

Assessment of PFAS Mobility in Soil–Groundwater Systems Based on Adsorption Characteristics

JongHyun Yoon

National Institute of Environmental Research

Kyungjin Han

Korea National University of Transportation

Hyeonhee Choi

National Institute of Environmental Research

Seunghwan Park

National Institute of Environmental Research

JongBeom Kwon

National Institute of Environmental Research

KyungEung Ha

National Institute of Environmental Research

Seong-Yu Noh

National Institute of Environmental Research

Yong Sik Ok

Korea University

Moonsu Kim

National Institute of Environmental Research

Sunhwa Park

parksu@korea.kr

National Institute of Environmental Research

Research Article

Keywords: PFAS, groundwater chemistry, soil organic matter, relative mobility, carbonaceous sorbents, hydrogeochemical controls

Posted Date: October 8th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10464069/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.
[Read Full License](#)

Additional Declarations: No competing interests reported.

1 **Assessment of PFAS Mobility in Soil–Groundwater Systems Based on**
2 **Adsorption Characteristics**

3
4 JongHyun Yoon¹, Kyungjin Han², Hyeonhee Choi¹, Seunghwan Park¹, JongBeom Kwon¹, KyungEung Ha¹,
5 Seong-Yu Noh¹, Yong Sik Ok³, Moon-su Kim¹, Sunhwa Park^{*1}

6 ¹ National Institute of Environmental Research, Hwangyong-ro 42, Seo-gu, Incheon, 404-708, Republic of
7 Korea

8 ² Korea Biochar Research Center & Division of Environmental Science and Ecological Engineering, Korea
9 University, Seoul 02841, Republic of Korea

10 ³ Department of Environmental Engineering, Korea National University of Transportation, Chungju, 27469,
11 Republic of Korea

12

13 * Corresponding author email: parksu@korea.kr

14

Abstract

Per- and polyfluoroalkyl substances in soil–groundwater systems are influenced by molecular structure, soil characteristics, and groundwater chemistry, which determine their mobility and leaching behavior. This study evaluated PFAS adsorption using soils collected from three depth intervals (0–30, 30–60, and 60–90 cm) and groundwater matrices with contrasting ionic compositions. Apparent distribution coefficients and screening-level retardation factors were estimated from batch experiments to assess relative PFAS mobility. Adsorption increased with carbon-chain length and was greater in shallow soils with higher organic matter contents than in deeper soils. Retardation factors decreased with depth, indicating enhanced mobility in subsurface layers. Groundwater matrices reduced adsorption compared with deionized water, particularly for short-chain PFASs, suggesting that dissolved ions limited sorption. Among the tested carbonaceous sorbents, activated carbon exhibited the highest adsorption capacity, although removal efficiencies for short-chain PFASs remained moderate in contaminated groundwater. Overall, PFAS mobility in soil–groundwater systems were governed by PFAS structure, soil characteristics, and groundwater geochemistry. These findings provide a screening-level framework for evaluating PFAS leaching under groundwater-relevant conditions.

Keywords: PFAS, groundwater chemistry, soil organic matter, relative mobility, carbonaceous sorbents, hydrogeochemical controls

1. Introduction

Per- and polyfluoroalkyl substances (PFASs) are synthetic compounds with exceptional chemical stability and resistance to environmental degradation. Due to their water- and oil-repellent properties, PFASs are widely used across various industries, notably in nonstick cookware, waterproof coatings, and stain-resistant textiles (Arvaniti and Stasinakis, 2015; Du et al., 2014; Li et al., 2020; Oliver et al., 2019; Pereira et al., 2018). The strong carbon–fluorine bonds allow PFASs to persist in the environment for decades (Drobny, 2007; Harsanyi and Sandford, 2015; Riess, 2009).

39 PFAS contamination has become a global concern, with detectable levels reported in diverse environments
40 such as glaciers, riversides, agricultural fields, and urban groundwater sources (Chen et al., 2016; Gallo et
41 al., 2020; Liu et al., 2018; Loos et al., 2010; McMahon et al., 2022; Miao et al., 2017; Murakami et al.,
42 2009; Park et al., 2020; Peshoria et al., 2020; Savoca and Pace, 2021). Their persistence and widespread
43 occurrence have led to increasing regulatory attention, including classification as persistent organic
44 pollutants (POPs) and the development of management and remediation strategies (Agency, 2021).

45 Research on PFAS remediation has mainly focused on drinking water treatment, with activated carbon
46 (AC), anion exchange resins, and coagulation treatment emerging as the leading methods due to their high
47 removal efficiencies (Crone et al., 2019; Dickenson and Higgins, 2016, Park et al., 2021). Activated carbon
48 has been widely applied because of its high adsorption capacity under various water chemistry conditions
49 (Appleman et al., 2013; Falciglia et al., 2020; Hansen et al., 2010; Hashim et al., 2011; Inyang and
50 Dickenson, 2017; Marsh and Reinoso, 2006; Mohan and Pittman Jr, 2006; Montaña et al., 2013). More
51 recently, biochar has gained attention as a low-cost alternative due to its variable pore structure, with
52 favorable adsorption performance (Chen et al., 2011; Dong et al., 2011; Inyang and Dickenson, 2015;
53 Mukherjee et al., 2011; Wang et al., 2015).

54 In subsurface environments, PFAS risk is governed not only by removal efficiency but also by transport
55 processes along soil–groundwater flow paths. Although previous studies have provided valuable
56 information on PFAS adsorption by soils and carbonaceous materials, the combined influence of soil
57 characteristics and groundwater chemistry on PFAS mobility remains insufficiently understood. In
58 particular, limited information is available on the relationships among soil organic matter, groundwater
59 ionic composition, and PFAS molecular structure. This distinction is important because adsorption
60 behavior observed in deionized water or simplified aqueous systems may overestimate PFAS attenuation,
61 particularly for short-chain PFASs (Molé et al., 2024).

62 In this study, PFAS adsorption by soils collected from three depth intervals and carbonaceous sorbents was
63 evaluated using groundwater matrices with contrasting ionic compositions. The objective was to determine
64 how PFAS structure, soil organic matter, and groundwater chemistry affect PFAS mobility in soil–
65 groundwater systems as previous contaminant transport test in soil column (Patil et al., 2023). Apparent

distribution coefficients and screening-level retardation factors were estimated from batch experiments to interpret PFAS transport behavior. We hypothesized that (i) PFAS adsorption increases with carbon-chain length, (ii) shallow soils enriched with organic matter exhibit greater adsorption than deeper soils, and (iii) groundwater chemistry reduces adsorption more strongly for short-chain PFASs.

2. Materials and Methods

2.1. Standard solution for PFASs

High-purity standard solutions were utilized to examine the adsorption characteristics of per- and polyfluoroalkyl substances (PFASs). These included PFAC-MXA (>98% purity), PFAC-MXB (>98% purity), PFUnDA (>98% purity), and MPFAC-MXA (>98% purity), all sourced from Wellington Laboratories (Southgate, Canada). PFAC-MXA comprises ten PFAS compounds, such as perfluorobutanoic acid (PFBA), perfluoropentanoic acid (PFPeA), perfluorohexanoic acid (PFHxA), perfluoroheptanoic acid (PFHpA), perfluorooctanoic acid (PFOA), perfluorononanoic acid (PFNA), perfluorodecanoic acid (PFDA), perfluorobutanesulfonic acid (PFBS), perfluorohexanesulfonic acid (PFHxS), and perfluorooctanesulfonic acid (PFOS). PFAC-MXB includes a wider array of fifteen PFAS compounds, expanding upon PFAC-MXA with additional long-chain compounds, such as perfluoroundecanoic acid (PFUnDA), perfluorododecanoic acid (PFDoDA), perfluorotridecanoic acid (PFTrDA), perfluorotetradecanoic acid (PFTeDA) and perfluorodecanesulfonic acid (PFDS). The MPFAC-MXA internal standard, containing nine labeled PFAS analogs (MPFBA, MPFHxA, MPFOA, MPFNA, MPFDA, MPFUdA, MPFDoA, MPFHxS, and MPFOS), ensured analytical consistency. These standards facilitated precise quantification of adsorption dynamics in both deionized water (DIW) and groundwater matrices.

2.2. Soil and adsorbent preparation

Three soil types, representing depths of 0–30 cm, 30–60 cm, and 60–90 cm, were selected to evaluate PFAS adsorption in DIW and groundwater. These soils, with organic matter contents of 3.9%, 2.9%, and 1.8%, respectively, were sieved through a 10-mesh screen for uniformity in adsorption testing.

Activated carbon (AC) and two biochar variants wood charcoal (WC) and chaff biochar (CF) served as adsorbents. Each adsorbent was sieved through a 100-mesh screen for particle consistency. WC and CF were acquired from KD Development (Gyeonggi-do, Korea) and Yougi Industry Co. (Jeollabuk-do, Korea), respectively, and were produced via pyrolysis at 300 °C and 500–650 °C, resulting in organic contents of 65–70% for WC and 62% for CF.

