Editor Helen Dahlke.

Funding information

European Union's Horizon 2020 Research and Innovation Programme, Grant/Award Number: 101036449; Vienna Science and Technology Fund (WWTF), Grant/Award Number: 10.47379/ESR20013

Abstract

Five column experiments were conducted using a mixture of 10 per- and polyfluoroalkyl substances (PFASs) to explore sampling techniques for the PFAS injection solution concentration in order to accurately determine the tracer mass within the experimental system and close the mass balance. Samples of the injection solution were first taken by the method of pouring from the injection container into sampling tubes and analyzed for PFAS concentration. The results showed a drastic increase in the concentration of certain PFASs over the course of injection (up to 763%), leading to incomplete mass balances and low recovery rates. By contrast, when the injection solution was sampled by pipetting away from the air–water interface, the mass balance greatly improved (PFAS recovery percentages increased from an average of 62%–102%). The observed concentration increase by the method of pouring can be attributed to the attraction of certain PFASs to the air–water interface. Factors such as carbon chain length and solubility were found to impact this attraction most, while surprisingly, the air–water interfacial sorption coefficients did not appear to be significantly influential. This phenomenon is important to column experiments, as elevated local concentrations may promote micelle or hemi-micelle formation, consequently affecting the transport and sorption characteristics of the compounds under study. These aspects should be thoroughly considered in future studies to ensure a correct calculation of mass balance and therefore to correctly characterize the behavior of PFASs in the environment, and may also be relevant in remediation investigations, such as column tests with granular activated carbon.

ABBREVIATIONS: 9CL-PF3ONS, 9-chlorohexadecafluoro-3-oxanonane-1-sulfonic acid; CMC, critical micelle concentration; CT, column test; PFAS, per- and polyfluoroalkyl substance; PFDS, perfluorodecanesulfonic acid; PFOS, perfluorooctanesulfonic acid; PFOSA, perfluorooctane sulfonamide; VIC PFAS, varying injection concentration PFAS.

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Plain Language Summary

This study looked at how 10 different per- and polyfluoroalkyl substances (PFASs), which are harmful chemicals, stick to sand and natural soil. The researchers wanted to see if the way they collected samples affected the measured PFAS levels. When samples were poured, some PFAS concentrations appeared to increase, giving incomplete results. But when samples were taken with a pipette, recovery improved. The concentration increase, seen when using the pouring method, is caused by PFAS gathering at the air–water surface, influenced mainly by their chain length and solubility. This matters because high local concentrations can change how PFASs move and stick to materials. Understanding this helps scientists accurately measure PFASs and design better cleanup methods for contaminated water.

1 | INTRODUCTION

Per- and polyfluoroalkyl substances (PFASs) comprise a class of fluorinated chemicals used in various consumer products and numerous industrial processes, having been in production for over 80 years (Buck et al., 2011; Smeltz et al., 2023). Despite many desirable properties, the non-reactivity and resistance to degradation of PFASs raise growing concerns regarding its occurrence and persistence in the environment (Evich et al., 2022; Li et al., 2023; Moody & Field, 2000). Consequently, research into the fate and transport of PFAS in the environment is highly important (Bräunig et al., 2017; Marchiandi et al., 2021; Sharifan et al., 2021). Injection-extraction experiments with soil columns provide an essential, long-established approach, especially for groundwater investigations, and are particularly useful for studying the transport of chemicals through porous media and their interaction with grain surfaces (May et al., 2023).

The interpretation of results from injection-extraction experiments, such as column tests aiming to ascertain tracer sorption rates, heavily relies on a closed or semi-closed mass balance (Bi et al., 2010; Pang et al., 2005; Schijven & Hasanizadeh, 2000; Shackelford, 1994). The critical aspect here is identifying the tracer mass within the system, as the overestimation of the mass may lead to the overestimation of sorption rates. Thus, accurately measuring the concentration of the injection fluid is crucial.

