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Potential of micropollutants originated from irrigation water to contaminate soil and groundwater

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Abstract: Sorption of organic contaminants in soils and sediments is a crucial factor affecting their mobility in the vadose zone environment. Freundlich sorption isotherms were evaluated for six micropollutants identified in areas irrigated with river-water and sixteen soils. The highest Freundlich sorption coefficients, K_F, were obtained for 1,3-diphenylguanidine (11.6 ± 5.0 $\text{cm}^{3/n}\mu\text{g}^{1-1/n}/\text{g}$) followed by triethyl citrate (4.57 ± 4.91), 4-acetamidoantipyrine (1.43 ± 0.24), 6 : 2 fluorinated telomer sulfonate (1.18 ± 0.42), benzo(d)thiazole-2-sulfonic acid (1.12 ± 0.33), and naphthalene-2-sulfonic acid (0.28 ± 0.17). The K_F values for the individual compounds were correlated with soil properties. Multiple linear regressions were used to derive equations for predicting the K_F values using the soil properties. Sorption of cationic molecules was positively affected by cation exchange capacity or clay content, indicating strong sorption of cations on negatively charged sorption sites. Sorption of anionic molecules was positively correlated with organic carbon content and wettability index, suggesting hydrophobic interactions with soil organic matter. Anion sorption was also positively influenced by magnetic susceptibility, which could indicate sorption of anions on the positively charged sorption sites. Sorption of acids was in some cases also positively affected by cation exchange capacity, which could imply their sorption via cation bridges.

Keywords: identification of pollutants in the environment; industrial chemicals; soil properties; sorption isotherms; surfactants; pharmaceuticals' metabolites; vulcanization accelerators

Agricultural soil can be contaminated by various organic micropollutants. Common micropollutants are various pesticides used for plant protection and weed reduction, and their metabolites (e.g., Sabzevari & Hofman 2022; Alaoui et al. 2024). Another source of contamination can be irrigation water. In areas with a shortage of water, treated wastewater that may contain, for example, pharmaceuticals, hormones, per-

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sonal care products and various industrial chemicals, can be used directly for irrigation (e.g., Mordechay et al. 2021; Kodešová et al. 2024). However, even river water, which is often used for irrigation, can be contaminated by compounds via wastewater discharged into rivers, runoff from agricultural or urban land, etc. (e.g., Huntscha et al. 2013; Schulze et al. 2019; Foscari et al. 2024; Jin et al. 2024; Kuntz et al. 2024; Xu et al. 2025). The accumulation of various pollutants in the soil, or their leaching from the soil and migration into groundwater, depends on climatic conditions, the properties of the vadose zone environment, and the behaviour of the compounds, i.e., their sorption into soils and sediments and their stability in the soil-water environment. Sorption is a key property of stable compounds that may occur in contaminated rivers, determining their spread in the vadose zone. For simplicity, the sorption of compounds in the soil environment is usually characterised by an equilibrium state between the concentration in the soil solution and the concentration sorbed on soil components. The distribution coefficients or parameters of the sorption isotherm describing this equilibrium state are not known for many micropollutants, and, moreover, these parameters can vary considerably in different soils. Therefore, efforts are being made to develop models for predicting sorption coefficients based on soil properties. For organic micropollutants, a close relationship to the soil organic carbon content is generally assumed. However, this assumption is insufficient for many substances, because the sorption of many depends on their dissociation in the environment, which depends on its pH (e.g., Schaffer & Licha 2015). As found in the previous studies (e.g., Schmidtová et al. 2020; Kodešová et al. 2023), a close positive correlation was observed between the Freundlich sorption coefficients (K_F) and organic carbon content, specifically for neutral organic molecules. Nonpolar organic pollutants tend to associate with hydrophobic regions of soil material. The K_F values for mostly cationic compounds were usually positively correlated with the cation exchange capacity or the base cation saturation (i.e., exchangeable cations except for H^+). Cationic compounds are very strongly bound in the soil due to electrostatic interactions with predominantly negatively charged soil components (e.g., organic matter and clay). On the other hand, the K_F values for mostly anionic compounds are frequently positively correlated with their hydrolytic capacity, which unfortunately does not help to clarify the sorption mechanisms of these compounds (Kodešová et al. 2023). It is assumed that the sorption of these compounds is generally low because the molecules are repulsed by the negatively charged soil surface. Sorption of the anionic compounds (like others) can be driven by nonionic intermolecular forces such as hydrogen bonds, π-π interactions, and Van der Waals forces. However, anionic compounds can also bind via cation bridging or through electrostatic interactions with the positively charged surfaces of soil components (e.g., amorphous materials, Fe and Al oxides, sesquioxide hydrates). Anion exchange capacity is not typically studied because it is generally lower than cation exchange capacity, except in cases such as heavily weathered tropical soils. Therefore, its role in compound sorption in soils is usually negligible but can increase with decreasing pH (i.e., also with increasing hydrolytic capacity).

