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Sorption of pharmaceutically active compounds to soils: a review

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Abstract

Pharmaceutically active compounds (PACs) are ubiquitous contaminants that can pollute the environment. This study critically analyzes the sorption of PACs to soil materials based on 137 published papers encompassing 106 PACs and 212 soil materials. The batch technique is commonly employed for sorption studies of PACs to soil, but the experimental setups vary in terms of the type and number of PACs, mixing time, solid to liquid (S/L) ratio, solution type, range of initial concentration, and bio-inhibition method. Sorption competition among PACs or between PACs and dissolved organic matter occurs for certain cases. Linear or close to linear behavior was reported for sorption of many PACs to soil, but sorption of some PACs deviates from linearity. The reaction of PACs to soil is fast at the initial stages but slows down as it approaches equilibrium. PACs characteristics, soil properties, and solution attributes intricately influence the sorption process. Zwitterionic PACs exhibit the highest sorption affinity, whereas neutral PACs display increased sensitivity to soil hydrophobicity. The average sorption coefficient (K) ranges from 0.0915 mL/g for anionic sulfonamides to 84725.5 mL/g for zwitterionic norfloxacin. An increase in the molar volume corresponds to heightened sorption for cationic PACs and reduced sorption for anionic PACs. Increasing solubility, soil organic carbon, cation exchange capacity, S/L ratio, and soil surface area while decreasing pH, ionic strength, and temperature result in an increase in K. The values of K determined by the batch technique are higher than their column-determined counterparts, possibly due to variations in the employed residence times between the two systems. Several models have been developed to estimate K of PACs, but they are limited in their applicability to specific PACs and soil types. Future research related to sorption of PACs to soils has been suggested.

Keywords Batch reactors, Column reactors, Emerging pollutants, Groundwater, Modeling, Pharmaceuticals, Prediction, Soil, Sorption nonideality

Introduction

Pharmaceutically active compounds (PACs) are organic molecules used to treat, inhibit, and reduce different diseases in human and animal bodies [126, 137]. The production of PACs has gained more attention over the last two decades, resulting in an increase in their production rate to meet the higher demand and consumption rate of people and animals [99]. PACs used by humans or animals are not completely utilized in the body, but some are excreted in urine and feces with a slight transformation or unchanged form [15, 17, 20, 22, 23, 45, 54]. Consequently, PACs have entered the environment through various sources, such as human waste [3], animal waste [69, 99], septic tanks [18], hospital waste [66,

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68], domestic waste [6, 16, 81], industrial waste [17], urban runoff [30], and landfills [51]. Figure 1 illustrates the possible pathways through which PACs could reach different environmental systems. PACs from septic tanks and landfills contaminate the unsaturated zone and could reach the aquifers and contaminate groundwater. PACs from farms and urban runoff contaminate the top surface and root zone and could reach surface water by surface runoff and groundwater by infiltration [64]. PACs from wastewater treatment plants (WWTPs) could be discharged directly into surface water, they could reach the soil surface using treated sewage effluent (TSE) for irrigation [16], or they could reach groundwater through surface or artificial aquifer recharge. Sludge from WWTPs if discharged to landfills could leach PACs and contaminate the unsaturated zone and groundwater. PACs could also reach surface water or groundwater through industrial discharge. Contaminated groundwater with PACs could reach surface water through natural discharge, while PACs in marine water could reach groundwater when the groundwater table is lowered below the sea level. PACs in surface water or groundwater may undergo several mechanisms that affect their fate including advection, dispersion, sorption, and degradation.

Several studies have investigated the presence of PACs in natural systems. For example, Ternes [119] found that 40 different rivers and streams in Germany contain 31 different PACs, with at least one compound found in every sample. Kolpin et al. [65] indicated that TSE inflows represent a major source of human PACs in surface waters. PACs were also found in aquifers underlying agricultural areas irrigated with TSE [5, 46, 61, 112]. Therefore, PACs could reach the natural system from different sources, one of which is TSE [81, 86]. Some PACs can also be sorbed or accumulate in the soil [88, 101]. The presence of PACs in environmental systems can lead to different complications. They can lead to the evolution of antibiotic-resistant bacteria, resulting in reduced drug efficacy [102]. Furthermore, leaching of PACs from top to lower soil layers can cause contamination of groundwater, posing a threat to indirect potable water reuse [25, 74, 89, 134], as they could affect humans and plants due to chronic exposure [127]. The large number of produced PACs, the inability to determine many of them, and the lack of data about their toxicity make it challenging to assess their potential risk. Moreover, many PACs do not have actual guidelines specifying their concentration in treated wastewater or soil [75, 97].

Sorption of PACs to soils could affect their fate in the environment [74]. Some PACs have higher sorption abilities than others. Their sorption depends on their physicochemical properties and on the characteristics of the sorbent and those of the solution. Tremendous efforts have been made in the last two decades to understand how PACs sorb to soil materials. Investigators typically tend to analyze the impact of a certain parameter on the sorption of a limited number of PACs. Among these studies, variations occur in the types of the investigated PACs, characteristics of the used soils, and properties of the solution. Variations also occur in the experimental protocols used and reactor type. These variations sometimes lead to discrepancies in the findings among different studies. Thus, there is a need to compile data from the conducted work to gain a better insight into the factors that control the sorption behavior of PACs to soil material.