2.3. Groundwater preparation

Three groundwater matrices (JH, FH, and DH) were used in the adsorption tests. JH and FH were collected from sites without detectable PFAS contamination and were used to evaluate PFAS retention in soils under uncontaminated groundwater conditions. DH was collected from a PFAS-contaminated site and was used to evaluate PFAS removal by activated carbon under contaminated groundwater conditions.

2.4. Experiment procedure for adsorption tests

2.4.1. PFAS adsorption tendency test (STT)

The STT was conducted to evaluate PFAS retention in soils under DIW and groundwater conditions. For this test, 1 g of soil was combined with 10 mL of DIW, JH groundwater, or FH groundwater. The physical and chemical properties of the soils are provided in Table 1, and the cation and anion compositions of DIW, JH, and FH are provided in Table 3. Fifteen PFASs were tested at the initial concentrations listed in Table 2 using PFAC-MXB as the standard mixture. The mixtures were agitated at 70 rpm and maintained at 20 °C for 14 days in polypropylene (PP) containers to minimize container-related adsorption. Analytical conditions for PFAS quantification are provided in Tables 3 and 4.

2.4.2. PFAS adsorption kinetic test (SKT)

The SKT was conducted to evaluate the time-dependent adsorption of PFASs by activated carbon (AC), wood charcoal (WC), and chaff biochar (CF). PFAC-MXA and PFUnDA were used to prepare an 11-PFAS mixture in DIW at the initial concentrations listed in Table 5. Each adsorbent (0.05 g) was placed in a PP container with the PFAS solution and agitated at 40 rpm. Samples were collected after 0.25, 1, 3, 6, and 10 days. The test was conducted at 20–25 °C, and the pH was maintained between 6.5 and 7.5.

2.4.3. PFAS removal efficiency test (REAG)

The REAG test was conducted to evaluate PFAS removal by AC in contaminated groundwater from site DH. The initial PFAS concentrations in DH groundwater are listed in Table 5. Samples were collected after 0.25, 0.5, 1, 3, 5, and 8 days. The ionic composition of DH groundwater, including major anions and cations, is provided in Table 2.

2.5. PFAS extraction and analysis method

PFASs were extracted from groundwater and batch test samples by following a systematic protocol involving suspended solid filtration, cartridge activation, sample loading, cartridge drying, and final elution. The extraction was performed using a Visiprep vacuum manifold (Supelco) equipped with Oasis HLB cartridges (Waters).

To prepare the cartridges for PFAS capture, activation was carried out by passing HPLC-grade methanol followed by DIW through each cartridge in sequence. Subsequently, the filtered groundwater or batch test samples were introduced to the activated cartridges at a controlled flow rate of 10–15 mL/min, ensuring thorough interaction with the adsorbent media. Following sample loading, each cartridge was dried under vacuum conditions for approximately 30 minutes to remove residual moisture.

For PFAS desorption, 8 mL of HPLC-grade methanol was applied in two separate 4 mL aliquots, ensuring optimal recovery of PFAS analytes from the cartridges into a 15 mL polypropylene vial. The eluted PFAS solution was then concentrated using an N-EVAPTM 112 evaporator (Organomation Associates Inc., USA), after which it was rinsed three times with 1 mL portions of HPLC-grade methanol to eliminate any potential contaminants. The final sample volume was adjusted to 0.4 mL by adding HPLC-grade methanol.

High-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) analysis was conducted using a TSQ Altis Plus instrument (ThermoFisher). Detection and quantification were achieved via electrospray ionization (ESI), employing both precursor and product ions for each PFAS analyte. Analytical conditions, as well as precursor and product ion parameters, are detailed in Tables 3 and 4. These procedures ensured precise quantification and identification of PFAS concentrations in both groundwater and batch samples, facilitating comprehensive analysis of adsorption behaviors.

2.6. Data analysis

2.6.1. Calculation of PFAS concentration in soil

The concentration and mass of PFAS adsorbed onto soil and other absorbents were determined using indirect calculation methods as described in Eq. (1) and (2) (OECD, 2000).

$$m_s^{abs}(eq) = m_0 - m_{aq}(eq) = [C_0 - C_{aq}(eq)]V_0 \quad \text{Eq. (1)}$$

$$C_s^{abs}(eq) = \frac{[C_0 - C_{aq}(eq)]V_0}{m_{absorbent}} \quad \text{Eq. (2)}$$

Where, V_0 represents the initial liquid volume (L); m_0 denotes the initial mass of PFAS in the liquid (μg); $m_{absorbent}$ is the mass of the absorbent (g); $m_{aq}(eq)$ is the PFAS mass in the liquid at adsorption equilibrium (μg); $m_s^{abs}(eq)$ represents the PFAS mass adsorbed onto the absorbent at equilibrium (μg); C_0 is the initial PFAS concentration in the liquid ($\mu\text{g/L}$); $C_{aq}(eq)$ is the PFAS concentration in the liquid at equilibrium ($\mu\text{g/L}$) and $C_s^{abs}(eq)$ is the concentration of PFAS adsorbed onto the absorbent at equilibrium ($\mu\text{g/g}$).

2.6.2. Estimation of apparent distribution coefficients and retardation factors

To interpret the STT results in terms of relative subsurface mobility, apparent distribution coefficients (K_d) were estimated from the batch adsorption data using the soil-to-solution ratio applied in the experiment:

$$K_d = \frac{V}{m} \times \frac{C_0 - C_e}{C_e} \quad \text{Eq. (3)}$$

Where V is the solution volume (L), m is the dry soil mass (kg), C_0 is the initial aqueous PFAS concentration, and C_e is the equilibrium aqueous PFAS concentration. Because the STT used 1 g of soil and 10 mL of solution, $\frac{V}{m}$ was 10 L/kg. Screening-level retardation factors (R_f) were then estimated as:

$$R_f = 1 + \frac{\rho_b K_d}{n} \quad \text{Eq. (4)}$$

Where ρ_b is the soil bulk density and n is porosity. The soil bulk density and porosity values used for this calculation were obtained from the soil characterization results. These values were used to compare relative

PFAS mobility across soil depths and water matrices. The calculated K_d and R_f values should be interpreted as batch-derived screening indicators rather than field-scale transport parameters.

2.6.3. Empirical kinetic models for SKT

Empirical kinetic models were applied to the SKT results to describe time-dependent adsorption behavior on the tested carbonaceous sorbents. Four models were considered: pseudo-first-order (PFO), pseudo-second-order (PSO), pseudo-third-order (PTO), and Elovich models.

Pseudo-first-order (PFO)

The PFO model, as shown in Eq. (5), describes the rate of adsorption onto absorbents over time (Aitali et al., 2016; Lagergren, 1898; Wang et al., 2020).

$$q_t = q_{e,1}(1 - e^{-k_1 \times t}) \quad \text{Eq. (5)}$$

Where, q_t ($\mu\text{g/g}$) is the adsorption amount at time t (hours); $q_{e,1}$ ($\mu\text{g/g}$) is the equilibrium adsorption capacity, and k_1 (h^{-1}) is the PFO rate constant.

Pseudo-second-order (PSO)

The PSO model, presented in Eq. (6), is widely used to describe adsorption processes by estimating rate constants and predicting adsorption trends (Aitali et al., 2016; Wang et al., 2020).

$$q_t = q_{e,2}^2 k_2 t / (1 + q_{e,2} k_2 t) \quad \text{Eq. (6)}$$

Where, $q_{e,2}$ ($\mu\text{g/g}$) is the equilibrium adsorption capacity, and k_2 ($\text{g}/\mu\text{g/h}$) is the PSO rate constant.

Pseudo-third-order (PTO)

The PTO model, described in Eq. (7), was applied as an empirical higher-order kinetic model to describe nonlinear adsorption trends (Özer, 2007; Wang et al., 2020).

$$[1/(q_{e,3} - q_t)]^{1/2} = 2k_3 t + (1/q_t)^{1/2} \quad \text{Eq. (7)}$$

Where, k_3 ($\text{g}^2/\mu\text{g}^2/\text{hr}$) is the rate constant for the Pseudo-Third Order (PTO).

Elovich model

The Elovich model, given in Eq. (8), is used for adsorption systems with uneven surfaces and variable activation energy over time (Elovich et al., 1962; Wang et al., 2020).

$$q_t = \frac{1}{b} \ln(1 + \alpha b t) \quad \text{Eq. (8)}$$

Where, α ($\mu\text{g/g/hr}$) is the initial adsorption rate constant, and b ($\text{g}/\mu\text{g}$) is the desorption rate constant. These models provide a comprehensive framework for understanding PFAS adsorption kinetics across various adsorbents and conditions, facilitating comparison of equilibrium behaviors and adsorption rates (Chien et al., 1980; Ho et al., 1999; Lagergren, 1898).