This study focused on pollutants that may be present in surface water used in irrigated areas and the threat of their accumulation in soil or leaching into groundwater. The goals were: (1) to identify representative micropollutants with different sorption behaviour in irrigated soils; (2) to evaluate sorption of these compounds in the representative soils; (3) to derive equations for predicting the Freundlich sorption coefficients using soil properties. To achieve these goals, compounds with different sorption behaviour were first selected from the list of compounds identified in irrigated lands, with greater emphasis on compounds with expected high mobility. In addition to the typically measured soil properties, the wettability of soil organic matter was investigated using the potential wettability index (PWI), and magnetic susceptibility was measured, indicating the presence of ferrimagnetic particles. The reason was to extend the set of soil properties by including those that could better correlate with sorption coefficients and indicate sorption mechanisms, primarily with respect to anionic compounds.

MATERIAL AND METHODS

Compounds of interest. The compounds were selected based on the results of our 2023 screening, which aimed to map the occurrence of micropollutants in surface and groundwater, as well as in soils, in intensively irrigated agricultural areas around the Elbe and Dyje rivers in the Czech Republic (unpublished data). The main criteria were: (1) Frequent occurrence in the analysed water and soil samples;

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(2) Different sources of contamination of substances; (3) Different characteristics of substances determining their behaviour in the soil environment, and thus different potential for accumulation of substances in soil, or conversely, contamination of groundwater. Six compounds were identified and selected (Table S1 in Electronic Supplementary Material (ESM): 1,3-diphenylguanidine (DPG), triethyl citrate (TEC), 4-acetamidoantipyrine (4-AAA), napthalene-2-sulfonic acid (NSA), benzo(d)thiazole-2-sulfonic acid (BTSA), and 6 : 2 fluorinated telomer sulfonate (6 : 2 FTS). Since these compounds were found in the environment, they are relatively stable. The compounds DPG and BTSA have also been recognised as emerging contaminants that can be found in water (Foscari et al. 2024; Jin et al. 2024; Zhang et al. 2024; Xu et al. 2025; Zhuang et al. 2025) and even in aerosols (Kuntz et al. 2024) in urban and industrial areas. Their source in soil can be irrigation water, as well as surrounding traffic (e.g., Li et al. 2023). Fluorotelomer molecules (e.g., 6 : 2 FTS) that have been widely employed as replacements to perfluorooctane sulfonic acid (PFOS) in aqueous film-forming foam and perfluorooctanoic acid (PFOA) in other products are increasingly identified in environmental settings, including surface and groundwater, soil and sediments (e.g., Høisæter & Breedveld 2022; Loganathan et al. 2025). Similarly, NSA can be found in wastewater plant products (e.g., Lara-Martín et al. 2025) and 4-AAA in river and groundwater (Huntscha et al. 2013). TEC is used for various purposes, including food processing, and therefore probably should not be considered a hazardous contaminant. However, due to its widespread use, it was chosen to indicate the behaviour of similar molecules in the environment.

Soils and soil properties. Sixteen different soil types were selected to study the sorption of the identified compounds in soils (Table S2 in ESM). Soil samples for sorption experiments and for mapping of soil properties were taken from a depth of 0–25 cm. The samples were air-dried, disintegrated, and passed through a 2-mm mesh sieve. Next, the following chemical and physical soil properties were measured under constant laboratory conditions (t = 20 °C): active soil reaction ($\mathrm{pH_{H_2O}}$) and potential soil reactions ($\mathrm{pH_{KCl}}$, $\mathrm{pH_{CaCl_2}}$) (ISO 10390:2005), oxidizable organic carbon content (Cox) (Skjemstad & Baldock 2008), soil salinity in water (Rhoades 1996), particle density (ρ_s) (Flint & Flint 2002), particle size distribution (Gee & Or 2002), cation exchange capacity (CEC) (Bower & Hatcher 1966), hydrolytic acidity (Klute 1996), base cation saturation (BCS, the difference between CEC and HA), and sorption complex saturation (SCS, the percentage of BCS in CEC).

The PWI was further assessed using diffuse reflectance infrared spectroscopy, as described, for example, by Pavlů et al. (2023, 2024). Powdered samples, gold mirror as background reference, 64 scans in spectral range 4 000–400 1/cm with 4 1/cm resolution, and Nicolet iS10 (Thermo Fisher Scientific Inc., USA) was used for analysis. OMNIC 9.2.41 software (Thermo Fisher Scientific Inc., USA) was used to process the measured spectra. The PWI value was calculated as the ratio of the spectral bands of the hydrophobic (aliphatic) C-H groups (2 950–2 820 1/cm), and the bands of the hydrophilic groups (1 740–1 600 1/cm). The PWI value indicates the degree of hydrophobicity of soil organic matter, which can play a significant role in the sorption of the studied organic compounds through hydrophobic interactions.