Preliminary experiments with PFASs in empty columns showed that throughout the injection phase, during which the water level in the container decreased, PFAS concentrations varied. We hypothesized that this was due to a non-homogeneous injection solution. Potential explanations for this phenomenon include PFAS hydrophobicity, interactions at the air–water interface, and micelle formation (Brusseau & Van Glubt, 2021; Honda et al., 2007; Kancharla et al., 2022). A varying injection concentration complicates

the closing of the mass balance, resulting in challenges in determining PFAS transport parameters, such as sorption rates. As of now, there is scarce knowledge about the incidence of these issues in column test studies, their origins, and avenues to address them (Grieco et al., 2021; Niarchos et al., 2022; Umeh et al., 2024).

The objective of this study was to explore sampling techniques for the PFAS injection solution concentration in order to accurately determine the tracer mass within the experimental system and ultimately close the mass balance for injection-extraction experiments with PFASs.

2 | MATERIALS AND METHODS

Five column tests (CT1–5) were conducted. The injection fluid contained Viennese tap water, which is oxic Alpine karstic spring water with low ionic content, a pH of approximately 8, and an electrical conductivity of 250 $\mu\text{S}/\text{cm}$ (Oudega et al., 2021), and a mix of 10 PFASs (with the exception of CT3, in which eight PFAS were used). The 10 PFASs were selected to represent a diverse range of substances present in the environment, in terms of type, functional group, chain length and usage (Table 1).

The experimental set-up (see graphical abstract) comprised a glass Erlenmeyer injection container with a magnetic stirrer, polypropylene tubes, and a glass column filled with either lab-grade quartz sand measuring 0.6–1.3 mm in diameter (CT1–3) and natural soil (CT4–5). The magnetic stirrer was used to generate a vortex intended to prevent the accumulation of PFASs at the air–water interface. The injection volume in all tests was two pore volumes, corresponding to 1500 mL for CT1–3 and 600 mL for CT4–5. Each PFAS had a target concentration of 2.5 $\mu\text{g}/\text{L}$ in CT1–4 and a target concentration of 250 ng/L in CT5 (Table 2). Following the injection of the PFAS solution, flushing was carried out with the same tap

TABLE 1 Per- and polyfluoroalkyl substances (PFASs) used in the column experiments.

PFAS	Full name	CAS number	Type	Chain length	Charge state (pH ~7)
PFPeA	Perfluoropentanoic acid	2706-90-3	Carboxylic acid (PFCA)	C5	Anionic
PFOA	Perfluorooctanoic acid	335-67-1	Carboxylic acid (PFCA)	C8	Anionic
PFDODA	Perfluorododecanoic acid	307-55-1	Carboxylic acid (PFCA)	C12	Anionic
PFPeS	Perfluoropentanesulfonic acid	2706-91-4	Sulfonic acid (PFSA)	C5	Anionic
PFOS	Perfluorooctanesulfonic acid	1763-23-1	Sulfonic acid (PFSA)	C8	Anionic
PFDS	Perfluorodecanesulfonic acid	335-77-3	Sulfonic acid (PFSA)	C10	Anionic
6:2 FTS	6:2 Fluorotelomer sulfonic acid	27619-97-2	Fluorotelomer sulfonate	C8	Anionic
PFOSA	Perfluorooctane sulfonamide	754-91-6	Sulfonamide precursor	C8	Neutral
ADONA	4,8-Dioxa-3H-perfluorononanoic acid	919005-14-4	Ether-based PFCA	C6 (perfluorinated segment)	Anionic
9Cl-PF3ONS	9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid	73606-19-6	Perfluoroether PFSA	C6 equivalent	Anionic

water. A total of 12 pore volumes of tap water were injected for the flushing phase of the experiment, which lasted 24 h.