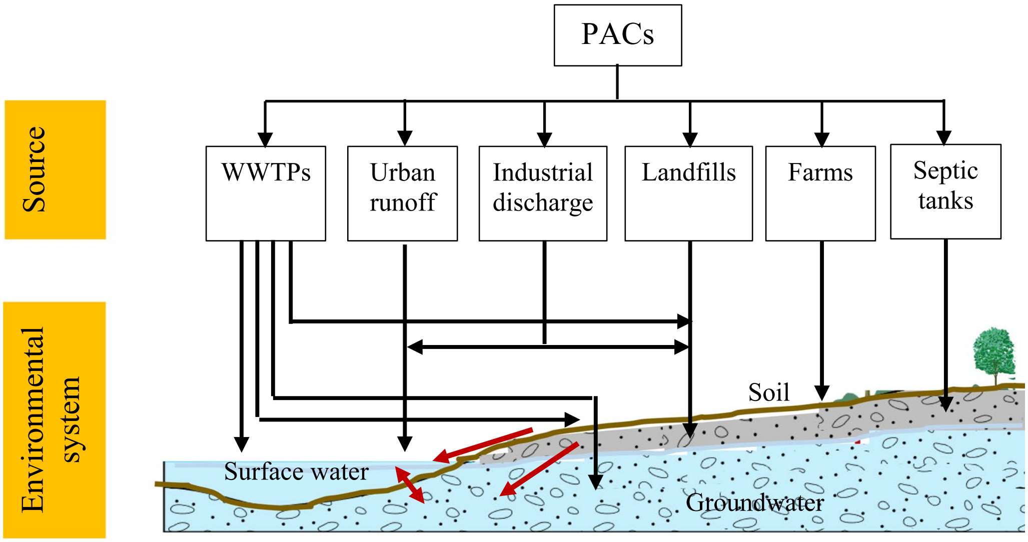

Fig. 1 Possible pathways for PACs to reach environmental systems

Tolls' [120] review of the literature on the sorption of veterinary pharmaceuticals to soil suggested that the sorption of these compounds cannot be solely predicted based on hydrophobic partitioning. Gworek et al. [47] reviewed the fate of PACs in soil and plants and concluded that the mobility of these compounds and their availability to plants depends on the soil and the PAC properties. Mejías et al. [87] reviewed the occurrence of PACs and their metabolites in sewage sludge. They concluded that the most critical PACs found in sludge-amended soil are ciprofloxacin, 17α-ethinylestradiol, 17β-estradiol, triclocarban, and triclosan. Xu et al. [129] reviewed the sorption of pharmaceuticals and personal care products (PPCPs) on soil components (humic acids, montmorillonite, kaolinite, and goethite). They also discussed the sorption mechanisms of PPCPs and assessed the influence of pH, ionic strength, organic matter, and temperature on sorption. Wang and Wang [124] reviewed the sorption of antibiotics to soil, with emphasis on the physicochemical properties of antibiotics and the influence of environmental factors on sorption. They concluded that the sorption of antibiotics to soil is a highly intricate process, reflecting the complex interplay of various factors. To our knowledge, no review compiles data from the literature for all the factors that influence the sorption of PACs to soil material. Previous reviews also limited the discussion to sorption in batch reactors and did not consider sorption in column reactors. A review of recent efforts to predict the sorption of PACs to soil is also lacking. Hence, this paper aims to critically review the research performed on the sorption of PACs to soil material in batch and column reactors. The discussion focuses on the experimental protocols employed, methods of determination of sorption parameters, nonideal sorption behavior, factors that affect the extent of PAC sorption, and established predictive relationships for the sorption of PACs to soils.

Description of the reviewed studies

Literature search

A bibliometric analysis [28] was conducted using a comprehensive search query to obtain insights regarding the status of the literature on sorption of PACs to soil. The obtained studies were categorized then into subgroups based on the type of experiment conducted, nature of the study, and general analysis attributes. Finally, selected papers were chosen from each category to extract essential data and information to carry out further analysis and discussions.

The bibliometric analysis was conducted utilizing the Scopus database. The search query used for searching the articles, mainly through the titles, keywords, and abstract, included the terms (Pharmaceuticals OR "Pharmaceutically Active Compounds" OR "Active Pharmaceutical Compounds") AND (Soil OR Sediment) AND (Sorption OR Absorption OR Adsorption OR Partitioning OR Interaction). The selection of keywords in the search query was based on obtaining the broadest number of publications related to the topic. The total articles initially obtained was 1,213 studies. Following that, a filtering stage was initiated by keeping only publications in the last 30 years (1994 to 2024), reducing the number of papers to 1,189. Another exclusion criterion was then applied to keep only peer-reviewed papers (removing conferences, book chapters, editorials), and to remove articles that are still in-press and non-English papers. The total number of obtained studies after applying the exclusion criteria was 974 studies. The obtained articles were then analyzed using VOSviewer, Bibliometrix (R-Studio open-source package), and Microsoft Excel, for trends and keywords analysis.

Annual publications in the present research field (Figure SM1) suggest that the topic was not a major focus of research in the 1990s and early 2000s. However, beginning 2003, an upward trend occurred, which could be attributed to increasing awareness and concern regarding environmental contamination of PACs to soil ecosystems. A more significant rise in publications started around 2009, accelerated from 2016 onwards, and reached a peak value of 98 articles in 2023. This spike could be linked to regulatory pressures for better environmental protection and public health strategies coupled with available funding as well as advancements in analytical techniques.

Figure 2 shows the cooperation exchange map between the 25 leading countries which conducted research on sorption of PACs to soil. Out of 974 publications, China leads with 130, followed by the United States with 115. This prominence could be attributed to their substantial research infrastructure, funding availability, and a high priority placed on environmental science and technology. Moreover, notable thick links were observed between countries like the United States and China or between Germany and Spain, suggesting robust cooperation. In terms of continental analysis, Europe leads with 314 articles, reflecting the strong research framework and collaborative policies in science within the continent. Asian countries follow with 261 publications, mostly contributed by China. North America (United States and Canada) shows a solid contribution (142 articles), led predominantly by the United States. South America, represented with 26 articles, suggests lesser focus or resource allocation towards this specific area of research. Notably, no studies have been conducted in Africa, and very limited studies have been conducted in the arid and semi-arid countries of the Gulf Cooperation Council, where the utilization of TSE for irrigation or aquifer recharge is widely promoted. Such an imbalance in global research efforts, where some regions are underrepresented, suggests the

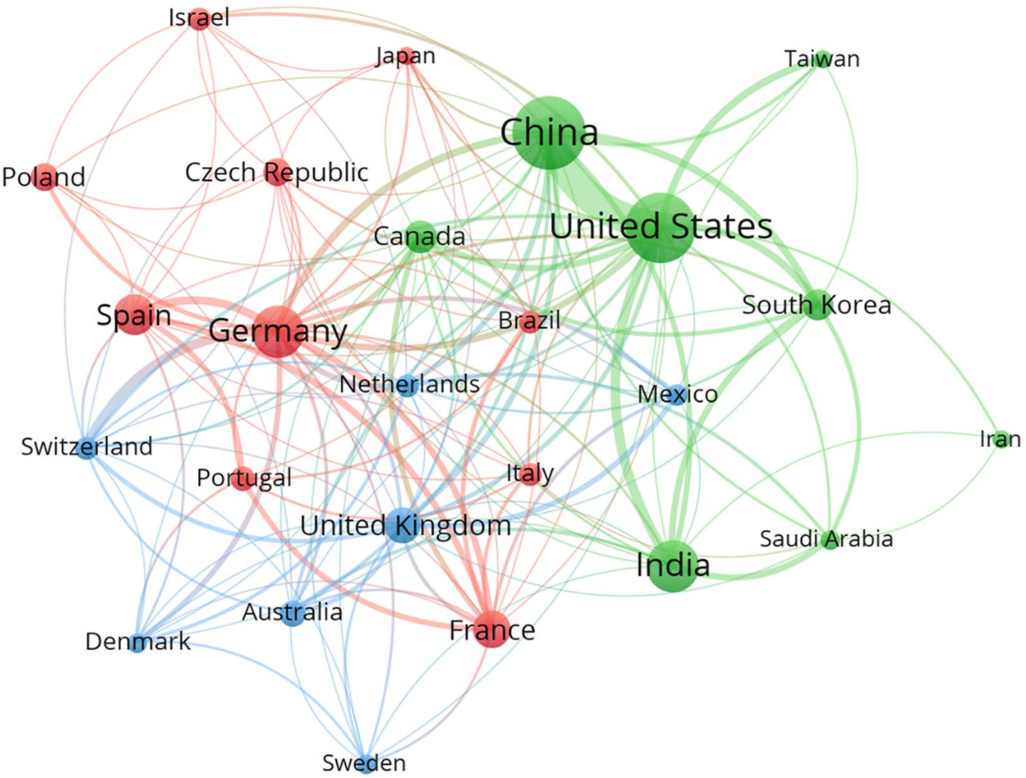

Fig. 2 Cooperation exchange between the 25 leading countries in the present research field

need for local strategic initiatives to bolster research capacities and outputs in these areas.