Finally, magnetic susceptibility was also measured at low (0.47 kHz) and high frequencies (4.7 kHz) on dry soil samples packed in 10 mL containers using the Bartington MS2 meter and MS2B sensor (Bartington 2008). This sensor provided the volume-specific magnetic susceptibility at low (κLF) and high frequency (κHF), from which the mass-specific magnetic susceptibility at low (χLF) and high (χHF) frequency were calculated as follows:

$$\chi = \frac{\kappa \times V}{m} \tag{1}$$

where:

χ – the mass magnetic susceptibility ($\mathrm{cm^3/g}$);

κ – the volume magnetic susceptibility (–);

V – the volume of the cup ($\mathrm{cm^3}$);

m – the mass of the soil sample (g).

Magnetic susceptibility indicates the presence of ferrimagnetic particles (mainly ultrafine ferrimagnetics formed by pedogenetic processes, e.g., Fe and Mn oxides). It may also indicate the presence of sesquioxide hydrates, which can release $\mathrm{OH^-}$ and provide sorption sites for anion sorption. The correlation coefficients describing the relationships among the soil properties are shown in Table S3 in ESM.

Sorption experiment. Sorption isotherms were evaluated using the standard batch equilibrium method (OECD 2000), a method also employed by Kodešová et al. (2023) and Schmidtová et al. (2020). Ten grams of the dry soil sample and 20 $\mathrm{cm^3}$

of a solution of one compound in 5 different concentrations (0.5, 1, 2, 5, or 10 μg/cm^3 in 0.01 M $CaCl_2$) were placed into a plastic centrifuge tube. Duplicate tubes for each soil-solution suspension were shaken on an analogue reciprocating shaker (GFL 3006, GFL Gesellschaft für Labortechnik mbH) at 20 °C for 24 h, centrifuged for 10 min at 6 000 rpm, and the remaining solution was filtered through a regenerated cellulose syringe filter (0.45 μm).

The actual initial concentrations, c_{ini} (μg/cm^3), and final equilibrium concentrations, c_{eq} (μg/cm^3), were quantified using liquid chromatography-tandem mass spectrometry (LC-MS/MS) for all compounds, following the same procedure as described by Kodešová et al. (2015) and Schmidtová et al. (2020). An isotope dilution or an internal standard (IS) method was used for quantification. Matrix effects were corrected using the matrix-matching standards (calibration points prepared in corresponding soil leachate without added analytes). Briefly, approximately 1 cm^3 of the filtrate was transferred to the autosampler vial, and the IS was added for LC-MS/MS analysis. The samples were analysed by direct injection of 10 μL into an LC-MS/MS system, where a triple quadrupole mass spectrometer (TSQ Altis, Thermo Scientific, USA) was coupled with a Dionex Ultimate 3000SD pump and an autosampler (Thermo Scientific, USA). For 6 : 2 FTS analysis, a hybrid quadrupole-orbital trap high-resolution mass spectrometer QExactive HF coupled with Dionex Vanquish LC and an autosampler (all instruments Thermo Scientific, USA). To shorten the analysis time, we used an Arion Plus C18 Column (30 × 2.1 mm, 5 μm, Chromservis s.r.o., Czech Republic), preceded by a precolumn (10 × 2.1 mm, 5 μm particle size) from the same producer for separation. Detailed information on both methods, including the LOQ range for the given analytes, is provided in the supplementary materials (Tables S4 to S6 in ESM).

The concentrations of compounds sorbed onto soil, s (μg/g), were calculated:

$$s = 2\,(c_{\text{ini}} - c_{\text{eq}}) \tag{2}$$

Experimental sorption isotherms, i.e., the final equilibrium concentrations ($c_{\text{eq}} = c$) in each tube paired with the calculated s values, were fitted using the Freundlich equation:

$$s = K_F \times c^{1/n} \tag{3}$$

where:

K_F – empirical coefficient (cm$^{3/n}$ μg$^{1-1/n}$/g);

n – empirical coefficient (–) (Table S7, Figure S1 in ESM).

As discussed by Kodešová et al. (2023) and Schmidtová et al. (2020), the K_F values depend on the n values, and therefore it would not be mathematically correct to directly use these K_F values to assess the influence of soil properties on their sorption affinity. Therefore, the average coefficient n_{avg} was calculated for each compound using the n values for all sixteen soils. The exponent n in Equation (3) was fixed at the value n_{avg}. The experimental points were then refitted once more using this modified equation, resulting in a new set of K_F values (Table 1, Figure S1 in ESM). These values were next used for the statistical analyses. The potential mobility of compounds in soils was also assessed using the following criteria (Kodešová et al. 2023): $K_F < 2.5$ – very high mobility, $2.5 \leq K_F \leq 5$ – high mobility, $5 < K_F \leq 10$ – moderate mobility, $10 < K_F \leq 20$ – low mobility, $20 < K_F \leq 40$ – very low mobility, $40 < K_F$ – immobility.