During the injection phase, four or five samples were collected from the injection fluid. During CT1, sampling was conducted by pouring 5 mL from the injection container directly into a sample test tube, with the goal of minimizing the amount of materials and surface area that the PFAS solution would come in contact with, and thereby reducing potential PFAS adsorption. During CT2–5, two sampling methods were utilized: pouring 5 mL as well as pipetting 5 mL, which was done from the bottom of the water column adjacent to the entry of the tube that drains the injection fluid from the injection container. Both during the injection and flushing phases, samples of 5 mL were extracted from the column effluent at intervals ranging from 5 to 30 min. All samples were diluted with 5 mL of methanol to enhance solubility. The analysis of PFAS was performed using liquid chromatography coupled with mass spectrometry, adhering to United States Environmental Protection Agency draft method 1633 (Environmental Protection Agency, 2022), as described in Obeid et al. (2023).

To close the mass balance post experiment, all materials used in the experiments (the stirrer, tubes, glass column, interior of the injection container, and in CT2–5, the pipet) were washed with ethanol, which was collected and analyzed for PFASs. In addition, three representative 20 g samples of the porous media were taken from the top, middle, and bottom of the column. These samples were mixed with a 50 mL 0.3% ammonium methanol solution in a shaker for 2 h. Subsequently, the solution was analyzed using the method previously described.

3 | RESULTS AND DISCUSSION

In all tests, five PFAS—namely perfluorododecanoic acid, perfluorooctanesulfonic acid (PFOS), perfluorodecanesulfonic acid (PFDS), perfluorooctane sulfonamide (PFOSA), and 9-chlorohexadecafluoro-3-oxanonane-1-sulfonic acid (9CL-PF3ONS; henceforth collectively referred to as VIC PFASs, varying injection concentration PFASs)—showed an increase in injection concentration during the injection phase when using the pouring method. In CT2, concentration increases during the injection phase varied from 266% to 764%, depending on the substance, while the injection concentrations of non-VIC PFASs remained relatively constant (Figure 1). The mass balance for CT2 demonstrated that the measurement of the injection mass of the VIC PFASs was markedly improved by using the pipetting method, yielding an average recovery of 109% for the pipetting method versus 55% for the pouring method (Table 2). This shows that the liquid at the surface (preferentially sampled by the pouring method) contains a higher concentration of PFAS than liquid deeper in the water column (preferentially sampled by the pipetting method), that is, PFASs accumulated at the air–water interface, which is a well-established phenomenon (Brusseau, 2019; Silva et al., 2019; Vierke et al., 2013). This likely causes the high injection concentrations observed when using the pouring method, especially toward the end of the injection phase when (due to the abstraction of the injection solution, as well as due to the shape of the Erlenmeyer injection flask) the air–water interface becomes large compared to the volume of the injection fluid (Figure 1).

TABLE 2 Mass of per- and polyfluoroalkyl substances (PFASs) (ng) measured pre- and post-injection in different reservoirs of the experimental set-up.

Column test	Measurement	PFPeA	PFOA	PFDoDA	PFPeS	PFOs	PFDS	6:2 FTS	PFOSA	ADONA	9CI-PF3ONS	PFAS average
Test 1	Injection—pour	3330	3162	11,564	2915	3793	15,273	2970	6553	3305	6819	5968
	Effluent	3028	2755	102	2812	2772	88	2740	4007	2958	2731	2399
	Porous media	3	142	1439	2	113	1915	128	72	1	1021	484
	Column system	3	7	33	3	21	27	8	25	5	54	19
	Total mass	3034	2904	1574	2817	2906	2030	2876	4105	2963	3806	2901
	Pour recovery (%)	91	92	14	97	77	13	97	63	90	56	49
Test 2	Injection—pour	4133	3428	14,170	3543	5313	17,546	3724	7534	3822	7756	7097
	Injection—pipet	3967	3488	2063	3552	3781	2798	3791	4808	3733	3993	3598
	Injection—both	4050	3458	8117	3548	4547	10,172	3758	6171	3777	5875	5347
	Effluent	4168	3416	87	3583	3949	35	3762	5384	3655	3503	3154
	Porous media	59	35	1933	0	58	2832	0	65	3	733	572
	Column system	9	15	765	7	83	737	16	133	11	204	198
Total mass	4236	3466	2785	3589	4090	3603	3778	5581	3668	4440	3924	
Pour recovery (%)	103	101	20	101	77	21	101	101	74	96	57	
Pipet recovery (%)	107	99	135	101	108	129	100	116	98	98	111	
Both methods (%)	105	100	34	101	90	35	101	90	97	97	76	
Test 3	Injection—pour	3858	4313	—	3705	7045	—	4521	11742	3996	10,529	6214
	Injection—pipet	3794	3920	—	3568	3789	—	3967	5081	3815	4949	4110
	Injection—both	3826	4116	—	3636	5417	—	4244	8411	3905	7739	5162
	Effluent	4431	4537	—	3564	8990	—	4479	10,457	4029	6639	5891
	Porous media	0	33	—	0	198	—	57	463	0	1850	325
	Column system	3	26	—	6	168	—	24	473	14	345	132
Total mass	4434	4595	—	3570	9356	—	4560	11,393	4042	8835	6348	
Pour recovery (%)	115	107	—	96	133	—	101	97	101	101	84	
Pipet recovery (%)	117	117	—	100	247	—	115	224	106	106	178	
Both methods (%)	116	112	—	98	173	—	107	135	104	104	114	