The database set showed a total of 2,670 authors' keywords, with the ones that occurred at least 10 times are visualized in Fig. 3. The keywords "pharmaceuticals," "sorption," and "adsorption" are the most frequently occurring terms. Thick lines connecting keywords denote a high frequency of co-occurrence in the literature. Furthermore, Fig. 3 shows three distinct clusters, each colored differently to represent various thematic focuses. The red cluster includes terms like "pharmaceuticals," "sorption," "biodegradation," and "wastewater." The common theme here revolves around the pathways and processes through which PACs interact with and impact water-related environments. The green cluster, featuring "soil, pharmaceuticals and personal care products ("PPCPs"), "plant uptake", and "risk assessment," focuses on the terrestrial impacts and risks of PACs. The blue cluster, including keywords like "sediment," "desorption," "metabolites," and "environmental risk assessment," is oriented towards understanding the fate and impacts of pharmaceutical residues in sedimentary environments and their broader ecological implications. This keyword analysis is beneficial for identifying the focal points of the conducted research and reveals the interconnectedness of different study areas within the field. The obtained insights can guide future research directions by highlighting firm paths and less explored areas that might be useful for a holistic understanding of the topic.

A further breakdown of the obtained 974 studies revealed that 107 involved batch experiments, 34 involved column experiments, 36 related to nonideal sorption of PACs to soil, and 11 related to predictive modeling. Other categories include review papers (148), risk assessment (97), remediation (281), toxicity (98), plant uptake (32), and metabolites (99). It should be noted that an overlap could occur among the different categories. For example, there are 7 publications that involved batch and column experiments and 37 publications that involved remediation and batch experiments.

Some research papers were selected for information and data extraction that are essential to carry out further analysis and discussion in this study. However, additional papers, not obtained from the search queries, were added to the selected papers. The added papers were not originally identified through the search queries for two reasons: (1) keywords may not always capture all pertinent studies due to variations in terminology, and (2) these papers, although not captured in the initial search, were identified through citations or references within the

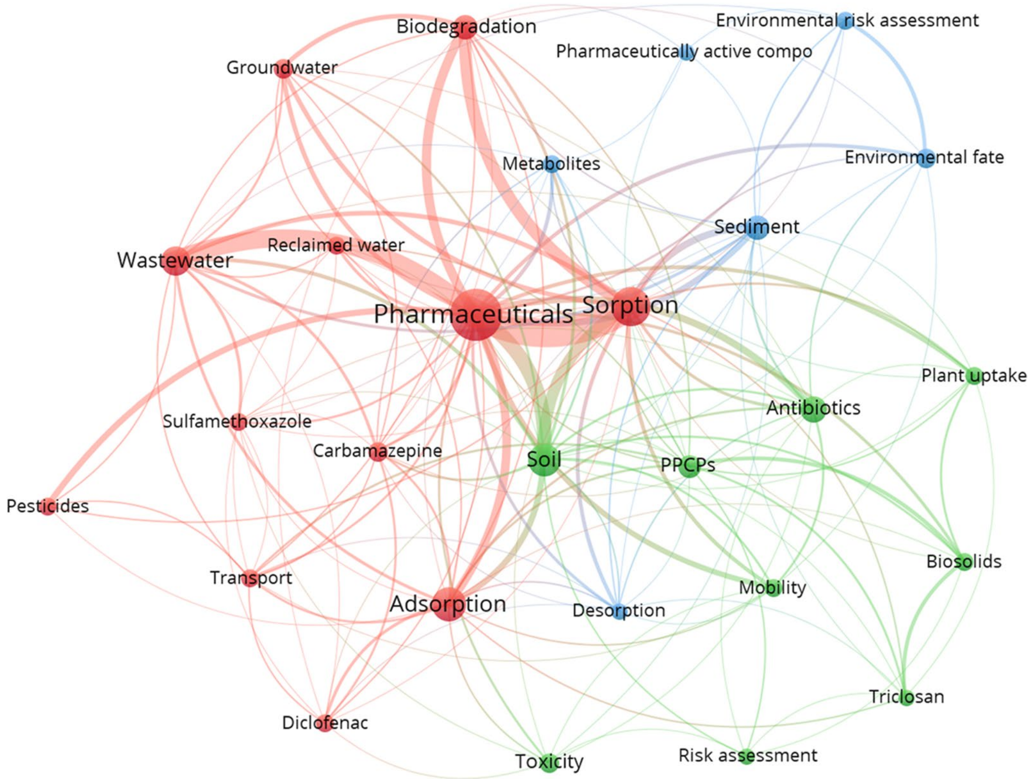

Fig. 3 Co-occurrence network of the top keywords in the present research field

primary dataset. A total of 137 studies were reviewed in this work, of which 59 batch- and column-related studies were used comprehensibly to make comparisons and to evaluate different factors that affect the sorption of PACs.

Table 1 briefly describes the reviewed batch and column studies including the number of PACs used and the type of the sorption study (rate or/and equilibrium). As noted before, limited work has been done to investigate the sorption of PACs in column compared with the batch reactor. Also, a few studies investigated the sorption of PACs in both reactors. Most of the reviewed studies that involved more than one PAC, have conducted sorption experiments with all tested PACs in the solution except those of Markiewicz et al. [82], Miroslav et al. [88], Srinivasan et al. [115], who studied the effect of sorption competition among the tested PACs.

Tested PACs

Table 2 provides a list of the PACs investigated in the reviewed studies along with their abbreviations. Table SM1 provides details about the chemical characteristics of the PACs, including their negative logarithmic base of 10 of the acid dissociation constants (pK_{a1}, pK_{a2}, and pK_{a3}), octanol–water partition coefficient (pK_{ow}), molecular mass (M_w), density (ρ), molecular volume (V_m), and water solubility (S_w). Figure SM2 presents the frequency at which these PACs appear in the reviewed studies. ATL, CBZ, DIC, SMTZ, and IBU have been reported in 10 or more of the reviewed studies.

Soil material

The characteristics of the used soil in the investigated studies including fraction of organic carbon (OC), cation exchange capacity (CEC), pH, and sorbent texture are presented in Table SM2. Some investigators manipulated the soil by changing the soil organic matter [60, 115] or by adding oxides to the soil material [131]. For studies where no significant differences were observed in the sorption behavior across different soil depths [88, 136], average values were considered. For studies reporting soil organic matter, it is assumed that soil organic matter contains 67% organic carbon [116].

Types of solution

The solution used for conducting the PACs sorption experiments varies among the reviewed studies. Many of the investigations used $CaCl_2$ at 0.01 M [27, 29, 135], 0.001 M [90], or 0.0037 M [48]. Others used 0.02 M phosphate buffer [130], artificially-made groundwater [107],