Statistical analyses. To assess the relationships between the Freundlich sorption coefficients, K_F (for n_{avg} value) obtained for various compounds, between different soil properties, and between the K_F values and soil properties, correlation analyses were performed using the Pearson correlation coefficient (Table S8 in ESM). The statistical significance of the estimated correlations was evaluated using the P-value. Next, multiple linear regressions were used to obtain models for estimating the K_F values based on soil properties (Table 2). Two approaches were considered: (A) including only the properties (Cox, clay content, and pH_{KCl}), which are usually available in soil maps and related databases (e.g., Kodešová et al. 2023); and (B) using all measured soil properties. It should be noted that some datasets did not exhibit normal distribution and were therefore logarithmically transformed. All statistical analyses were performed using STAGRAPHICS Centurion XV (Ver. 15.2.06.)

RESULTS AND DISCUSSION

Sorption of compounds in soils. The parameters of the Freundlich equations K_F and n obtained during the initial fitting of the experimental data are listed in Table S7 in ESM. The K_F values for n_{avg} are shown in Table 1, which also includes the

Table 1. The Freundlich sorption coefficients obtained for the average n exponent and values published for soils and other organo-mineral sorbents

	DPG		TEC		4-AAA		NSA		BTSA		6:2 FTS	
n_{avg}	1.37		1.90		1.31		1.25		1.68		1.28	
	K_F	R^2	K_F	R^2	K_F	R^2	K_F	R^2	K_F	R^2	K_F	R^2
HCa-B	9.7	0.983	1.85	0.942	1.46	0.942	0.17	0.907	0.39	0.505	0.87	0.693
GP	10.9	0.987	6.42	0.972	1.79	0.999	0.25	0.782	1.14	0.848	1.54	0.888
HCh	16.3	0.988	5.59	0.905	1.15	0.953	0.54	0.834	1.26	0.927	0.87	0.447
AR-A	3.3	0.836	0.40	0.517	1.04	0.776	NC		0.62	0.646	0.93	0.481
GF	8.4	0.950	2.28	0.885	1.37	0.960	0.14	0.822	1.37	0.898	1.01	0.553
HF-A	10.7	0.976	7.14	0.996	1.50	0.884	0.14	0.861	0.96	0.855	1.29	0.766
HCa-A	9.0	0.956	1.35	0.838	1.68	0.992	0.28	0.863	1.12	0.858	1.48	0.765
ACh-A	4.4	0.867	0.24	0.037	1.26	0.880	NC		0.97	0.900	0.76	0.727
AR-B	9.8	0.988	1.31	0.905	1.11	0.981	0.20	0.715	1.18	0.842	0.90	0.744
HF-B	9.2	0.969	0.52	0.632	1.21	0.940	0.18	0.763	1.27	0.886	1.13	0.897
HL	13.6	0.996	2.22	0.784	1.70	0.993	0.14	0.895	0.94	0.902	0.98	0.814
ACh-C	15.6	0.995	7.53	0.942	1.77	0.809	0.25	0.862	1.22	0.913	1.14	0.817
DCa	13.9	0.995	1.77	0.887	1.42	0.837	0.62	0.872	1.75	0.961	2.28	0.949
SChS	18.5	0.991	19.39	0.967	1.48	0.693	0.58	0.887	1.61	0.923	1.82	0.906
HF-C	22.5	0.995	9.03	0.912	1.60	0.904	0.26	0.771	1.13	0.830	1.09	0.931
ACh-B	9.4	0.964	6.03	0.906	1.39	0.932	0.19	0.193	1.05	0.724	0.80	0.635
Avg.	11.6		4.57		1.43		0.28		1.12		1.18	
St.Dev.	5.0		4.91		0.24		0.17		0.33		0.42	
Max.	22.5		19.39		1.79		0.62		1.75		2.28	
Min.	3.3		0.24		1.04		0.14		0.39		0.76	
Range	19.2		19.15		0.74		0.49		1.36		1.52	
Literature values	1.6–2.88 for n = 0.75 – 1.16[a]				2.42 and 0.64 for n = 1[b]						1.04–5.55 for n = 1[c] 18.08 for n = 1[d] 0.69–2.5 for n = 1[e] 0.67–1.1 for n = 0.91–1.35[f] 0.3–0.63 for n = 1[g]	

[a] engineered geomedium (40% compost and 60% silica sand) and four soils (Tang & Kolodziej 2022); [b] clinoptilolite and palygorskite clay (Leal et al. 2017); [c] ten soils (Nguyen et al. 2020); [d] soil (of high Cox) from a contaminated site at an airport, desorption (Hubert et al. 2023); [e] soils from four contaminated areas (Høisæter & Breedveld 2022); [f] six soils (Barzen-Hanson et al. 2017); [g] two soils (Cai et al. 2022)

K_F (cm$^{3/n}$ μg$^{1-1/n}$/g) – Freundlich sorption coefficient; n_{avg} (–) – average n values; R^2 – coefficients of determination; DPG, TEC, 4-AAA, 6:2 FTS, BTSA, and NSA – studied compounds; soils: SChS – Stagnic Chernozem Siltic on marlite; HCh – Haplic Chernozem on loess; ACh-A and ACh-B – two Arenic Chernozems on sand and gravel; ACh-C – Arenic Chernozem on sandy marlstone; GP – Greyic Phaeozem on loess; HL – Haplic Luvisol on loess; HCa-A and HCa-B – two Haplic Cambisol on paragneiss; DCa – Dystric Cambisol on orthogneiss; HF-A, HF-B, HF-C, and GF – three Haplic Fluvisols and Gleyic Fluvisol on fluvial sediments; AR-A and AR-B – two Arenic Regolols on sand or sand and gravel

K_F values published for soils and other organomineral sorbents in the available literature. The coefficients of determination R^2 in Tables S7 in ESM and 1 show that using the average n value for all soils did not significantly worsen the resulting fits of the data points.