(Continues)

TABLE 2 (Continued)

Column test	Measurement	PFPeA	PFOA	PFDoDA	PFPeS	PFOs	PFDS	6:2 FTS	PFOsA	ADONA	9CI-PF3ONS	PFAS average	
Test 4	Injection—pour	1220	1354	6796	1261	1851	11,776	1046	4235	1455	3366	3436	
	Injection—pipet	1089	1146	1170	1050	1355	2119	940	2036	1191	2207	1430	
	Injection—both	1154	1250	3983	1155	1603	6947	993	3135	1323	2787	2433	
	Effluent	954	945	105	896	913	75	722	1267	943	1483	830	
	Porous media	50	32	273	0	0	221	0	0	0	0	58	
	Column system	2	3	364	3	21	370	3	77	3	53	90	
	Total mass	1006	981	743	898	934	666	725	1344	945	1536	978	
	Pour recovery (%)	82	72	11	71	50	6	69	32	65	65	46	28
	Pipet recovery (%)	92	86	63	86	69	31	77	66	79	79	70	68
	Both methods (%)	87	78	19	78	58	10	73	43	71	71	55	40
Test 5	Injection—pour	177	226	238	136	467	329	182	112	161	1490	352	
	Injection—pipet	177	160	12	134	125	18	130	32	147	626	156	
	Injection—both	177	193	125	135	296	174	156	72	154	1058	254	
	Effluent	565	368	1195	148	169	105	984	39	160	165	390	
	Porous media	0	0	34	0	0	101	0	0	0	0	13	
	Column system	0	2	50	0	20	49	2	8	1	1	13	
	Total mass	565	370	1279	148	189	254	986	47	161	167	417	
	Pour recovery (%)	319	164	538	109	41	77	542	42	100	11	118	
	Pipet recovery (%)	319	231	10614	111	152	1431	760	149	109	27	267	
	Both methods (%)	319	192	1025	110	64	147	632	66	104	16	164	

Note: Injection masses are averages, weighted to the amount of injection fluid left in the injection container. The column system includes all materials used, excluding the porous media in the column. Abbreviations: 6:2 FTS, 6:2 fluorotelomer sulfonic acid; 9CI-PF3ONS, 9-chlorohexadecafluoro-3-oxanonane-1-sulfonic acid; ADONA, 4,8-dioxo-a-3H-perfluorononanoic acid; PFDoDA, perfluorododecanoic acid; PFDS, perfluorododecanesulfonic acid; PFOs, perfluorooctanesulfonic acid; PFOA, perfluorooctanoic acid; PFOsA, perfluorooctanoic acid; PFPeA, perfluoropentanesulfonic acid; PFPeS, perfluoropentanesulfonic acid.