Table 1 Summary of the reviewed batch and column studies

Reference	Number of PACs	Batch	Column	Rate	Equilibrium
Accinelli et al. [1]	2	•		•	•
Al-Khazrajy and Boxall [2]	5	•		•	•
Arye et al. [4]	1		•	•	•
Białk-Bielińska et al. [10]	2	•		•	•
Boulard et al. [12]	27	•		•	•
Burke et al. [14]	1		•	•	
Calisto and Esteves [16]	1	•		•	•
Chefetz et al. [20]	3	•	•	•	•
Doretto and Rath [24]	1	•		•	•
Drillia et al. [25]	6	•		•	•
Durán–Álvarez et al. [27]	3	•	•	•	•
Estevez et al. [29]	1	•		•	•
Fan et al. [31]	1	•	•	•	•
Filep et al. [34]	9	•		•	•
Foolad et al. [35]	2	•		•	•
González-Naranjo et al. [44]	1	•		•	•
Haham et al. [48]	1	•		•	•
Hiller and Šebesta [50]	1	•		•	•
J. Li et al. [72]	54	•		•	•
Karnjanapiboonwong et al. [57]	5	•		•	•
Kiecak et al. [58]	7		•	•	
Kiecak et al. [59]	9	•		•	•
Kim et al. [60]	3	•		•	•
Klement et al. [62]	3	•		•	•
Kodešová et al. [63]	7	•		•	•
Leal et al. [70]	9	•		•	•
Lin and Gan [74]	5	•		•	•
Maoz and Chefetz [77]	2	•			•
Markiewicz et al. [82]	2	•		•	•
Martínez-Hernández et al. [84]	6	•		•	•
Maszkowska et al. [85]	3	•		•	•
Miroslav et al. [88]	3	•		•	•
Mutavdžić Pavlović et al. [90]	1	•		•	•
Mutavdžić Pavlović et al. [91]	1	•		•	•
Navon et al. [92]	1	•		•	•
Nowara et al. [93]	1	•		•	•
Pan and Chu [94]	5	•		•	•
Paz et al. [95]	2	•		•	•
Peruchi et al. [96]	1	•		•	•
Rabølle and Spliid [99]	3	•		•	•
Revitt et al. [101]	5	•		•	•
Schaffer et al. [105]	8		•	•	•
Scheytt et al. [106]	3		•	•	•
Scheytt et al. [107]	3	•		•	•
Scheytt et al. [108]	4		•		•
Schübl et al. [109]	5		•	•	
Shen et al. [111]	2	•		•	•
Srinivasan et al. [115]	1	•		•	•
Srinivasan et al. [114]	4	•		•	•

Table 1 (continued)

Reference	Number of PACs	Batch	Column	Rate	Equilibrium
ter Laak et al. [117]	3	•		•	•
Vulava et al. [122]	2	•		•	•
Wang et al. [125]	1	•		•	•
X. Li et al. [73]	9	•		•	•
Xu et al. [128]	5	•		•	•
Yamamoto et al. [130]	8	•		•	•
Yao et al. [131]	1	•		•	•
Yu et al. [133]	2	•		•	•
Zhang et al. [136]	4	•		•	•
Zhang et al. [135]	3	•		•	•

groundwater [58, 109], river water [105], freshwater [44], distilled water [125], or TSE with 0.005 M $CaCl_2$ [20].

Some investigators manipulated the solution by changing the dissolved organic matter (DOM) (e.g., [35]), altering solution pH (e.g., [131]), varying the ionic strength (e.g., [91]), or changing the solution temperature (e.g., [50]).

Methods of determination of sorption parameters

Batch studies

Batch experiments are conducted in bottles by adding a certain mass of the sorbent to a volume of the liquid solution containing a known concentration of the target PACs. The applied experimental conditions of the batch experiments in the reviewed studies are shown in Table 3. Based on the reviewed articles, the solid/liquid (S/L) ratio ranged from 1:1 [24, 29] to 1:1000 [122]. Typically, the S/L ratio is selected based on the extent of interaction between the target PACs and the sorbent. The initial concentration (C_o) employed in the isotherm (equilibrium) experiments of the reviewed studies varied from 0.01 μg/L [27] to 200 mg/L [131]. The reactor material used in the batch experiments was made of glass or PTFE [111, 133]. Biodegradation was inhibited in the reviewed studies by using NaN_3, $HgCl_2$, or by sterilization (using UV or Gamma-radiations or by autoclaving). Photodegradation could be inhibited by using amber bottles or by covering the bottles with aluminum foil [1]. Generally, control bottles were used to check for the disappearance of PACs in the absence of the sorbent.

Quantitation of PACs in solution was commonly done using either liquid chromatography (LC) [25, 114] or gas chromatography (GC) [107, 128, 133], coupled with various types of detectors as detailed in Table 3. Some researchers used solid phase extraction (SPE) to concentrate the analyte and achieve a better detection [4, 111].

The most used models to describe sorption rates in batch reactors are pseudo first order (PFO) and pseudo second order (PSO) models [91, 125]. The PFO model (Eq. 1) is applicable during the first stage of the sorption process, whereas the PSO model (Eq. 2) is applicable over a longer time period [100]. The PSO model assumes that the sorption capacity is directly proportional to the number of active sites occupied by the sorbent [91, 96]. Other models, such as Elovich [41, 73, 96], intra-particle diffusion [73, 91], and Boyd [73] have been used.

$$q_t = q(1 + e^{-k_1 t}) \tag{1}$$

$$q_t = \frac{k_2 q^2 t}{1 + q k_2 t} \tag{2}$$

where q_t is the concentration of the sorbate (μg/g) on the sorbent at time t (h), q is the concentration of the sorbate on the sorbent at equilibrium (μg/g), k_1 is the PFO rate constant (1/h), and k_2 is the PSO rate constant (μg/g.h).

The commonly used models in analyzing the batch isotherm results are the linear [31, 50, 70], the Freundlich [1, 27, 34, 42], and the Langmuir models [34, 59]. These models are presented in Eq. 3–5, respectively. Other models, such as Dubinin-Radushkevich and Temkin have been used [72, 73, 82, 90, 91].

$$q = KC \tag{3}$$

$$q = K_F C^N \tag{4}$$

$$q = \frac{q_m bC}{1 + bC} \tag{5}$$

where C is the equilibrium liquid phase concentration (μg/L), K is the linear sorption distribution coefficient (L/g), K_F is the Freundlich coefficient ($L^n.\mu g^{(1-n)}/g$), N is the Freundlich exponent, q_m is the maximum sorption capacity (μg/g), and b is the Langmuir constant (L/μg).

Table 2 List of PACs investigated in the reviewed articles

PACs	Abbreviation	PACs	Abbreviation
17α-ethynylestradiol	EE2	Metformin	MTF
17β estradiol or estradiol	E2	Methotrexate	MTX
1-acetyl-1-methyl-2-dimethyl-oxamoyl-2-phenylhydrazide	AMDOPH	Metoprolol	MET
1-Acetyl-1-methyl-2-phenyl hydrazide	AMPH	Metronidazole	MNZ
5-fluorouracil	5-FU	Naproxen	NAP
Acetaminophen	AMP	Nevirapine	NVP
Acetyl amino antipyrine	AAA	Nicotine	NCT
Amitriptyline	APL	N-methyl Phenacetin	N-MAPC
Amoxicillin	AMOX	Norethisterone	NTS
Antipyrine	ANP	Norfloxacin	NOR
Artemisinin	AMS	Ofloxacin	OFX
Atenolol	ATL	Oxazepam	OZP
Bezafibrate	BEZA	Oxytetracycline	OTC
Caffeine	CAF	Para-toluene sulfonamide	p-TSA
Carbamazepine	CBZ	Phenacetin	APC
Cetirizine	CTZ	Phenobarbital	PBB
Chloramphenicol	CAP	Phenyl ethyl malonamide	PEMA
Cimetidine	CMD	Phenytoin	PNT
Ciprofloxacin	CIPRO	Pregabalin	PGL
Citalopram	CTP	Primidone	PRI
Clarithromycin	CAM	Propranolol	PPOL
Clindamycin	CLN	Propranolol hydrochloride	PPOL HCl
Clofibric acid	CFA	Propyphenazone	PPZ
Codeine	COD	Ranitidine	RTD
Cotinine	COT	Roxithromycin	RXM
Danofloxacin	DFX	Salbutamol	SBT
Desvenlafaxine	DVF	Sitagliptin	SGP
Diazepam	DZ	Sotalol	STL
Diclofenac	DIC	Sulfa chloro pyridazine	SCP
Diltiazem	DLZ	Sulfadiazine	SDI
Enrofloxacin	ENR	Sulfadimethoxine	SMX
Erythromycin	ETM	Sulfadimidine	SDM
Estrone	E1	Sulfaguanidine	SGI
Fexofenadine	FXFD	Sulfamethazine	SMZ
Fluconazole	FCZ	Sulfamethizole	SUT
Fluoxetine	FXT	Sulfamethoxazole	SMTZ
Formyl amino antipyrine	FAA	Sulfapyridine	SPI
Gabapentin	GPN	Sulfathiazole	STZ
Glipizide	GPZ	Sulfisoxazole	SSZ
Hydrocodone	HYC	Sulfonamides	SFM
Ibuprofen	IBU	Temazepam	TMZ
Ifenprodil	IFP	Tetracycline	TTC
Indomethacin	IND	Thiabendazole	TBD
Irbesartan	IBS	Tolyltriazole	TTRI
Ketoprofen	KET	Tramadol	TMD
Ketotifen	KTF	Tramadol hydrochloride	TMD HCl
Lamotrigine	LTG	Triamterene	TMR
Lidocaine	IDC	Triclosan	TCS
Lidocaine hydrochloride	IDC HCl	Trimethoprim	TMP