The K_F values for DPG varied between 3.3 and 22.5 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.37), which is higher than the K_F values (Table 1) published by Tang and Kolodziej (2022) for the engineered geomedium (40% compost and 60% silica sand) and four soils. It should be noted, however, that their isotherms were not as curved as in our study and even had a concave shape in three cases ($n < 1$), which could have resulted in the reduced K_F values. Nevertheless, their study showed an overall lower sorption of DPG in soils compared to our study. Similar range, but lower K_F values that varied between 0.24 and 19.39 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.37) were found for TEC. No data was found in the literature for comparison, likely because this compound is not considered a hazardous contaminant. Both compounds exhibited highly variable sorption in different soils, resulting in varying mobility in the soil environment, ranging from high to very low mobility (DPG) and from very high to low mobility (TEC).

The K_F values for other compounds were below 2.5 $cm^{3/n}$ $μg^{1-1/n}$/g, which indicates that their mobility is very high. The K_F values for 6 : 2 FTS varied between 0.76 and 2.28 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.28). These values are like those (Table 1) published by Barzen-Hanson et al. (2017), Nguyen et al. (2020), Cai et al. (2022), and Høisæter and Breedveld (2022), for various soils, but considerably lower than values (Table 1) published by Hubert et al. (2023) for soil of high Cox content. The K_F values for 4-AAA varied between 1.04 and 1.79 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.31), which is within the range of the K_F values (Table 1) published by Leal et al. (2017) for clinoptilolite and palygorskite clay. Two other compounds were selected as representatives of organic acids, for which high mobility in soil was expected. The K_F values for BTSA varied between 0.39 and 1.75 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.68), and even lower K_F values that varied between 0.14 and 0.62 $cm^{3/n}$ $μg^{1-1/n}$/g (for n_{avg} = 1.25) were found for NSA. No published data has been found for the sorption of these two substances in soils and sediments. However, very high sorption of NSA on polystyrene resin under acidic conditions or on granular activated carbon has been documented by Sun et al. (2019) and Song et al. (2006), respectively.

Correlations between the K_F values for different compounds and their relationships to soil properties. The correlation coefficients between the K_F values for different compounds (Table S8 in ESM) indicated the significant positive correlations between all three acids, BTSA, NSA (logarithmically transformed), and 6 : 2 FTS (logarithmically transformed): R = 0.641 (BTSA and 6 : 2 FTS), R = 0.649 (BTSA and NSA), and R = 0.574 (NSA and 6 : 2 FTS). Significant positive correlations were also found between DPG and TEC (logarithmically transformed) (R = 0.776), TEC (logarithmically transformed) and 4-AAA (R = 0.534), and DPG and NSA (logarithmically transformed) (R = 0.549). While positive correlation between the neural compounds TEC and 4-AAA, and even between the positively charged compound DPG and TEC (electrically neutral but polar molecules) can be expected, positive correlation between DPG (positively charged molecules) and NSA (negatively charged molecules) is surprising.

Similarities in sorption of different compounds were also reflected in their correlations with soil properties (Table S8 in ESM). The K_F values for BTSA, NSA (logarithmically transformed), and 6 : 2 FTS (logarithmically transformed) were mainly positively related to the Cox content (R = 0.705, 0.521, and 0.614, respectively), and BTSA and 6 : 2 FTS (logarithmically transformed) to PWI (logarithmically transformed) (R = 0.596 and 0.635, respectively). This suggests that the primary role of organic matter content and its hydrophobicity is in the sorption of these compounds in soil, specifically through hydrophobic interactions, π-π interactions, and hydrogen bonding. Interestingly, no positive correlations were found between the K_F values for these compounds and HA, as was the case in the previous studies (e.g., Kodešová et al. 2023). However, significant positive correlations with CEC were observed for the K_F value of BTSA and 6 : 2 FTS (logarithmically transformed) (R = 0.588 and 0.591, respectively). Negatively charged organic molecules should be repelled from the mostly negatively charged surface of soil components. The positive correlation with CEC for these weakly sorbing molecules can be explained by the sorption of these molecules via cation bridges (e.g., Yi et al. 2024). In the case of 6 : 2 FTS, Loganathan et al. (2025), who studied interfacial adsorption and dynamics of fluorotelomers with soil minerals, concluded that 6 : 2 FTS exhibits surface complexation. For example, the adsorption of 6 : 2 FTS was characterised by H-bond interactions with the basal hydroxyl surface of kaolinite or hydrophobic interactions between the carbon backbone and the hydrophobic region of the basal surface of montmorillonite. In addition, the mobility of surface adsorbed 6 : 2 FTS was substantially restricted by the coordination with surface adsorbed Ca^{2+} ions. Additionally, Cai et al. (2022) found that polyvalent cations (Ca^{2+} and Mg^{2+}) enhanced the sorption of 6 : 2 FTS in two soils. The sorption of DPG and TEC (logarithmically transformed) was positively related to clay content (R = 0.835 and 0.665, respectively), CEC (R = 0.731 and 0.589, respectively), and BCS (R = 0.762 and 0.736, respectively), which may indicate bonding mainly due to electrostatic interactions between positively charged compounds and negatively charged soil constituents. The K_F values for DPG were also positively correlated with all three pH values, which may be partly attributed to the positive correlations between the pH values and the clay or BCS content. However, correlations between the K_F values for TEC (logarithmically transformed) and all three pH values were much higher than those with other soil properties. In the case of 4-AAA, the only significant positive correlation of the K_F value was found with CEC (R = 0.512).