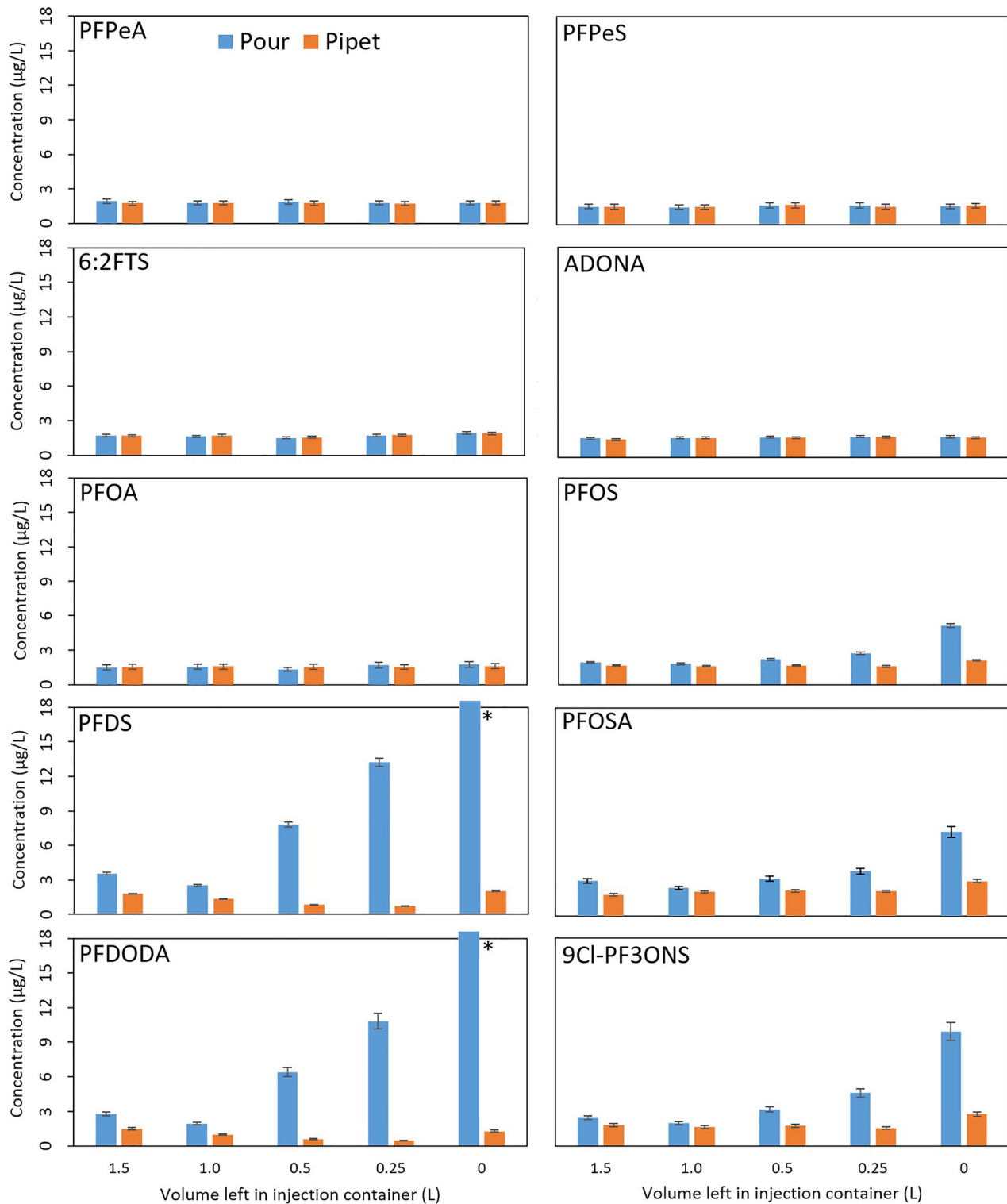


FIGURE 1 Measured per- and polyfluoroalkyl substance (PFAS) concentrations in the injection container during CT2 injection, using the pouring method versus the pipetting method. A concentration of 2.5 µg/L was intended. *Concentration above axis (26.6 µg/L for perfluorodecanesulfonic acid [PFDS] and 21.3 µg/L for perfluorododecanoic acid [PFDODA]). ADONA, 4,8-dioxa-3H-perfluorononanoic acid; PFOS, perfluorooctanesulfonic acid; PFOA, perfluorooctanoic acid; PFOSA, perfluorooctane sulfonamide; PFPeA, perfluoropentanoic acid; PFPeS, perfluoropentanesulfonic acid.