Table 2 (continued)

PACs	Abbreviation	PACs	Abbreviation
Lincomycin	LNY	Tylosin	TYL
Loratadine	LTD	Venlafaxine	VFX
Mefenamic acid	MFA	Verapamil	VPM
Meprobamate	MPB	Warfarin	WFR

One of the objectives of this study was to quantitatively assess the effect of various factors (related to the sorbate, sorbent, or the solution) on the sorption of the PACs. For cases where sorption is linear, the comparison was made based on the values of K. For cases with a nonlinear sorption behavior, the process was not straightforward as two parameters affected the extent of sorption (K_F and N for a Freundlich behavior and q_m and b for a Langmuir behavior). To resolve this, a linearized sorption distribution coefficient (K_L) was estimated for the reported cases with nonlinear sorption behavior as described by Genuchten et al. [39]. The equations used for linearization (Eq. SM1 to SM5) are provided in the supplementary material.

Column studies

Column experiments are commonly used to evaluate the transport of pollutants through porous media. Compared with the batch method, the column method provides a better representation of contaminant transport through the sorbent in the field. The setup of a column experiment in the reviewed studies varied in terms of the average pore water velocity (v_o), column length (L) and internal diameter (ID), column material, injected solution concentration, and injection type. Although high pore-water velocities lead to faster experimentation and allow for more repetitions, slow velocities may need to be applied for better representation of natural systems. Based on the reviewed articles, the average pore water velocity ranged from 0.267 to 62.4 cm/h [4, 27]. The column length reported in the reviewed studies ranged from 7 cm [27, 31] to 51 cm [109], whereas the column internal diameter ranged from 3 to 10 cm [4, 14]. The column material was either stainless steel [14, 27], or glass [4, 20].

Table 4 lists the experimental conditions of the reviewed articles involving column experiments. The methods used for obtaining sorption parameters from the column breakthrough data varied among the reviewed studies. For example, the retardation factor (R_f) was found by either the number of pore volumes at $C/C_o = 0.5$, fitting breakthrough data to an equilibrium transport model, or by fitting the breakthrough data to a two-site nonequilibrium transport model. The 1-D transport equation under steady-state conditions in a homogenous soil is given as:

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{\theta}\frac{\partial q}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v_o\frac{\partial C}{\partial x} \tag{6}$$

where D is the hydrodynamic dispersion coefficient (m^2/h), v_o is average pore-water velocity (m/h), ρ_b is soil bulk density (g/cm^3), θ is volumetric water content, t is time (h), and x is distance (m).

The two-site sorption nonequilibrium model assumes that sorption on a fraction of the soil (F) is instantaneous, while it is rate-limited on the remaining part. For a first-order rate reaction with a nonlinear sorption behavior, the sorption rate on these soil fractions is expressed as [79]:

$$\frac{\partial q_1}{\partial t} = FKC^{N-1}\frac{\partial C}{\partial t} \tag{7}$$

$$\frac{\partial q_2}{\partial t} = k[(1 - F)KC^N - q_2] \tag{8}$$

where k is the first-order sorption/desorption rate coefficient (1/h) and $q_1 + q_2 = q$. Equations 6–8 constitute the two-site first order nonequilibrium model with nonlinear sorption. The retardation factor (R_f) for a linear sorption behavior is given as:

$$R_f = 1 + \frac{\rho_b K}{\theta} \tag{9}$$

All the investigations listed in Table 4 that use curve fitting to obtain R_f assumed that sorption of the tested PACs is linear. The column experiments listed in Table 4 were conducted under saturated conditions except for the study of Durán–Álvarez et al. [27] and Scheytt et al. [108] who conducted their experiments under unsaturated flow conditions. In addition, all the studies packed the soil homogeneously in the columns (i.e., disturbed soil column experiments), except for the study of Durán–Álvarez et al. [27] where undisturbed soil columns were used.

Table 3 Applied experimental conditions of the batch sorption study of the reviewed articles