Prediction of the K_F values from soil properties. The equations for predicting the K_F values resulting from the multiple linear regressions are shown in Table 2. The suitability of the models is documented both by the coefficients of determination (R^2 in Table 2) and graphically in Figure 1. The first equation for each compound was derived using a limited set of soil properties, specifically model A. The second equations were obtained considering all measured soil properties, i.e., model B. The equation for DPG shows a dominant influence of clay content, which is present in both equations. The Cox content in the A equations was replaced by CEC in the B equations, which resulted in a slight improvement in the coefficient of determination (R^2). The equations for TEC show a strong relationship with pH_{KCl} and either clay content or CEC. The third model, C, was also proposed for DPG and TEC, both of which include BCS instead of CEC. However, this resulted in only a slight increase in R^2 values. Both equations for NSA include the Cox and clay content, and pH_{KCl} in the first equation was replaced by χHF, which considerably increased the R^2 value. All other equations A and B constructed for the remaining compounds differed significantly. While equation A for BTSA shows a positive relationship with Cox and clay content, an improved B equation indicates a positive relationship with CEC, ln(PWI), and χHF. The A equation for 4-AAA shows a weak, insignificant relationship with considered properties, i.e., a negative relationship with Cox content and a positive relationship with pH_{KCl} and clay content. The equation B for 4-AAA indicates a significant negative relationship with Cox content and a positive relationship with CEC and ln(PWI). The equation A for 6 : 2 FTS shows a weak positive relationship with Cox content. The B equation for 6 : 2 FTS again indicates a significant negative relationship with Cox content and a positive relation-

Table 2. Equations for predicting the Freundlich sorption coefficients

Compound	Model	Equation	R^2
1,3-Diphenylguanidine (DPG)	A	$K_{F\text{-DPG}} = 0.173 + 0.395\ \text{Clay}^{***} + 1.48\ \text{Cox}$	72.9***
	B	$K_{F\text{-DPG}} = 0.168 + 0.319\ \text{Clay}^{**} + 0.256\ \text{CEC}$	77.1***
	C	$K_{F\text{-DPG}} = 1.253 + 0.302\ \text{Clay}^{**} + 0.259\ \text{BCS}^{*}$	78.3***
Triethyl citrate (TEC)	A	$K_{F\text{-TEC}} = 2.718 \wedge (-3.74 + 0.682\ \text{pH}_{\text{KCl}}^{***} + 0.0347\ \text{Clay})$	73.9***
	B	$K_{F\text{-TEC}} = 2.718 \wedge (-3.98 + 0.719\ \text{pH}_{\text{KCl}}^{***} + 0.0532\ \text{CEC})$	76.1***
	C	$K_{F\text{-TEC}} = 2.718 \wedge (-3.342 + 0.618\ \text{pH}_{\text{KCl}}{}^{**} + 0.0598\ \text{BCS})$	77.0***
4-Acetamidoantipyrine (4-AAA)	A	$K_{F\text{-4-AAA}} = 1.09 - 0.0679\ \text{Cox} + 0.0492\ \text{pH}_{\text{KCl}} + 0.00740\ \text{Clay}$	22.3
	B	$K_{F\text{-4-AAA}} = 2.62 - 0.443\ \text{Cox}^{**} + 0.0387\ \text{CEC}^{***} + 0.295\ \ln(\text{PWI})$	62.0**
Napthalene-2-sulfonic acid (NSA)	A	$K_{F\text{-NSA}} = 2.718 \wedge (-2.36 + 0.427\ \text{Cox}^{*} + 0.0262\ \text{Clay} - 0.0644\ \text{pH}_{\text{KCl}})$	54.4*
	B	$K_{F\text{-NSA}} = 2.718 \wedge (-3.19 + 0.497\ \text{Cox}^{**} + 0.0217\ \text{Clay}^{*} + 0.0143\ \chi\text{HF}^{*})$	83.7***
Benzo(d)thiazole-2-sulfonic acid (BTSA)	A	$K_{F\text{-BTSA}} = 0.462 + 0.318\ \text{COX}^{**} + 0.00777\ \text{Clay}$	54.3**
	B	$K_{F\text{-BTSA}} = 1.73 + 0.0284\ \text{CEC}^{**} + 0.336\ \ln(\text{PWI})^{*} + 0.00682\ \chi\text{HF}^{*}$	68.2**
6 : 2 Fluorinated telomer sulfonate (6 : 2 FTS)	A	$K_{F\text{-FTS}} = 2.718 \wedge (-0.261 + 0.249\ \text{Cox}^{*})$	27.2*
	B	$K_{F\text{-FTS}} = 2.718 \wedge (2.34 - 0.283\ \text{Cox} + 0.0297\ \text{CEC}^{*} + 0.595\ \ln(\text{PWI})^{*})$	61.2**