3. Results and discussion

3.1. PFAS retention across soil-depth and water-matrix gradients

The STT results showed that PFAS retention varied systematically with PFAS molecular structure, soil depth, and water matrix (Fig. 1). Under DIW conditions, adsorption generally increased with increasing carbon-chain length for both PFCAs and PFASs. Longer-chain compounds showed substantially higher retention than shorter-chain compounds, with maximum adsorption reaching 98.8% for the strongly retained PFASs. This pattern indicates that PFAS molecular structure, particularly carbon-chain length, was a primary factor controlling retention in the tested soils.

Soil depth also influenced PFAS retention. For example, PFOA adsorption decreased from 30.5% in the 0–30 cm soil to 23.2% in the 30–60 cm soil and only 0.3% in the 60–90 cm soil (Fig. 1a). This decrease is consistent with the decline in soil organic matter content from 3.9% in the surface soil to 2.9% in the middle soil and 1.8% in the deep soil (Table 1). Because organic matter provides important sorption domains for PFASs, particularly for compounds with longer perfluorinated chains, the lower retention in deeper soils indicates a reduced attenuation capacity with depth (Fabregat-Palau et al., 2021; Milinovic et al., 2021; Mohona et al., 2023; Pereira et al., 2018).

The effect of water matrix was also evident. Although chain-length-dependent retention was observed in both DIW and groundwater matrices, adsorption was generally lower in groundwater, particularly for shorter-chain PFASs (Fig. 1). In groundwater, adsorption efficiencies decreased to below 20% for PFCAs with fewer than nine carbons and for PFASs with six or fewer carbons. This suggests that groundwater constituents weakened PFAS retention, especially for compounds that already had low sorption affinity (Du et al., 2014; Walters et al., 1991; Wang et al., 2012).

The contrast between FH and JH further supports the role of groundwater chemistry. FH contained higher concentrations of major ions, including Cl^- , Na^+ , Ca^{2+} , and Mg^{2+} , than JH (Table 2), and PFDA adsorption was lower in FH than in JH. These results indicate that groundwater ionic composition can suppress PFAS retention even when the same soil matrix is used. Therefore, retention patterns observed in DIW should not be directly extrapolated to groundwater conditions without considering groundwater geochemistry (Chen et al., 2016; Yu et al., 2016).

3.2. Apparent distribution coefficients and screening-level retardation factors

Apparent distribution coefficients K_d and screening-level retardation factors R_f were estimated from the STT results to translate batch adsorption behavior into a relative mobility context (Table 6 and Table 7). The calculation 7 used the soil-to-solution ratio applied in the STT and the soil bulk density and porosity values for each depth interval (Table 1). Because these values were derived from batch adsorption data, they should be interpreted as apparent and screening-level indicators rather than direct field-scale transport parameters.

The estimated K_d and R_f values showed that PFAS retardation potential decreased with soil depth. For example, PFOA adsorption decreased from 30.5% in the 0–30 cm soil to 23.2% in the 30–60 cm soil and 0.3% in the 60–90 cm soil (Fig. 1a). These adsorption values corresponded to estimated K_d values of approximately 4.39, 3.02, and 0.03 L/kg, respectively, and the corresponding R_f values decreased from approximately 8.1 to 5.1 and 1.1 (Table 7). This result indicates that the surface soil had a measurable capacity to retard PFOA, whereas the deep soil provided little retardation, with an R_f value close to unity.

The depth-dependent decrease in R_f was consistent with the decrease in soil organic matter content from 3.9% in the surface soil to 2.9% in the middle soil and 1.8% in the deep soil (Table 1). This relationship suggests that the greater retention observed in shallow soil was associated with higher organic matter content, while deeper low-organic-matter soil had lower attenuation capacity. Therefore, once PFASs migrate below the organic-matter-rich surface layer, their relative mobility may increase substantially, particularly for compounds with weak sorption affinity.

The K_d and R_f values also clarified compound-specific mobility differences. Short-chain PFASs such as PFBA, PFHxA, and PFBS generally showed low estimated retardation, especially under groundwater conditions, whereas longer-chain compounds such as PFDA and PFOS showed higher K_d and R_f values (Table 7). This pattern indicates that the mobility risk is not uniform across PFASs. Short-chain compounds are more likely to remain in the aqueous phase and migrate with groundwater, while longer-chain compounds are more likely to be delayed by soil or sorbent retention.

Groundwater chemistry further modified these mobility patterns. Compared with DIW, the groundwater matrices generally reduced adsorption and lowered estimated retardation for weakly retained PFASs (Fig. 1 and Table 7). This effect was particularly relevant for short-chain compounds, which already had low K_d and R_f values. The higher ionic composition of FH relative to JH (Table 2) supports the interpretation that groundwater geochemistry can suppress PFAS retention and increase relative mobility under aquifer-relevant conditions.

Overall, the K_d and R_f estimates strengthen the hydrogeochemical interpretation of the STT results. Adsorption percentages alone show how much PFAS was removed from solution under batch conditions, whereas R_f provides a transport-relevant indicator of how strongly PFAS movement may be delayed relative to groundwater flow. The results therefore indicate that PFAS relative mobility in soil–groundwater systems is controlled by the combined effects of PFAS structure, soil depth-associated organic matter, and groundwater chemistry (Appleman et al., 2014; Carter et al., 2010; Du et al., 2014; Kupryianchyk et al., 2016; Ochoa-Herrera et al., 2008; Yu et al., 2009).

3.3. Structure-dependent PFAS retention in carbonaceous sorbents

The SKT results were used to evaluate whether carbonaceous sorbents altered the structure-dependent retention patterns observed in the soil and groundwater matrices. Adsorption generally increased rapidly during the initial contact period and approached equilibrium within approximately three days (Fig. 2). Among the tested sorbents, activated carbon showed the highest adsorption capacity, followed by chaff biochar and wood charcoal (Fig. 2 and Fig. 3).

The higher retention by activated carbon was most evident for longer-chain PFASs. For example, PFUnDA and PFOS showed greater adsorption on activated carbon than on the two biochars (Fig. 2 and Table 6). The modeled equilibrium capacities also increased with increasing carbon-chain length for PFCAs and were generally higher for PFASs than for shorter-chain PFCAs (Fig. 3 and Table 6). These results indicate that activated carbon enhanced PFAS retention, but the relative adsorption hierarchy remained strongly dependent on PFAS molecular structure (Gagliano et al., 2020; Li et al., 2018; Wei et al., 2017).

Empirical kinetic models were applied to describe the time-dependent adsorption patterns (Table 6). However, the model-specific fitting results are interpreted here as supporting information rather than as the main mechanistic finding. The high model fits confirm rapid initial uptake and stronger affinity of activated carbon relative to the two biochars, but assigning different best-fit kinetic models to individual compounds does not by itself explain PFAS mobility in soil–groundwater systems. Therefore, the SKT results are used mainly to support the conclusion that sorbent type modifies retention capacity, whereas compound structure continues to govern the relative retention hierarchy.

The sorbent results also provide an important practical perspective on compound-specific retention. Activated carbon showed strong PFAS retention in the SKT, but the lower adsorption of short-chain PFASs across the tested sorbents indicates that engineered sorption does not fully eliminate compound-specific mobility differences. Therefore, sorption-based management strategies should not be evaluated only by total PFAS removal, because overall removal efficiency may mask the persistence of the more mobile short-chain fraction.

3.4. Short-chain PFAS persistence under contaminated groundwater conditions

The REAG results showed that PFAS removal by activated carbon in DH groundwater remained strongly compound-specific (Fig. 4). Removal increased with contact time, but the extent of removal differed substantially among the ten PFASs tested. Longer-chain compounds such as PFDA and PFOS reached approximately 80–90% removal after 8 days, whereas shorter-chain compounds such as PFBA and PFPeA remained only moderately removed, generally in the range of 20–40% (Fig. 4).

This result indicates that activated carbon can improve PFAS retention under contaminated groundwater conditions, but it does not fully overcome the low retention of short-chain PFASs. The DH groundwater contained multiple major ions, including HCO_3^- , Cl^- , SO_4^{2-} , Na^+ , Ca^{2+} , and Mg^{2+} (Table 2). These solutes may reduce PFAS adsorption by competing for interaction sites, altering surface charge conditions, or changing PFAS partitioning behavior in solution. Although the present study did not isolate the effect of individual ions, the results show that chemically complex groundwater can constrain sorption performance (Chen et al., 2017; Crone et al., 2019; Deng et al., 2015; Johnson et al., 2007; Zhi et al., 2015; Zhi et al., 2016).