Reference	PACs	S/L ratio	C_o (mg/L)	Time (h)	Bio-inhibition	Analytical method
Accinelli et al. [1]	SCP, SMZ	1:2	0.001–0.1	14	NR	HPLC[a]
Al-Khazrajy and Boxall [2]	APL	1:25	20–100	24	NR	HPLC-PDA[b]
Al-Khazrajy and Boxall [2]	ATL, CMD, MFA	1:10	20–100	24	NR	HPLC–PDA
Al-Khazrajy and Boxall [2]	DLZ	1:30	20–100	24	NR	HPLC–PDA
Białk-Bielińska et al. [10]	SGI	1:25	0.625–80	24	NR	HPLC-UV[c]
Białk-Bielińska et al. [10]	SMX	1:5	0.625–80	24	NR	HPLC–UV
Boulard et al. [12]	ATL, BEZA, CBZ, CTP, CAM, DIC, FXFD, FCZ, FXT, GPN, IBS, LTG, IDC, MET, NAP, OZP, PNT, PGL, PRI, RXM, SGP, STL, SMTZ, TMD, TMP, CLN, MTF	1:5, 1:25[m]	0.0002–0.04	24	NR	LC–MS/MS[d]
Calisto and Esteves [16]	CBZ	1:2	2–8	4	NR	HPLC–UV
Chefetz et al. [20]	CBZ, NAP	NR	0.1–10	72	NaN_3	LC–MS/MS
Chefetz et al. [20]	DIC	NR	0.1–10	48	NaN_3	LC–MS/MS
Doretto and Rath [24]	SDI	1:1	4–75	48	NaN_3	HPLC–PDA
Drillia et al. [25]	CBZ, SMTZ, DIC, CFA	1:2	1–12	24	NR	HPLC–UV
Drillia et al. [25]	OFX	1:50	1–12	24	NR	HPLC–UV
Drillia et al. [25]	PPOL HCl	1:25	1–12	24	NR	HPLC–UV
Durán–Álvarez et al. [27]	E1, E2, IBU	1:5	0.00001–0.01	24	NR	GC[e]-MS[f]
Estevez et al. [29]	IBU	1:1, 1:5[13]	1–200	24	Autoclaved at 121 °C for 45 min	HPLC–UV
Fan et al. [31]	SMZ	1:5	0.012–1.219	168	NR	TLC[g]
Filep et al. [34]	CBZ, DIC, E1, E2, EE2, IDC HCl, LTG, OZP, TMD HCl	1:12	0.1–5	2	NaN_3	HPLC–PDA
Foolad et al. [35]	AMP, CBZ	1:25	0.1–1	24	Sterilized (NR)	LC–MS/MS
González-Naranjo et al. [44]	IBU	1:5	0–10	24	NR	HPLC–UV
Haham et al. [48]	SPI	1:10	0.04–11	96	NaN_3	HPLC–PDA
Hiller and Šebesta [50]	IBU	3:5	1–20	48	NaN_3	HPLC-FLD[h]
J. Li et al. [72]	APL, AMS, ATL, CAF, CBZ, CTZ, CMD, CIPRO, CTP, CAM, COD, COT, DVF, DZ, DLZ, ENR, ETM, FXFD, FXT, FCZ, GPN, GPZ, HYC, KTF, IDC, LNY, LTD, MTF, MNZ, NAP, NVP, NCT, NTS, OTC, AMP, PNT, PGL, PPOL, RTD, SBT, SGP, SDI, SUT, SMTZ, TMZ, TTC, TBD, TMD, TMR, TMP, TYL, VFX, VPM, WFR	1:5[n], 1:3[o], 1:2[p]	0.01–0.04	24	NR	HPLC–MS/MS
Karnjanapiboonwong et al. [57]	E1, E2, EE2, TCS, CAF	1:30	1–4	24	NR	HPLC–UV
Kiecak et al. [59]	ANP, ATL, CAF, CBZ, CIPRO, OFX, SMTZ, KET, DIC	1:5	0.5–7.5	96	NaN_3	LC–MS/MS
Kim et al. [60]	AMOX, OTC, STZ	1:10	1–40	24	Sterilized (NR)	HPLC–UV
Klement et al. [62]	CTP, FXFD, IBS	1:2	1–10	24	NR	LC–MS/MS
Kodešová et al. [63]	ATL, TMP CAM, CBZ, CLN, MET, SMTZ,	1:2	0.5–10	24	NR	LC–MS/MS
Leal et al. [70]	CIPRO, DFX, ENR, STZ NOR,	1:15	1–6	24	NR	HPLC–PDA and FLD
Leal et al. [70]	SCP, SDI, SDM, SMTZ	1:2	1–6	24	NR	HPLC- PDA and FLD
Lin and Gan [74]	DIC, IBU, NAP, SMTZ, TMP	1:5	0.002–0.04	24	NaN_3	LC–MS/MS
Maoz and Chefetz [77]	CBZ, NAP	NR	0–10	48	NaN_3	HPLC–PDA
Markiewicz et al. [82]	MTX	1:15	0.625–100	24	NaN_3	HPLC–UV
Markiewicz et al. [82]	5-FU	1:25[q], 1:5[p]	0.625–100	24	NaN_3	HPLC–UV
Martínez-Hernández et al. [84]	AMP, ATL, CAF, CBZ, NAP, SMTZ	1:4	0.001–0.1	24	NaN_3	LC–MS TripleTOF[i]
Maszkowska et al. [85]	PPOL HCl	1:50	0.625–80	24	NR	HPLC–UV
Maszkowska et al. [85]	SGI	1:5	0.625–80	24	NR	HPLC–UV
Maszkowska et al. [85]	SSZ	1:2	0.625–80	24	NR	HPLC–UV
Miroslav et al. [88]	ATL, CBZ, SMTZ	1:2	1–10	24	NR	LC–MS/MS
Mutavdžić Pavlović et al. [90]	SMZ	1:5[18]	1–50	24	NaN_3	LC–MS/MS

Table 3 (continued)

Reference	PACs	S/L ratio	C_o (mg/L)	Time (h)	Bio-inhibition	Analytical method
Mutavdžić Pavlović et al. [90]	SMZ	1:2[19]	1–50	24	NaN_3	LC–MS/MS
Mutavdžić Pavlović et al. [91]	CIPRO	1:25	0.1–25	4	NaN_3	HPLC-FLD
Navon et al. [92]	CBZ	1:5	0.005–0.1	96	NaN_3	LC–MS/MS
Nowara et al. [93]	ENR	1:20	0.1–10	6	NR	HPLC-SEC[j]
Pan and Chu [94]	TTC, SMZ, NOR, ETM, CAP	1:5	0.01–0.1	24	NaN_3	LC–MS/MS
Paz et al. [95]	LTG	1:5	0.05–5	168	NaN_3	LC–MS
Paz et al. [95]	CBZ	1:1	0.05–5	168	NaN_3	LC–MS
Peruchi et al. [96]	NOR	1:100	1–50	50	NaN_3	HPLC–PDA
Rabølle and Spliid [99]	MNZ, TYL	1:4	1.25–50	24	NR	LC–MS
Rabølle and Spliid [99]	OTC	1:8	1.25–50	24	NR	LC–MS
Revitt et al. [101]	BEZA, CAP, CBZ, DIC, TCS	1:2	1–10	24	Sterilized by Gamma radiation	LC–MS-IT[k]-TOF
Scheytt et al. [107]	CBZ, DIC, IBU	4:5	0.057–0.857	24	NR	GC–MS
Shen et al. [111]	SDI, SMTZ	1:5	0.5–10	24	Autoclaved at 121 °C for 20 min	LC–MS/MS
Srinivasan et al. [115]	SMTZ	1:15	1–15	24	NR	HPLC–UV
Srinivasan et al. [114]	TYL, SMTZ, SCP, SMZ	1:15	2.5–35	24	NR	HPLC–UV
ter Laak et al. [117]	OTC	1:300[t], 1:150[u]	0.05–5	24	NaN_3	HPLC–UV
ter Laak et al. [117]	SCP	1:2	0.05–5	24	NaN_3	HPLC–UV
ter Laak et al. [117]	TYL	1:2[u], 1:25[t]	0.05–5	24	NaN_3	HPLC–UV
Vulava et al. [122]	IBU, NAP	1:5 – 1:1000	0.01–20	168	NR	LC–MS/MS
Wang et al. [125]	OTC	1:20	5–25	24	NR	UPLC-TUV[l]
X. Li et al. [73]	SMZ	1:2	0.1–9.8	168	$HgCl_2$	HPLC–UV
Xu et al. [128]	CAF, DIC, IBU, NAP, TCS	1:2	0–10	24	Autoclaved at 120 °C for 45 min	GC–MS
Yamamoto et al. [130]	AMP, CBZ, IND	1:2	0.02–0.1	24	NaN_3	HPLC–UV
Yamamoto et al. [130]	ATL, IBU, IFP, MFA, PPOL	1:2	0.02–0.1	24	NaN_3	HPLC-FLD
Yao et al. [131]	OTC	1:100	0.5–200	24	NaN_3	HPLC-FLD
Yu et al. [133]	CBZ, TCS	1:10	0–1	24	NaN_3	GC–MS
Zhang et al. [136]	SFM, SMX, SPI, TMP	1:2.5	0.1–10	48	NR	HPLC–UV
Zhang et al. [135]	ATL, CAF, SDI	1:2.5	0.001–0.1	72	NR	LC–MS/MS