K_F ($\text{cm}^{3/n}\ \mu\text{g}^{1-1/n}/\text{g}$) – Freundlich sorption coefficient; Cox (%) – oxidizable organic carbon content; Clay – clay content (%); pH_{KCl} – potential soil reaction; CEC ($\text{mmol}^+/100$ g) – cation exchange capacity; BCS ($\text{mmol}^+/100$ g) – base cation saturation, χHF (–) – magnetic susceptibility measured at high frequency, PWI (–) – potential wettability index; $^{***}, ^{**}, ^{*}P < 0.001, 0.01, 0.05$

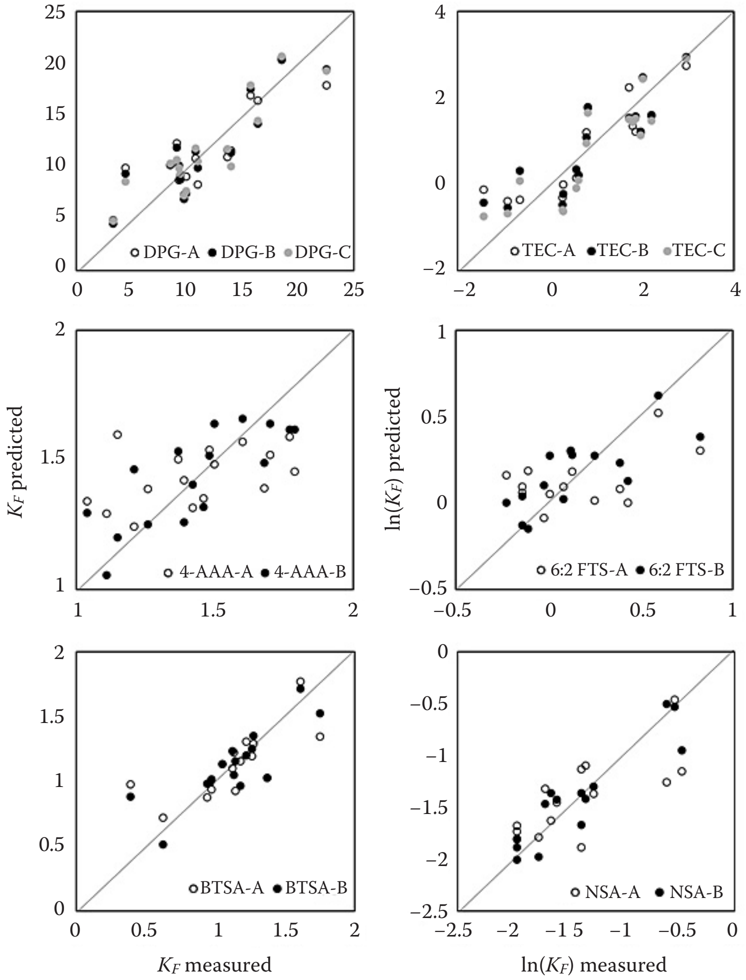

Figure 1. Measured and predicted Freundlich sorption coefficients

K_F (cm$^{3/n}$ μg$^{1-1/n}$/g) – Freundlich sorption coefficient; DPG, TEC, 4-AAA, 6:2 FTS, BTSA, and NSA –studied compounds; -A, -B, and -C – models in Table 2

ship with CEC and ln(PWI). From the above, it follows that while the soil properties usually available in the soil databases are sufficient for predicting K_F values of DPG and TEC, for other compounds, particularly 4-AAA and 6 : 2 FTS, it is necessary to consider other properties, such as CEC, ln(PWI), and χHF. The possible effects of various soil properties on the sorption of compounds have been discussed above, apart from χHF. Although no direct significant correlation was observed between the K_F values and χHF (Table S8 in ESM), this parameter is positively related to the K_F values in the equations obtained from the multiple linear regressions for both acids, NSA and BTSA (Table 2). This suggests that this parameter may indicate sorption sites for negatively charged compounds, which could be activated by the reduced pH of the solution-soil suspension due to the addition of both acids.