In all tests, the average observed injection mass of the VIC PFASs was lower (corresponding to higher observed recovery) when based on the pipetting method rather than on the pouring method (Table 2). Using the pouring method to measure injection mass resulted in challenges in distinguishing sorption processes, given the ambiguity surrounding whether the VIC PFAS were (1) actually present in the injection fluid at such high concentrations and subsequently sorbed to the porous media or (2) if their actual concentrations in the injection fluid were lower.

Pipetting improved the mass balance for VIC PFASs while not negatively impacting the mass balance of the non-VIC PFASs, with some exceptions. For example, in CT2, the recovery of perfluoropentanoic acid was calculated to be 107% while using the pipetting method and 103% while using the pouring method. This indicates that sampling the injection solution by pipetting can result in an underestimation of the injection concentration, suggesting that the accumulation of certain substances at the air–water interface leads to lower concentrations in the bulk of the injection solution, which can also be seen in Figure 1. This underestimation of the injection concentration is most pronounced in CT3 and CT5, where the majority of PFASs show recoveries exceeding 100% for the pipetting method, due to higher masses in the effluent than in the injection container (e.g., PFOSs in CT3). While this mainly points to an underestimation of the injection mass due to a heterogeneous injection solution, sampling biases might also have affected these mass balance discrepancies. Because different PFASs break through at different times, the effluent breakthrough curves (from which the effluent mass was calculated) are drawn with varying number of data points (effluent samples), which can lead to uncertainties. Further discrepancies might arise from the measurement of sorbed PFASs, as only three representative soil samples were measured post experiment. While in some of these cases, the pouring method yields better results for specific substances (e.g., 4,8-dioxo-3H-perfluorononanoic acid, CT3), in other cases, substances exhibit recoveries well below 100% (e.g., PFOS, CT5). However, when comparing the pipetting method, the pouring method, and the average between both methods for all tests, the pipetting method performs best overall (Figure 2).

CT5, similar to CT2–4, shows higher recovery rates when using the pipetting method than when using the pouring method. The lower injection concentrations in CT5 do not seem to negate the VIC phenomenon; aggregation at the air–water interface is as strong as it is in CT2–4, leading to a significant underestimation of injection concentrations, and thus overestimation of recovery rates, when using the pipetting method (Table 2). CT5 also shows significant increases in pouring concentrations during the injection phase, for example, for PFDS and PFOSA, like in CT2 (Figure 1). One explanation for this is that while the concentration at which

micelle formation occurs, known as the critical micelle concentration (CMC), is typically in the mg/L range, studies have shown that aggregation into hemi-micelles on surfaces, such as the glass container, could already occur at concentrations around $0.001 \times \text{CMC}$ (Alves et al., 2020; Kancharla et al., 2022). This indicates that the bulk of the PFASs in the injection container might be sorbed to either the glass Erlenmeyer or the air–water interface, instead of being homogeneously distributed. Because this mechanism was not directly measured, it is not possible to rule out aggregation at the glass walls. In fact, the case for this kind of sorption is supported by the higher mass sorbed to the column system of VIC PFAS than non-VIC PFAS in all tests (Table 2). During the injection phase, the falling air–water interface might “collect” these PFASs sorbed to the glass Erlenmeyer, which leads to increased concentrations at the air–water interface at the end of the injection phase.