[a] *HPLC* High-performance liquid chromatography

[b] *PDA* Photodiode array detector

[c] *UV* Ultraviolet detector

[d] *LC-MS/MS* Liquid chromatography with tandem mass spectrometry

[e] *GC* Gas chromatography

[f] *MS* Mass spectrometry

[g] *TLC* Thin layer chromatography

[h] *FLD* Fluorescence detector

[i] *TOF* Time of flight detector

[j] *SEC* Size exclusion chromatography

[k] *IT* Ion trap

[l] *UPLC-TUV* Ultrahigh performance liquid chromatography tunable ultraviolet detector

[m] Studied the effect of S/L for the same soil

[n] For Sandy loam 1 and Clay loam 3

[o] For Clay loam 1 and Sandy clay loam 2

[p] For the remaining soils in the study

[q] For Alluvial

[r] For Sand 3

[s] For the remaining soils

[t] For Clay loam

[u] For Loamy sand

Table 4 Experimental conditions of the column studies of the reviewed articles

Reference	PACs	Injection type	ρ_b[a] (g/cm^3)	θ[a]	ID (cm)	L (cm)	v_o (cm/h)	Bio-inhibition	Method of determining R_f
Arye et al. [4]	CBZ	Pulse	1.66	NR	3	20	62.4^{b}, 55.2^{c}, 57.6^{d}, 58.8^{e}	NR	Fitting an equilibrium or a two-site nonequilibrium sorption model
Burke et al. [14]	DZ, OZP, MPB, PRI, ANP, PPZ, AMDOPH, AMPH, AAA, FAA, ATL, PPOL, STL, MET, p-TSA, TTRI, APC, N-MAPC	Desorption	NR	0.45	10	30	0.612	NaN_3	Fitting a one-site nonequilibrium sorption model
Chefetz et al. [20]	CBZ, DIC, NAP	Desorption	NR	NR	3	25	16.8	NaN_3	Pore volume at $C/C_o = 0.5$
Durán–Álvarez et al. [27]	E1, E2, IBU	Pulse	1.1^{m}, 1^{n}	0.4^{m}, 0.41^{n}	9	15	0.267	NR	Fitting an equilibrium or a two-site nonequilibrium sorption model
Fan et al. [31]	SMZ	Pulse	1.01^{o}, 0.87^{p}, 0.91^{q}, 1.17^{m}, 1.67^{r}	0.62^{o}, 0.67^{p}, 0.66^{q}, 0.56^{m}, 0.37^{r}	8.4	15	20^{o}, 20.9^{p}, 19.8^{q}, 21.4^{m}, 39.4^{r}	NR	Fitting a two-site nonequilibrium sorption model
Kiecak et al. [58]	ANP, ATL, CAF, CBZ, DIC, KET, SMTZ,	Pulse	1.89^{g}, 1.51^{h}, 1.53^{f}	NR	$9^{f,g}$, 5^{h}	50	8.7^{f}, 5.3^{f}, 2.8^{f}, 10.8^{g}, 7.2^{g}, 4.2^{g}, 9.8^{h}, 2.6^{h}	NaN_3	Fitting an equilibrium sorption model with degradation
Schaffer et al. [105]	ATL, CBZ, CTZ, DZ, NAP, PBB, PRI, TMP	Step increase	1.78	NR	3.4	25	3.77	NR	Fitting an equilibrium sorption model
Scheytt et al. [106]	CFA, PPZ, DIC	Desorption	NR	0.32	13.59	35	1.25	NR	Pore volume at $C/C_o = 0.5$
Scheytt et al. [108]	CBZ, DIC, IBU, PPZ	Desorption	1.8^{i}, 1.86^{j}, 1.87^{k}, 1.73^{l}	$0.28^{i,j}$, 0.29^{k}, 0.26^{l}	13.6	35	3.21^{i}, 2.96^{j}, 3.5^{k}, 3.66^{l}	NR	Fitting a two-site nonequilibrium sorption model
Schübl et al. [109]	ANP, ATL, CAF, CBZ, SMTZ	Pulse	NR	NR	5, 9.1	51	1.2^{f}, 1.29^{f}, 3.5^{h}, 3.85^{h}	NaN_3	Fitting a two-site nonequilibrium sorption model with degradation

[a] ρ_b is bulk density and θ is moisture content

[b] Basin soil, 0–5 cm

[c] Basin soil, 5–25 cm

[d] Basin soil, 25–50 cm

[e] Basin soil, 50–75 cm

[f] Coarse sand

[g] Medium sand

[h] Sandy loam

[i] for CBZ

[j] for DIC

[k] for IBU

[l] for PPZ

[m] Loam

[n] Clay

[o] Silty clay loam

[p] Clay loam

[q] Silt loam

[r] Sand

Sorption nonideality

Ideal sorption behavior entails equilibrium, linear, singular, and non-competitive interaction between the sorbate and the sorbent. Deviations from ideality may occur due to rate limitations (nonequilibrium), nonlinear sorption, hysteresis (non-singular), or competitive/cooperative sorption.

Sorption nonequilibrium

Sorption kinetics of PACs in batch reactors can be influenced by the type of soil [63, 70], the nature of the PACs [118], and the type of solution used [20]. Based on the reviewed studies, the reaction kinetics of PACs in batch reactors is characterized by a fast reaction at the initial stages followed by a slow approach to equilibrium.

The time to reach equilibrium in batch reactors varied from 2 h [34] to 168 h [31, 72, 73, 95, 122]. The average and standard deviation for the equilibrium time based on the reviewed studies are 31 h and 26.4 h, respectively. A long equilibrium time could be attributed to slow chemical reactions or limitations in the transfer of the PAC to the sorption sites due to slow diffusion within the sorbent pores or soil organic matter.

Investigation of sorption kinetics in the reviewed studies was mainly intended to determine the equilibrium time. However, few studies have modeled sorption kinetics in batch reactors (Table SM3). Wang et al. [125] tested PFO and PSO rate models for OTC using three types of sediments and found that the PFO model was better than the PSO model. However, Mutavdžić Pavlović et al. [91] found that the sorption of CIPRO onto different soils followed the PSO model. These models, however, cannot be utilized to elucidate the sorption mechanism [91].

Sorption nonlinearity

Ideal sorption requires a linear relationship between the equilibrium solid phase concentration and the equilibrium liquid phase concentration (Eq. 3). In some cases, sorption deviates from linearity. In general, sorption linearity is influenced by the properties of PACs [34, 62], soil properties [62, 63], temperature [50, 91], pH [60, 105, 115], and ionic strength [60, 115]. The addition of DOM to soil causes an increase in the degree of sorption nonlinearity due to the heterogeneity of the system [135].

Sorption of IBU in the work of González-Naranjo et al. [44] was best described by the linear model. On the other hand, several investigators [16, 82, 84] showed a nonlinear sorption behavior following the Freundlich model. Kiecak et al. [59] did not find a specific pattern to generalize which model was the best for their investigated PACs.