It should be noted that the sorption of each compound may be influenced by simultaneous sorption of multiple compounds. Studies by Kočárek et al. (2016) and Schmidtová et al. (2020) have shown that sorption can be affected both negatively, i.e., in the case of substances competing for the same sorption site, and positively. For example, acid sorption may increase when cationic molecules of co-sorbed compounds bind to negative charges on the surface of soil components, thereby reducing the repulsion between the soil surface and acid molecules. These effects, however, are more likely to occur at higher concentrations and not at environmentally relevant levels.

Linking compound sorption to real-world soil and water contamination. To study the actual occurrence of these substances in groundwater and soils, soil and groundwater samples were collected from different areas along Elbe and Dyje rivers irrigated with river water in the spring and summer of 2024. Passive samplers (POCIS) were also used to sample compounds in surface and groundwater. Maps of the occurrence of the studied substances in various matrices were published by Kodeš et al. (2025). DPG was detected in all soil samples collected from both areas, and its concentrations, for example, ranged between 7.6 and 1.8 ng/g and 2.0 and 0.9 ng/g in the Elbe and Dyje regions, respectively, during the summer. Interestingly, NSA was also found in one soil sample from the Elbe region at a concentration of 3.2 ng/g. All other concentrations were below the limits of quantification (LOQ). Concentrations of DPG in groundwater were in several cases below LOQ, but it was found in two samples in the Elbe (410 and 48 ng/L) and two in the Dyje regions (3.4 and 2.9 ng/L). NSA was detected in almost all groundwater samples, with concentrations ranging from 76 to 3.9 ng/L and from 96 to 6.6 ng/L in the Elbe and Dyje regions, respectively. 6 : 2 FTS was also quantified in some groundwater samples, i.e., 3.3, 2.3, and 1.9 ng/L (Dyje) and 1.9 ng/L (Elbe). 4-AAA was detected in two samples at concentrations of 2.6 ng/L (Elbe) and 2.5 ng/L (Dyje). Concentrations of BTSA and TEC were below LOQs that were an order of magnitude higher than LOQs for other compounds (19–35 for BTSA and 25–34 ng/L for TEC), with the exception of TEC in one groundwater sample in the Dyje region, where TEC concentration was 180 ng/L. In the case of compounds detected in passive samplers installed in groundwater in the Elbe and Dyje regions, the following values were found: DPG 2.8–0.3 and 1.2–0.36 ng/POCIS, NSA 150– < 33 and 120– < 33, 4-AAA 4.6– < 0.1 and 8.2– < 0.07, 6 : 2 FTS 3.0– < 0.31 and 1.6– < 0.31, TEC 150– < 10 and 120– < 10, and BTSA < 36 and < 36, respectively. The concentrations of compounds detected in passive samplers installed in the Elbe and Dyje rivers were: DPG 1300–180 and 74–16 ng per POCIS, NSA 800–750 and 43–9.4, 4-AAA 78–53 and 66–31, 6:2 FTS 8.1–9.1 and 3.7–0.73, TEC 33–27 and 33–12, and BTSA 210–63 and 49–19, respectively. The results of this monitoring campaign clearly demonstrated that these substances are present in the water and soil environment. The study could not confirm whether the detected contamination of these shallow aquifers is directly related to irrigation or whether these compounds reach groundwater through other pathways. However, their occurrence in different matrices corresponded to their sorption behaviour (i.e., potential mobility) in both the soil and the vadose zone environment.

CONCLUSION

The Freundlich sorption isotherms were measured for six compounds (whose source is not agricultural practice) identified in two agricultural areas irrigated with river water and sixteen soils. Multiple linear regressions were used to derive the equations for predicting the Freundlich sorption coefficients K_F. While cationic molecules strongly sorbed mainly via electrostatic interactions between the positively charged molecules and negatively charged soil constituents, sorption of anionic molecules was affected by several mechanisms. Mechanisms related to soil organic matter, i.e., hydrogen bonding, π-π and particularly hydrophobic interaction, were documented by the positive correlations between the sorption coefficients and organic carbon content or wettability index. Electrostatic interactions between negatively charged molecules and positively charged soil components were also probably involved, as was assumed based on the positive correlations between The K_F values and magnetic susceptibility. Finally, based on the positive correlation between K_F values and cation exchange capacity, cation bridges between negatively charged molecules and negatively charged soil components were inferred. The information obtained on the sorption of the substances investigated in the soil environment has wide application in subsequent studies dealing with the spread of these contaminants in the vadose zone environment, i.e. both their movement and accumulation in soil, uptake by plants, and leaching into the water sources. The K_F values indicated that while GPG and TEC have the potential to accumulate in soil, the other substances (4-AAA, NSA, BTSA, and 6 : 2 FTS) are highly mobile and have an increased potential to contaminate groundwater, which was confirmed by the results of the monitoring campaign. The mechanisms described may help to understand the behaviour of other similar micropollutants.

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