The REAG results are consistent with the STT and K_d/R_f interpretations. Short-chain PFASs showed lower retention in soils and groundwater matrices, lower estimated retardation potential, and lower removal by activated carbon in contaminated groundwater. This repeated pattern across natural soils, groundwater matrices, and engineered carbonaceous sorbents indicates that short-chain PFASs have greater relative mobility under groundwater-relevant conditions.

The findings also show that adsorption results obtained in DIW or simple aqueous systems can overestimate PFAS attenuation in groundwater. Even though activated carbon was the most effective sorbent in the SKT, its performance in DH groundwater remained limited for shorter-chain compounds. Therefore, groundwater chemistry should be considered together with sorbent type and PFAS structure when evaluating sorption-based approaches for contaminated groundwater.

3.5. Hydrogeochemical implications for PFAS mobility in soil–groundwater

systems

Taken together, the STT, SKT, REAG, and K_d/R_f results indicate that PFAS retention and relative mobility in soil–groundwater systems are governed by interacting hydrogeochemical controls. PFAS molecular structure determined the baseline retention tendency, with longer-chain compounds showing stronger retention and short-chain compounds remaining more mobile. Soil depth-associated organic matter modified this behavior by increasing retention in shallow soils and reducing attenuation capacity in deeper soils. Groundwater chemistry further modified retention by suppressing adsorption under ion-rich conditions, particularly for weakly retained PFASs.

These findings have direct implications for PFAS leaching assessment. Shallow soils with higher organic matter content may delay PFAS movement, but this attenuation capacity decreases substantially with depth. Once PFASs migrate into deeper low-organic-matter layers, weakly sorbing compounds may move with limited retardation. This pattern is especially important for short-chain PFASs because they combine low sorption affinity with greater sensitivity to groundwater-matrix effects. Therefore, PFAS site assessment should consider PFAS-specific structure, soil depth-associated properties, and groundwater chemistry together rather than relying only on total PFAS concentrations or adsorption results obtained in simplified water matrices.

The principal contribution of this study is not the identification of activated carbon as the best-performing sorbent, but the demonstration that hydrogeochemical conditions control PFAS retention and relative mobility in soil–groundwater systems. Although the K_d and R_f values derived here are screening-level indicators based on batch tests, they provide a useful bridge between adsorption data and subsurface mobility interpretation. Further column experiments and field-scale transport modeling are needed to quantify actual migration rates, but the present results provide a screening-level hydrogeochemical basis for understanding why short-chain PFASs are more difficult to attenuate under groundwater-relevant conditions.

4. Conclusion

This study demonstrates that PFAS retention and relative mobility in soil–groundwater systems are jointly controlled by PFAS molecular structure, soil depth-associated properties, and groundwater geochemistry. PFAS retention generally increased with carbon-chain length and decreased with soil depth, consistent with the decline in organic matter content from shallow to deeper soils. These results indicate that organic-matter-rich shallow soils can provide greater attenuation capacity, whereas deeper low-organic-matter soils may allow more mobile PFAS transport.

The apparent distribution coefficients and screening-level retardation factors provided a transport-relevant interpretation of the batch adsorption results. The estimated retardation potential decreased markedly with soil depth, and short-chain PFASs generally showed low retention and low retardation under groundwater-relevant conditions. Groundwater matrices further reduced adsorption compared with DIW, particularly for short-chain compounds, indicating that groundwater ionic composition can weaken PFAS retention and increase relative mobility.

Activated carbon showed the highest PFAS retention among the tested carbonaceous sorbents, but the contaminated groundwater test confirmed that short-chain PFASs remained difficult to retain or remove even after prolonged contact. Therefore, the principal contribution of this study is not the identification of a single best-performing sorbent, but the demonstration that hydrogeochemical conditions govern PFAS retention and relative mobility in soil–groundwater systems. The batch-derived K_d and R_f values should be interpreted as screening-level indicators, and further column experiments or reactive transport modeling will be needed to quantify PFAS migration under dynamic flow conditions.

Acknowledgements

The authors acknowledged the financial contribution from the Ministry of Environment of the Republic of Korea.

Credit authorship contribution statement

JongHyun Yoon: Investigation, Data curation, Visualization. Kyungjin Han: Writing – original draft. Hyeonhee Choi: Investigation, Data curation, Visualization. Seunghwan Park: Investigation, Data curation, Visualization. JongBeom Kwon: Investigation, Data curation, Visualization, Writing – original draft. KyungEung Ha: Investigation, Data curation, Visualization. Seong-Yu Noh: Writing – review & editing. Yong Sik Ok: Writing – review & editing. Moonsu Kim: Writing – review & editing. Sunhwa Park: Conceptualization, Methodology, Writing – original draft, Supervision.

Funding

This work was supported by a grant from the National Institute of Environmental Research (NIER), funded by the Ministry of Environment (MOE) of the Republic of Korea (NIER-2026-01-01-063). The biochar samples were produced through the funding from the Korea Biochar Research Center and this work partly was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-00555967).

Data availability

All data generated or analyzed during this study are included in this article.

Declaration of competing interest

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

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors did not use any generative AI or AI-assisted technologies.

References

Agency, U. E. P. (2021). PFAS Strategic Roadmap: EPA's Commitments to Action 2021–2024, EPA-100-K-21-002.

378 Aitali, S., Kebiche-Senhadj, O., and Benamor, M. (2016), "Performance of an acidic extractant (D2EHPA)
379 incorporated in IM used for extraction and separation of Methylene Blue and Rhodamin B", *Membrane*
380 *and Water Treatment*, 7(6), 521-537.

381 Appleman, T. D., Dickenson, E. R., Bellona, C., & Higgins, C. P. (2013). Nanofiltration and granular
382 activated carbon treatment of perfluoroalkyl acids. *Journal of hazardous materials*, 260, 740-746.

383 Appleman, T. D., Higgins, C. P., Quiñones, O., Vanderford, B. J., Kolstad, C., Zeigler-Holady, J. C., &
384 Dickenson, E. R. (2014). Treatment of poly-and perfluoroalkyl substances in US full-scale water
385 treatment systems. *Water research*, 51, 246-255.

386 Arvaniti, O. S., & Stasinakis, A. S. (2015). Review on the occurrence, fate and removal of perfluorinated
387 compounds during wastewater treatment. *Science of the Total Environment*, 524, 81-92.

388 Carter, K. E., & Farrell, J. (2010). Removal of perfluorooctane and perfluorobutane sulfonate from water
389 via carbon adsorption and ion exchange. *Separation Science and Technology*, 45(6), 762-767.

390 Chen, S., Jiao, X. C., Gai, N., Li, X. J., Wang, X. C., Lu, G. H., ... & Yang, Y. L. (2016). Perfluorinated
391 compounds in soil, surface water, and groundwater from rural areas in eastern China. *Environmental*
392 *Pollution*, 211, 124-131.

393 Chen, W., Zhang, X., Mamadiev, M., & Wang, Z. (2017). Sorption of perfluorooctane sulfonate and
394 perfluorooctanoate on polyacrylonitrile fiber-derived activated carbon fibers: in comparison with
395 activated carbon. *RSC advances*, 7(2), 927-938.

396 Chen, X., Xia, X., Wang, X., Qiao, J., & Chen, H. (2011). A comparative study on sorption of
397 perfluorooctane sulfonate (PFOS) by chars, ash and carbon nanotubes. *Chemosphere*, 83(10), 1313-
398 1319.

399 Chien, S. H., & Clayton, W. R. (1980). Application of Elovich equation to the kinetics of phosphate release
400 and sorption in soils. *Soil Science Society of America Journal*, 44(2), 265-268.

401 Crone, B. C., Speth, T. F., Wahman, D. G., Smith, S. J., Abulikemu, G., Kleiner, E. J., & Pressman, J. G.
402 (2019). Occurrence of per-and polyfluoroalkyl substances (PFAS) in source water and their treatment in
403 drinking water. *Critical reviews in environmental science and technology*, 49(24), 2359-2396.

404 Deng, S., Nie, Y., Du, Z., Huang, Q., Meng, P., Wang, B., ... & Yu, G. (2015). Enhanced adsorption of
405 perfluorooctane sulfonate and perfluorooctanoate by bamboo-derived granular activated carbon. *Journal*
406 *of hazardous materials*, 282, 150-157.

407 Dickenson, E., & Higgins, C. (2016). Treatment mitigation strategies for poly-and perfluoroalkyl
408 substances. *Water research foundation web report*, 4322.

409 Dong, X., Ma, L. Q., & Li, Y. (2011). Characteristics and mechanisms of hexavalent chromium removal by
410 biochar from sugar beet tailing. *Journal of hazardous materials*, 190(1-3), 909-915.