To explain why particular PFASs accumulate at the air–water interface and/or glass walls, while other PFASs do not, we compared the air–water interfacial sorption coefficient (K_{AW}) and the chain length of the substances in this study (Psillakis et al., 2009). The K_{AW} range for the VIC PFAS species falls between -5.2 and -2.9 log, whereas the non-VIC PFASs have a K_{AW} ranging from -3.9 to -1.4 log (Mudlaff et al., 2024). This overlap suggests that differences in reported K_{AW} values alone do not fully explain the distinct air–water interface enrichment behavior observed here. However, it should be noted that literature K_{AW} values may not fully represent this system, particularly for ionic PFASs (all substances used in this study, except PFOSA), whose interfacial behavior is strongly influenced by solution chemistry (e.g., pH, ionic strength, and multivalent cations). As a result, these K_{AW} values may not accurately reflect the effective interfacial partitioning in the injection container. In contrast, carbon chain length is known to strongly influence PFAS surface activity and interfacial adsorption (Brusseau & Van Glubt, 2021). Therefore, carbon chain length may provide a better explanation of this distinct behavior of VIC PFAS, as each of the five VIC PFASs have a carbon chain length of 8 or more. However, as some PFASs in this study have a chain length of 8 (but not more) and do not show the same behavior (e.g., 6:2 fluorotelomer sulfonic acid), other characteristics must also contribute to this behavior. Solubility could be a significant factor, as the range for the VIC PFAS is -0.98 to 1.51 log₁₀ mg/L, in comparison with 1.34 – 3.09 log₁₀ mg/L for non-VIC PFASs (Sosnowska et al., 2023). Nevertheless, despite perfluorooctanoic acid and 9CL-PF3ONS both possessing a chain length of 8 and solubilities of 1.34 and 1.51 log₁₀ mg/L, respectively, the former is not a VIC PFAS, while the latter is. This discrepancy might be due to differences in molecular structure—9CL-PF3ONS contains an oxygen atom within its carbon skeleton, potentially altering its behavior (Allendorf et al., 2019). This shows that the

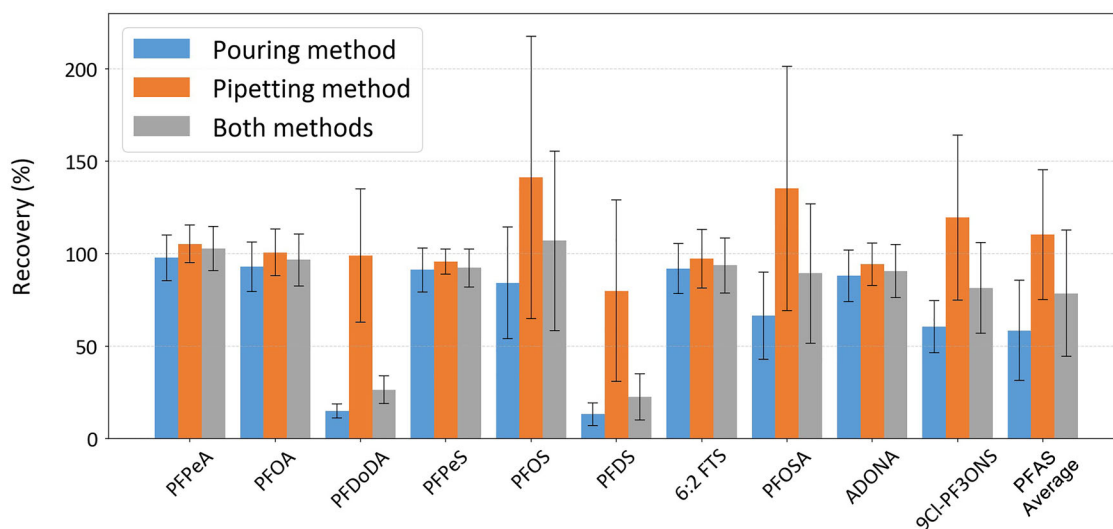


FIGURE 2 Average total mass recovery for CT1-4 as found by using the pouring method, pipetting method, and the average of these two methods to calculate injection mass. CT5 was excluded because of the significantly lower injection concentrations. 6:2 FTS, 6:2 fluorotelomer sulfonic acid; 9Cl-PF3ONS, 9-chlorohexadecafluoro-3-oxanonane-1-sulfonic acid; ADONA, 4,8-dioxa-3H-perfluorononanoic acid; PFDODA, perfluorododecanoic acid; PFDS, perfluorodecanesulfonic acid; PFOS, perfluorooctanesulfonic acid; PFOA, perfluorooctanoic acid; PFOSA, perfluorooctane sulfonamide; PFPeA, perfluoropentanoic acid; PFPeS, perfluoropentanesulfonic acid.