411 Drobny, J. G. (2007). Fluoropolymers in automotive applications. *Polymers for Advanced Technologies*,
412 18(2), 117-121.

413 Du, Z., Deng, S., Bei, Y., Huang, Q., Wang, B., Huang, J., & Yu, G. (2014). Adsorption behavior and
414 mechanism of perfluorinated compounds on various adsorbents—A review. *Journal of hazardous*
415 *materials*, 274, 443-454.

416 Elovich, S. Y., & Larinov, O. G. (1962). Theory of adsorption from solutions of non electrolytes on solid
417 (I) equation adsorption from solutions and the analysis of its simplest form (II) verification of the
418 equation of adsorption isotherm from solutions. *Izv. Akad. Nauk. SSSR, Otd. Khim. Nauk*, 2(2), 209-
419 216.

420 Fabregat-Palau, J., Vidal, M., & Rigol, A. (2021). Modelling the sorption behaviour of perfluoroalkyl
421 carboxylates and perfluoroalkane sulfonates in soils. *Science of the Total Environment*, 801, 149343.

422 Falciglia, P. P., Gagliano, E., Brancato, V., Malandrino, G., Finocchiaro, G., Catalfo, A., ... & Vagliasindi,
423 F. G. (2020). Microwave based regenerating permeable reactive barriers (MW-PRBs): proof of concept
424 and application for Cs removal. *Chemosphere*, 251, 126582.

425 Gagliano, E., Sgroi, M., Falciglia, P. P., Vagliasindi, F. G., & Rocco, P. (2020). Removal of poly-and
426 perfluoroalkyl substances (PFAS) from water by adsorption: Role of PFAS chain length, effect of
427 organic matter and challenges in adsorbent regeneration. *Water research*, 171, 115381.

428 Gallo, F., Fossi, C., Weber, R., Santillo, D., Sousa, J., Ingram, I., ... & Romano, D. (2018). Marine litter
429 plastics and microplastics and their toxic chemicals components: the need for urgent preventive
430 measures. *Environmental Sciences Europe*, 30(1), 13.

431 Hansen, M. C., Børresen, M. H., Schlabach, M., & Cornelissen, G. (2010). Sorption of perfluorinated
432 compounds from contaminated water to activated carbon. *Journal of Soils and Sediments*, 10(2), 179-
433 185.

434 Harsanyi, A., & Sandford, G. (2015). Organofluorine chemistry: applications, sources and sustainability.
435 *Green chemistry*, 17(4), 2081-2086.

436 Hashim, M. A., Mukhopadhyay, S., Sahu, J. N., & Sengupta, B. (2011). Remediation technologies for
437 heavy metal contaminated groundwater. *Journal of environmental management*, 92(10), 2355-2388.

438 Ho, Y. S., & McKay, G. (1999). Pseudo-second order model for sorption processes. *Process biochemistry*,
439 34(5), 451-465.

440 Inyang, M., & Dickenson, E. (2015). The potential role of biochar in the removal of organic and microbial
441 contaminants from potable and reuse water: A review. *Chemosphere*, 134, 232-240.

442 Inyang, M., & Dickenson, E. R. (2017). The use of carbon adsorbents for the removal of perfluoroalkyl
443 acids from potable reuse systems. *Chemosphere*, 184, 168-175.

444 Johnson, R. L., Anschutz, A. J., Smolen, J. M., Simcik, M. F., & Penn, R. L. (2007). The adsorption of
445 perfluorooctane sulfonate onto sand, clay, and iron oxide surfaces. *Journal of Chemical & Engineering*
446 *Data*, 52(4), 1165-1170.

447 Kupryianchyk, D., Hale, S. E., Breedveld, G. D., & Cornelissen, G. (2016). Treatment of sites
448 contaminated with perfluorinated compounds using biochar amendment. *Chemosphere*, 142, 35-40.

449 Lagergren, S. (1898). About the theory of so-called adsorption of soluble substances.

450 Li, F., Duan, J., Tian, S., Ji, H., Zhu, Y., Wei, Z., & Zhao, D. (2020). Short-chain per-and polyfluoroalkyl
 451 substances in aquatic systems: Occurrence, impacts and treatment. *Chemical Engineering Journal*, 380,
 452 122506.

453 Li, Y., Oliver, D. P., & Kookana, R. S. (2018). A critical analysis of published data to discern the role of
 454 soil and sediment properties in determining sorption of per and polyfluoroalkyl substances (PFASs).
 455 *Science of the Total Environment*, 628, 110-120.

456 Liu, Y., Ma, L., Yang, Q., Li, G., & Zhang, F. (2018). Occurrence and spatial distribution of perfluorinated
 457 compounds in groundwater receiving reclaimed water through river bank infiltration. *Chemosphere*, 211,
 458 1203-1211.

459 Loos, R., Locoro, G., Comero, S., Contini, S., Schwesig, D., Werres, F., ... & Gawlik, B. M. (2010). Pan-
 460 European survey on the occurrence of selected polar organic persistent pollutants in ground water. *Water*
 461 *research*, 44(14), 4115-4126.

462 Marsh, H., & Reinoso, F. R. (2006). *Activated carbon*. Elsevier.

463 McMahon, P. B., Tokranov, A. K., Bexfield, L. M., Lindsey, B. D., Johnson, T. D., Lombard, M. A., &
 464 Watson, E. (2022). Perfluoroalkyl and polyfluoroalkyl substances in groundwater used as a source of
 465 drinking water in the eastern United States. *Environmental science & technology*, 56(4), 2279-2288.

466 Miao, Y., Guo, X., Peng, D., Fan, T., & Yang, C. (2017). Rates and equilibria of perfluorooctanoate
 467 (PFOA) sorption on soils from different regions of China. *Ecotoxicology and environmental safety*, 139,
 468 102-108.

469 Milinovic, J., Lacorte, S., Vidal, M., & Rigol, A. (2015). Sorption behaviour of perfluoroalkyl substances
 470 in soils. *Science of the Total Environment*, 511, 63-71.

471 Mohan, D., & Pittman Jr, C. U. (2006). Activated carbons and low cost adsorbents for remediation of tri-
 472 and hexavalent chromium from water. *Journal of hazardous materials*, 137(2), 762-811.

473 Mohona, T. M., Ye, Z., Dai, N., & Nalam, P. C. (2023). Adsorption behavior of long-chain perfluoroalkyl
474 substances on hydrophobic surface: A combined molecular characterization and simulation study. *Water*
475 *Research*, 239, 120074.

476 Molé, R. A., Velosa, A. C., Carey, G. R., Liu, X., Li, G., Fan, D., ... & Lowry, G. V. (2024). Groundwater
477 solutes influence the adsorption of short-chain perfluoroalkyl acids (PFAA) to colloidal activated carbon
478 and impact performance for in situ groundwater remediation. *Journal of Hazardous Materials*, 474,
479 134746.

480 Montaña, M., Camacho, A., Serrano, I., Devesa, R., Matia, L., & Vallés, I. (2013). Removal of
481 radionuclides in drinking water by membrane treatment using ultrafiltration, reverse osmosis and
482 electrodialysis reversal. *Journal of environmental radioactivity*, 125, 86-92.

483 Mukherjee, A., Zimmerman, A. R., & Harris, W. (2011). Surface chemistry variations among a series of
484 laboratory-produced biochars. *Geoderma*, 163(3-4), 247-255.

485 Murakami, M., Kuroda, K., Sato, N., Fukushi, T., Takizawa, S., & Takada, H. (2009). Groundwater
486 pollution by perfluorinated surfactants in Tokyo. *Environmental science & technology*, 43(10), 3480-
487 3486.

488 Ochoa-Herrera, V., & Sierra-Alvarez, R. (2008). Removal of perfluorinated surfactants by sorption onto
489 granular activated carbon, zeolite and sludge. *Chemosphere*, 72(10), 1588-1593.

490 OECD (Organisation for Economic Co-operation and Development). (2000). Adsorption-desorption using
491 a batch equilibrium method. *OECD Guideline for Testing Chemicals*, 106, 1-42.

492 Oliver, D. P., Li, Y., Orr, R., Nelson, P., Barnes, M., McLaughlin, M. J., & Kookana, R. S. (2019). The role
493 of surface charge and pH changes in tropical soils on sorption behaviour of per-and polyfluoroalkyl
494 substances (PFASs). *Science of the total environment*, 673, 197-206.

495 Özer, A. (2007). Removal of Pb (II) ions from aqueous solutions by sulphuric acid-treated wheat bran.
496 *Journal of Hazardous Materials*, 141(3), 753-761.

497 Park, J. W., Noh, J. H., Yoon, S. W., Samiya, S., Choi, B. G., Kim, G. B., Oh, H. K., Maeng, S. K. (2021),
498 "Removal of short-and long-chain perfluorinated compounds from surface water by coagulation",
499 Membrane and Water Treatment., 12(4), 187-194.

500 Park, M., Daniels, K. D., Wu, S., Ziska, A. D., & Snyder, S. A. (2020). Magnetic ion-exchange (MIEX)
501 resin for perfluorinated alkylsubstance (PFAS) removal in groundwater: Roles of atomic charges for
502 adsorption. Water research, 181, 115897.

503 Patil, S. B., Chore, H. S., & Sawant, V. A. (2023). Assessing pollutants' migration through saturated soil
504 column. Membrane and Water Treatment, 14(2), 95-106.

505 Pereira, H. C., Ullberg, M., Kleja, D. B., Gustafsson, J. P., & Ahrens, L. (2018). Sorption of perfluoroalkyl
506 substances (PFASs) to an organic soil horizon—Effect of cation composition and pH. Chemosphere, 207,
507 183-191.

508 Peshoria, S., Nandini, D., Tanwar, R. K., & Narang, R. (2020). Short-chain and long-chain
509 fluorosurfactants in firefighting foam: a review. Environmental Chemistry Letters, 18(4), 1277-1300

510 Riess, J. G. (2009). Highly fluorinated amphiphilic molecules and self-assemblies with biomedical
511 potential. Current opinion in colloid & interface science, 14(5), 294-304.

512 Savoca, D., & Pace, A. (2021). Bioaccumulation, biodistribution, toxicology and biomonitoring of
513 organofluorine compounds in aquatic organisms. International journal of molecular sciences, 22(12),
514 6276.

515 Walters, F. H. (1991). Design of corrosion inhibitors: Use of the hard and soft acid-base (HSAB) theory.
516 Journal of chemical education, 68(1), 29.

517 Wang, J., & Guo, X. (2020). Adsorption kinetic models: Physical meanings, applications, and solving
518 methods. Journal of Hazardous materials, 390, 122156.

519 Wang, S., Gao, B., Zimmerman, A. R., Li, Y., Ma, L., Harris, W. G., & Migliaccio, K. W. (2015).
520 Physicochemical and sorptive properties of biochars derived from woody and herbaceous biomass.
521 Chemosphere, 134, 257-262.

522 Wang, T., Lu, Y., Chen, C., Naile, J. E., Khim, J. S., & Giesy, J. P. (2012). Perfluorinated compounds in a
523 coastal industrial area of Tianjin, China. Environmental Geochemistry and Health, 34(3), 301-311.

524 Wei, C., Song, X., Wang, Q., & Hu, Z. (2017). Sorption kinetics, isotherms and mechanisms of PFOS on
525 soils with different physicochemical properties. Ecotoxicology and Environmental Safety, 142, 40-50.

526 Yu, Q., Zhang, R., Deng, S., Huang, J., & Yu, G. (2009). Sorption of perfluorooctane sulfonate and
527 perfluorooctanoate on activated carbons and resin: Kinetic and isotherm study. Water research, 43(4),
528 1150-1158.

529 Yu, X., Takabe, Y., Yamamoto, K., Matsumura, C., & Nishimura, F. (2016). Biodegradation property of 8:
530 2 fluorotelomer alcohol (8: 2 FTOH) under aerobic/anoxic/anaerobic conditions. Journal of Water and
531 Environment Technology, 14(3), 177-190.

532 Zhi, Y., & Liu, J. (2015). Adsorption of perfluoroalkyl acids by carbonaceous adsorbents: Effect of carbon
533 surface chemistry. Environmental pollution, 202, 168-176.

534 Zhi, Y., & Liu, J. (2016). Surface modification of activated carbon for enhanced adsorption of
535 perfluoroalkyl acids from aqueous solutions. Chemosphere, 144, 1224-1232.

Figure legends

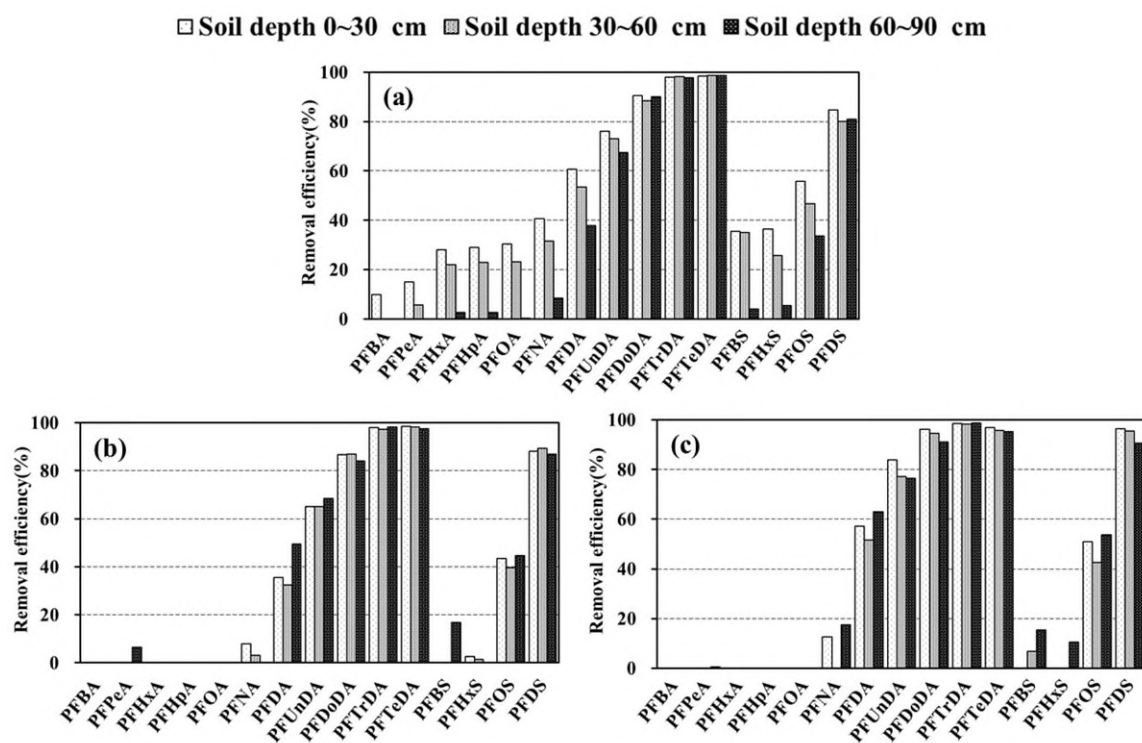


Fig. 1 Retention of 15 PFASs in DIW, FH, and JH groundwater across soil depths.