VIC phenomenon cannot be predicted on the basis of a single characteristic.

The phenomena in this study were observed under a specific experimental configuration, and injection container shape, material, and surface-area-to-volume ratios may influence the magnitude of the effect. We found that stirring alone does not resolve this problem, even if it disrupts the air–water interface by creating a vortex. Alternative solutions may include ensuring that the surface area to volume ratio does not become too large. This could be achieved, for instance, by using a larger injection volume that is not fully injected, or a differently shaped flask, such as a graduated cylinder or a cylindrical container. Despite these solutions, the surface area to volume ratio of the injection solution would still, to a certain extent, increase over time during injection. Furthermore, the material of the injection container may have influenced the concentrations due to potential sorption to the glass walls. Other materials, such as polypropylene or high-density polyethylene, might show better performance and should be considered in future experiments.

4 | CONCLUSIONS

Of the 10 investigated PFASs, five substances, characterized by longer carbon chain lengths and lower solubility than the others, were found to increasingly congregate at the air–water interface during injection, resulting in a non-homogenous distribution in the water column of the injection solution. While sampling the injection solution by pipet did not overcome

the difficulties in accurately establishing the injection mass for each PFAS in all experiments, it did show a significant improvement over pouring.

These findings suggest that care must be taken when determining concentrations of PFASs in injection solutions during soil column experiments. Factors that need consideration include the material and shape of the injection container, the sampling method, what point in the water column is sampled, and the frequency and intervals at which sampling is conducted. Furthermore, it should be considered to wash all materials that came into contact with PFASs using a solvent (such as ethanol). These samples should then be measured for PFAS concentration, as adsorption can occur on any material.

Addressing these challenges is crucial for accurately determining injection mass and closing the mass balance during injection–extraction experiments with PFASs, which in turn enables the correct determination of sorption rates. These considerations, as well as the phenomena discussed in this study, should be taken into account and documented thoroughly in future PFAS injection–extraction experiments, including remediation investigations.

AUTHOR CONTRIBUTIONS

Thomas J. Oudega: Conceptualization; data curation; investigation; methodology; visualization; writing—original draft; writing—review and editing. **Ali A. A. Obeid:** Conceptualization; data curation; methodology; visualization. **Nicolas Devau:** Conceptualization; methodology. **Ottavia Zoboli:** Conceptualization; writing—review and editing. **Claudia Gundacker:** Conceptualization. **Matthias Zessner:** Concep-

tualization. **Ernis Saracevic**: Conceptualization; formal analysis; investigation; methodology; resources. **Jörg Krampe**: Conceptualization. **Margaret E. Stevenson**: Conceptualization; supervision. **Julia Derx**: Conceptualization; methodology; supervision; writing—review and editing.

ACKNOWLEDGMENTS

This research was funded by the European Union's Horizon 2020 Research and Innovation Programme [grant number 101036449, "PROMISCES"] and by the Vienna Science and Technology Fund (WWTF) [grant number 10.47379/ESR20013]. Additional support came from the Vienna Water Resource Systems Project (ViWa 2020+), a research cooperation between Vienna Water (MA31) and the ICC Water & Health.


CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

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How to cite this article: Oudega, T. J., Obeid, A. A., Devau, N., Zoboli, O., Gundacker, C., Zessner, M., Saracevic, E., Krampe, J., Stevenson, M. E., & Dery, J. (2026). Effects of a variable air–water interface on injection of PFAS—Lessons learned from column tests with porous media. *Vadose Zone Journal*, 25, e70097. <https://doi.org/10.1002/vzj2.70097>