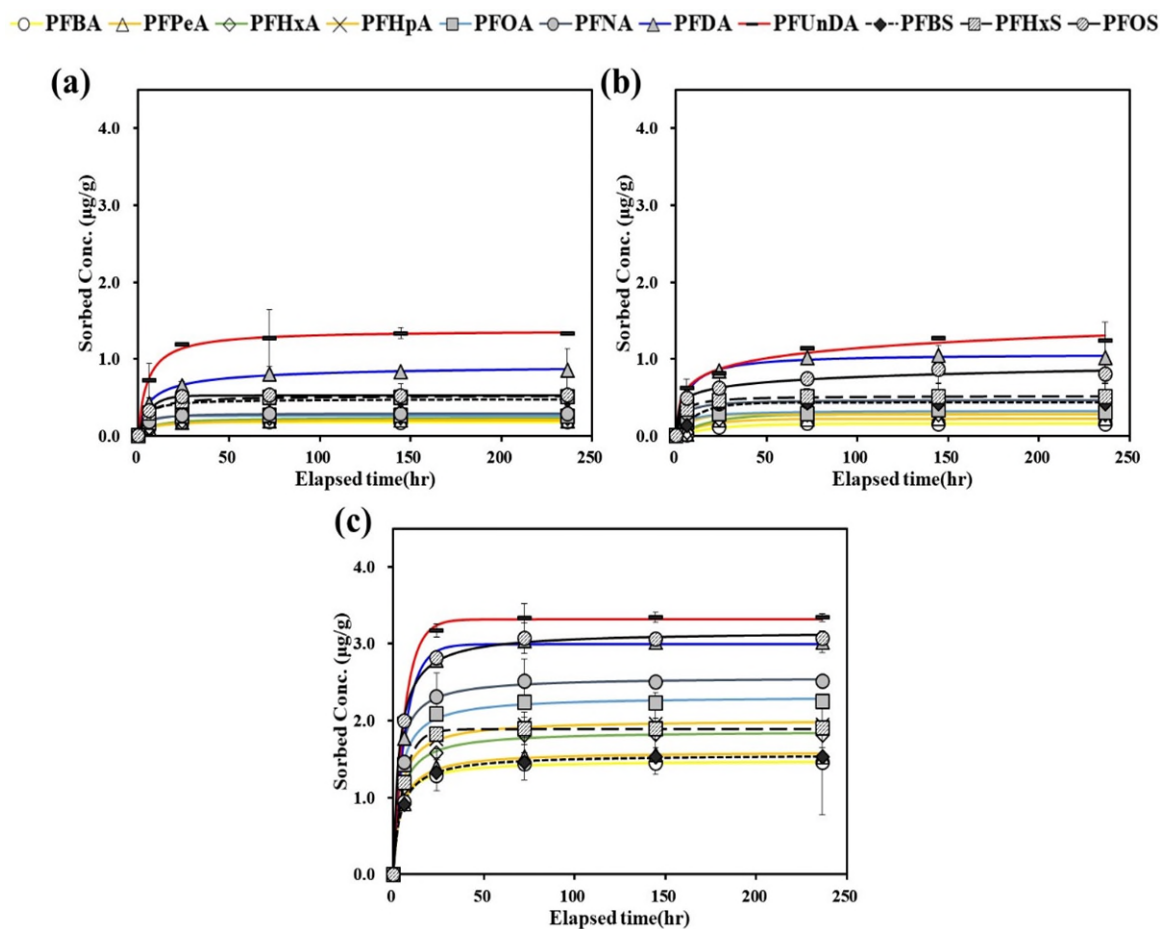


Fig. 2 Time-dependent adsorption of PFASs by chaff biochar, wood charcoal, and activated carbon.

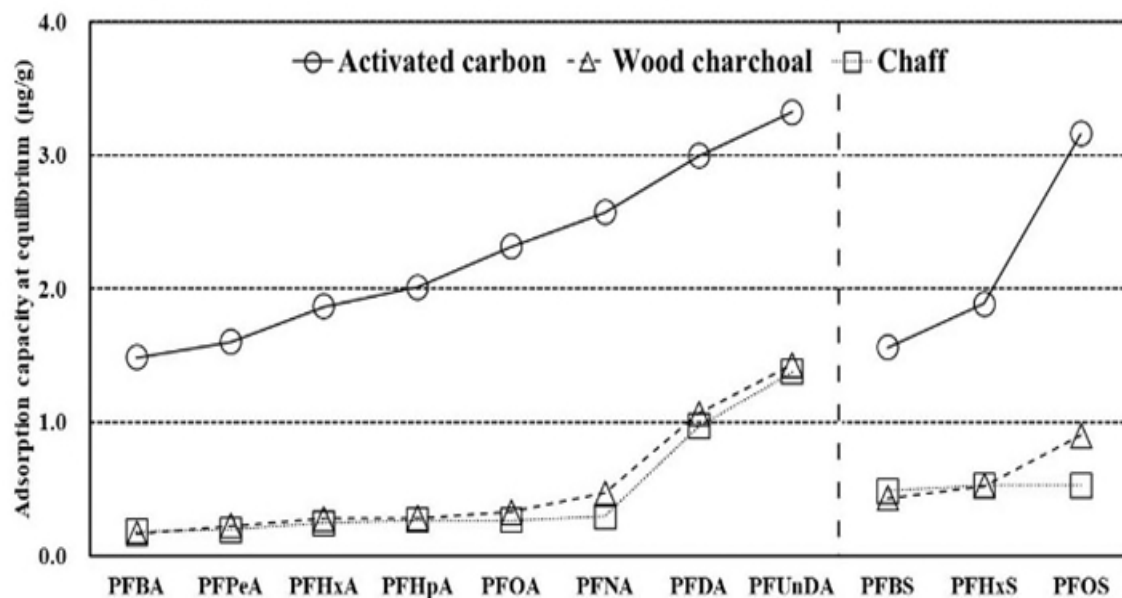


Fig. 3 Modeled equilibrium adsorption capacities of PFASs on carbonaceous sorbents.

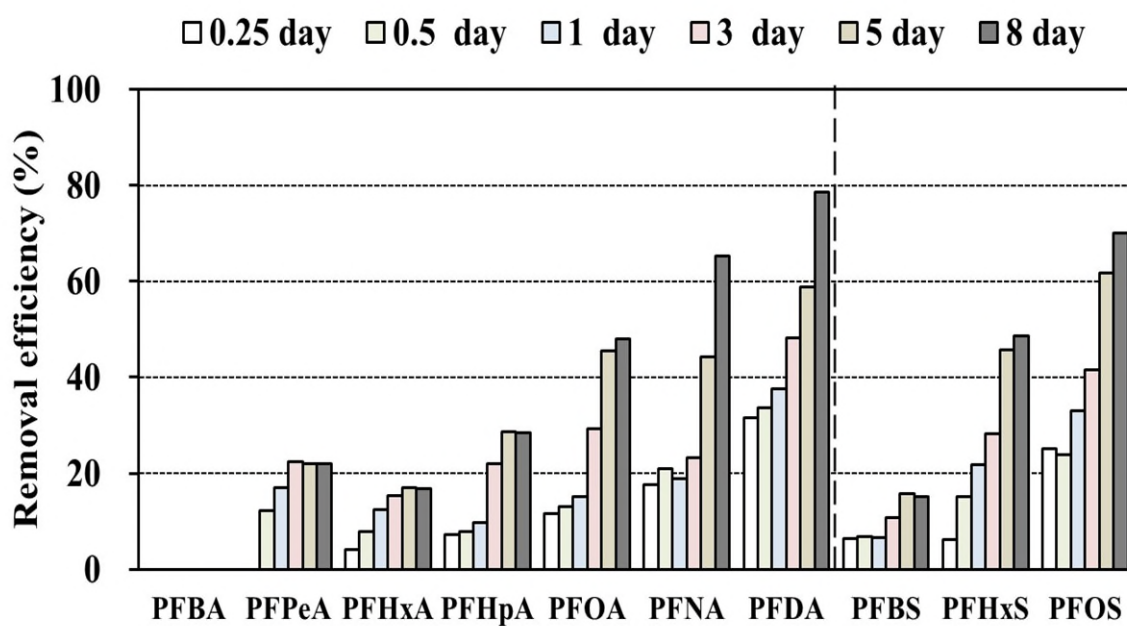


Fig. 4 Removal efficiency of 10 PFASs in DH groundwater using activated carbon.

Table legends

Table 1 Result of physical and chemical characterization of the soil for STT

pH	EC (dS/m)	OM (%)	CEC (cmol/kg)	Ca (mmol/kg)	Mg (mmol/kg)	K (mmol/kg)	Na (mmol/kg)	P ₂ O ₅ (mmol/kg)	Density (g/cm ³)	Porosity (%)	Soil texture
<u>Soil Adsorption – Surface (0~30 cm)</u>											
4.6	0.48	3.9	21.4	31.938	3.359	5.499	0.564	0.049	0.98(Bulk) 2.5(Particle)	60.8	Clay loam
<u>Soil Adsorption – Middle (30~60 cm)</u>											
4.6	0.41	2.9	20.9	28.844	2.743	4.604	0.527	0.018	0.88(bulk) 2.5(particle)	64.9	Loam
<u>Soil Adsorption – Deep (60~90 cm)</u>											
4.7	0.26	1.8	20.8	28.045	2.260	4.435	0.468	0.002	1.1(bulk) 2.5(particle)	54.4	Loam

Table 2 Results of cation and anion analysis in DIW, JH, and FH for STT (unit is mM).

Samples	Cl ⁻	NO ₃ ²⁻	SO ₄ ²⁻	K ⁺	Na ⁺	Ca ²⁺	Mg ²⁺
DIW	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
FH	2.15	0.13	0.27	0.06	0.90	0.93	0.53
JH	0.11	0.10	0.01	0.01	N.D.	N.D.	N.D.

N.D.: Not detected.

Table 3 Identities, carbon number and SRM conditions of measurement for PFCs.

Groups	Components			RT (min)	Precursor ion, m/z	Product ion, m/z (CE)
	Analyte	Acronym	Carbon number			
Carboxyl group	Perfluoro-n-butanoic acid	PFBA	4	5.27	212.912	169.000(8.12)
	Perfluoro-n-pentanoic acid	PFPeA	5	5.96	262.962	219.000(7.40)
	Perfluoro-n-hexanoic acid	PFHxA	6	6.34	313.050	269.143(8.54)
	Perfluoro-n-heptanoic acid	PFHpA	7	6.75	363.000	319.071(9.34)
	Perfluoro-n-octanoic acid	PFOA	8	7.18	413.000	369.054(9.47)
	Perfluoro-n-nonanoic acid	PFNA	9	7.57	463.062	419.125(9.30)
	Perfluoro-n-decanoic acid	PFDA	10	7.95	513.100	469.054(9.42)
	Perfluoro-n-undecanoic acid	PFUnDA	11	8.27	563.088	519.125(9.42)
	Perfluoro-n-dodecanoic acid	PFDoDA	12	8.54	613.050	568.982(10.18)
	Perfluoro-n-tridecanoic acid	PFTTrDA	13	8.81	663.038	619.125(11.40)
	Perfluoro-n-tetradecanoic acid	PFTeDA	14	9.04	713.100	669.125(11.15)
Sulfonyl group	Perfluoro-1-butane sulfonic acid	PFBS	4	6.02	299.050	80.000(31.58)
	Perfluoro-1-hexane sulfonic acid	PFHxS	6	6.76	399.088	80.000(36.89)
	Perfluoro-1-octane sulfonic acid	PFOS	8	7.57	499.038	80.000(40.55)
	Perfluoro-1-decane sulfonic acid	PFDS	10	8.24	599.050	80.000(45.78)
ISTD	Perfluoro-n- (13C4)butanoic acid	MPFBA	4	5.27	216.8	171.883(10.08)
	Perfluoro-n-(1,2- 13C2)hexanoic acid	MPFHxA	6	6.34	314.962	270.000(8.16)
	Perfluoro-n-(1,2,3,4- 13C4)octanoic acid	MPFOA	8	7.17	416.862	372.018(8.88)
	Perfluoro-n-(1,2,3,4,5- 13C5)nonanoic acid	MPFNA	9	7.57	468.012	423.000(9.42)
	Perfluoro-n-(1,2- 13C2)decanoic acid	MPFDA	10	7.95	514.912	469.929(9.38)
	Perfluoro-n-(1,2- 13C2)undecanoic acid	MPFUdA	11	8.27	564.912	520.000(10.10)
	Perfluoro-n-(1,2- 13C2)dodecanoic acid	MPFDoA	12	8.55	614.912	570.000(10.01)
	Sodium perfluoro-1- [1,2,3,4-13C4] octanesulfonate	MPFOS	8	7.58	502.962	99.000(39.20)

Table 4 HPLC-MS/MS condition for PFCs measurement.

Parameter	Condition
Column	Accucore™ RP-MS 100 × 2.1 mm
Mobile phase	A: 5 mM Ammonium acetate B: Methanol
Column flow rate	0.3 mL/min
Injection volume	5 µL
Column temp	40 °C
Ionization mode	Negative ion electrospray
Capillary voltage	3.50 kV
Gas temperature	250 °C
Gas flow	9 L/min (N ₂)

Table 5 Initial average concentration of PFASs at STT, SKT and REAG

Compound	STT (µg/L)			SKT (µg/L)	REAG (nM)
	DIW	FH	JH		
PFBA	2.01	1.68	1.67	2.44	0.40
PFPeA	2.08	2.09	2.10	2.35	1.16
PFHxA	2.13	1.78	1.70	2.54	1.51
PFHpA	2.10	1.71	1.68	2.50	0.80
PFOA	2.11	1.73	1.65	2.39	3.61
PFNA	2.05	1.70	1.59	2.25	0.24
PFDA	1.88	1.53	1.37	1.94	0.13
PFUnDA	1.69	1.51	1.12	2.02	-
PFDoDA	0.97	1.18	0.78	-	-
PFTTrDA	1.07	1.33	0.70	-	-
PFTeDA	1.06	0.99	0.41	-	-
PFBS	1.76	1.54	1.50	2.36	0.03
PFHxS	1.97	1.77	1.70	2.24	0.06
PFOS	2.04	2.06	1.71	2.21	0.03
PFDS	0.69	1.51	0.93	-	-

Table 6 Best fit model parameters for batch sorption kinetics

Absorbents	Compound	Model	Parameter 1	Parameter 2	R ²
Chaff	PFBA	PFO	q ₁ =0.1824	k ₁ =0.1345	0.9990
	PFPeA	PFO	q ₁ =0.1969	k ₁ =0.1060	0.9986
	PFHxA	PSO	q ₂ =0.2434	k ₂ =0.5947	0.9969
	PFHpA	PTO	q ₃ =0.2667	k ₃ =6.4024	0.9975
	PFOA	PFO	q ₁ =0.2638	k ₁ =0.1812	0.9992
	PFNA	PSO	q ₂ =0.2939	k ₂ =1.0572	0.9989
	PFDA	PTO	q ₃ =0.9720	k ₃ =0.1930	0.9989
	PFUnDA	PSO	q ₂ =1.3789	k ₂ =0.1432	0.9972
	PFBS	PSO	q ₂ =0.4871	k ₂ =0.6041	0.9976
	PFHxS	PSO	q ₂ =0.5259	k ₂ =0.4257	0.9987
	PFOS	PFO	q ₁ =0.5258	k ₁ =0.1603	0.9997
Wood charcoal	PFBA	PFO	q ₁ =0.1647	k ₁ =0.0450	0.9908
	PFPeA	PFO	q ₁ =0.2252	k ₁ =0.0613	0.9317
	PFHxA	PFO	q ₁ =0.2800	k ₁ =0.0533	0.9861
	PFHpA	PFO	q ₁ =0.2830	k ₁ =0.1211	0.9986
	PFOA	PSO	q ₂ =0.3263	k ₂ =0.6951	0.9828
	PFNA	PSO	q ₂ =0.4696	k ₂ =0.6444	0.9998
	PFDA	PSO	q ₂ =1.0680	k ₂ =0.1675	0.9980
	PFUnDA	Elovich	a=0.7589	b=5.2401	0.9876
	PFBS	PFO	q ₁ =0.4309	k ₁ =0.0857	0.9805
	PFHxS	PSO	q ₂ =0.5241	k ₂ =0.6447	0.9996
	PFOS	Elovich	a=2.5808	b=10.2384	0.9880
Activated carbon	PFBA	PSO	q ₂ =1.4870	k ₂ =0.1948	0.9998
	PFPeA	PSO	q ₂ =1.6006	k ₂ =0.1495	0.9981
	PFHxA	PSO	q ₂ =1.8672	k ₂ =0.1360	0.9990
	PFHpA	PSO	q ₂ =2.0126	k ₂ =0.1348	0.9991
	PFOA	PSO	q ₂ =2.3139	k ₂ =0.1246	0.9981
	PFNA	PSO	q ₂ =2.5701	k ₂ =0.1368	0.9995
	PFDA	PFO	q ₁ =2.9945	k ₁ =0.1456	0.9974
	PFUnDA	PFO	q ₁ =3.3218	k ₁ =0.1559	0.9993
	PFBS	PSO	q ₂ =1.5609	k ₂ =0.1505	0.9998
	PFHxS	PFO	q ₁ =1.8869	k ₁ =0.1675	0.9995
	PFOS	PSO	q ₂ =3.1604	k ₂ =0.0941	0.9989

Table 7 Apparent distribution coefficients (K_d) and screening-level retardation factors (R_f) estimated for selected PFASs across soil depth and water matrices

Matrix	Compound	0–30 cm			30–60 cm			60–90 cm		
		Ads (%)	K_d (L/kg)	R_f	Ads (%)	K_d (L/kg)	R_f	Ads (%)	K_d (L/kg)	R_f
DIW	PFBA	10.0	1.11	2.79	0.0	0.00	1.00	0.0	0.00	1.00
	PFHxA	28.0	3.89	7.27	22.0	2.82	4.82	3.0	0.31	1.63
	PFOA	30.5	4.39	8.07	23.2	3.02	5.10	0.3	0.03	1.06
	PFDA	60.0	15.00	25.18	53.0	11.28	16.29	38.0	6.13	13.39
	PFBS	35.0	5.38	9.68	35.0	5.38	8.30	5.0	0.53	2.06
	PFHxS	36.0	5.63	10.07	25.0	3.33	5.52	6.0	0.64	2.29
	PFOS	55.0	12.22	20.71	46.0	8.52	12.56	34.0	5.15	11.42
FH	PFBA	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00
	PFHxA	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00
	PFOA	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00
	PFDA	35.0	5.38	9.68	30.0	4.29	6.81	49.0	9.61	20.43
	PFBS	0.0	0.00	1.00	0.0	0.00	1.00	17.0	2.05	5.14
	PFHxS	3.0	0.31	1.50	1.0	0.10	1.14	0.0	0.00	1.00
	PFOS	43.0	7.54	13.16	37.0	5.87	8.96	45.0	8.18	17.54
JH	PFBA	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00
	PFHxA	0.0	0.00	1.00	0.0	0.00	1.00	1.0	0.10	1.20
	PFOA	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00
	PFDA	57.0	13.26	22.37	52.0	10.83	15.69	63.0	17.03	35.43
	PFBS	6.0	0.64	2.03	8.0	0.87	2.18	16.0	1.90	4.85
	PFHxS	0.0	0.00	1.00	0.0	0.00	1.00	10.0	1.11	3.25
	PFOS	51.0	10.41	17.78	42.0	7.24	10.82	54.0	11.74	24.75