Different mathematical models have been utilized to examine sorption isotherms of PACs, encompassing the linear, Freundlich, Langmuir, Temkin, and Dubinin models. The frequency of their usage among the reviewed studies is 38 times for the linear model, 45 for the Freundlich model, 11 for the Langmuir model, one for the Temkin model, and three for the Dubinin model. Table SM4 presents the sorption isotherm models used in the reviewed studies and the best model was found when multiple models were tested. The Freundlich's model was reported 14 times more than the linear model as the best fit. The average N value and standard deviation based on the reviewed studies were 0.828 and 0.2, respectively. The reported range of N values associated with the Freundlich model is presented in Fig. 4, showing that two-thirds of the reported values are between 0.7 and 1.1. Estevez et al. [29] found that the Langmuir and Freundlich models were suitable for describing their equilibrium sorption results. In the latter study, the results of the Freundlich model were used in the data analysis.

While linear or close to linear behavior was reported for sorption of many PACs to soil, sorption in some cases deviates from linearity and becomes more pronounced with the increase in the initial concentration [48, 92]. Consideration of nonlinear sorption is necessary in assessing the transport of PACs in groundwater as it could significantly affect the shape of contaminant plumes, causing back tails and sharp front ends [32, 110]. Meanwhile, the mean residence time (related to R_f) of a nonlinearly sorbed contaminant is influenced by the concentration at the source and the pore-water velocity [78].

Sorption hysteresis

Hysteresis (or non-singularity) occurs when the sorption and desorption isotherms do not coincide [13, 24, 25]. True hysteresis occurs when sorbed compounds strongly adhere to the sorbent and are not released during the desorption process (irreversible sorption). Sorption hysteresis may be explained by the presence of two distinct types of sorption sites: resistant and reversible. Additionally, it has been suggested that the sorption/desorption process can cause a physical alteration in the soil, leading to fluctuations in the number of available sorption sites [79]. About 14 reviewed studies investigated the sorption hysteresis of PACs.

Navon et al. [92] found that CBZ exhibits higher sorption hysteresis and higher non-linearity with silt loam soil than for clay soil. They attributed this to specific interactions of the compound to the polar soil organic carbon which is higher in silt loam than in clay soil. Durán–Álvarez et al. [27] also attributed the hysteresis in their studies to the amount of organic carbon in the soil. However, Paz et al. [95] reported reversible sorption isotherm for LTG and CBZ for their three tested soils while Chefetz et al. [20] reported reversible sorption isotherm for CBZ and NAP and hysteresis for DIC. The observed hysteresis for DIC was attributed by Chefetz et al. [20] to the entrapment of the adsorbed molecules in the organic and inorganic matrices. Furthermore, Yao et al. [131] found an increase in the hysteresis of OTC as the soil pH approached the pK_a value. Some investigators, however, cautioned that the observed hysteresis of organic compounds could be an artifact caused by slower desorption rates [24, 25], unaccounted for removal mechanisms, or analytical difficulties in measuring low desorbed concentrations [13].

Competitive/cooperative sorption

Sorption competition occurs when two or more substances compete for the same sorption sites. This could be influenced by the physicochemical properties

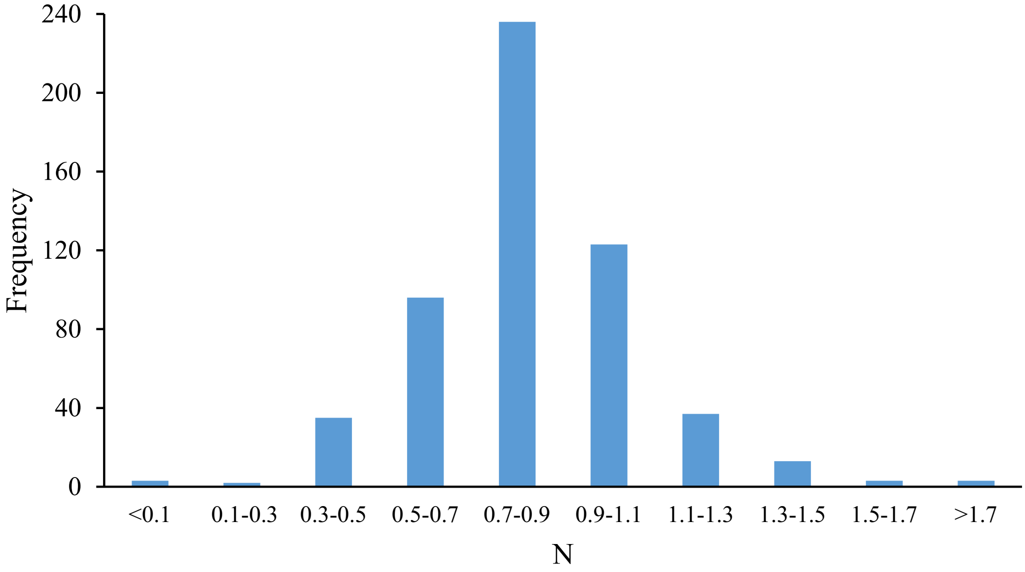

Fig. 4 Frequency distribution of N values based on reported best fit of Freundlich model

of the PACs [2], the type and properties of soil materials, and the environmental conditions. For instance, the presence of certain PACs [82] or DOM [35, 136] could impact the distribution of other PACs by competing for sorption sites. Yonge and Keinath [132] suggested that competition can arise due to differences in the solubilities of PACs.

Figure 5a presents the impact of adding DOM on the sorption of the cationic ATL, and neutral CAF and SDI to sandy loam soil [135]. The soil properties and experimental conditions are listed in Table SM2 and Table SM3, respectively. A significant reduction in the sorption of ATL was observed in the presence of DOM, but the effect of DOM on the sorption of CAF and DSI was not significant. The authors suggested that the reduction in ATL sorption could be due to the interaction of the compound's functional groups (NH and OH) with DOM via charge transfer rather than interaction with the soil material.

The presence of multiple PACs in solution could affect their sorption in different ways. Markiewicz et al. [82] examined the effect of the presence of MET in solution on the sorption of 5-FU and MTX to soil materials (Fig. 5b). The authors suggested that the presence of MET enhanced the sorption of 5-FU by creating new sorption sites, while it decreased the sorption of MTX by competing with 5-FU for sorption sites. Miroslav et al. [88] examined the sorption of ATL, CBZ, and SMTZ when tested both individually and in a mixture of the three. The study revealed that the sorption of CBZ and SMTZ increased, while the sorption of ATL remained the same. The authors attributed this behavior to the sorption of the cationic ATL to the negatively charged soil surface, which reduced the repulsion for anionic SMTZ. Additionally, they suggested that a cation bridging could be formed. The increased sorption of CBZ was attributed to the ionization of molecules and dipole-induced dipole interactions between non-polar and polar molecules in solution.

Factors affecting equilibrium sorption of PACs

Various factors can influence the equilibrium sorption of PACs to soils. These factors could be related to PACs properties, soil characteristics, or solution characteristics. One of challenges faced in making a comparative analysis of the effect of a particular factor using the data from the reviewed studies is the inability to isolate that factor from other possible influencing factors. To overcome this, most of the analyses presented here were made for cases where the considered factor changes while the other factors remain almost the same. A discussion of the effect of these factors is presented below with reference to the reviewed articles.

Characteristics of PACs

Hydrophobicity and ionization

Soils could be hydrophilic or hydrophobic depending on their composition and the availability of organic matter. Additionally, PACs could be hydrophilic, hydrophobic, or both, depending on the compound functional groups. Sorption of the hydrophobic PACs to soils could be controlled by the hydrophobic interaction, which is

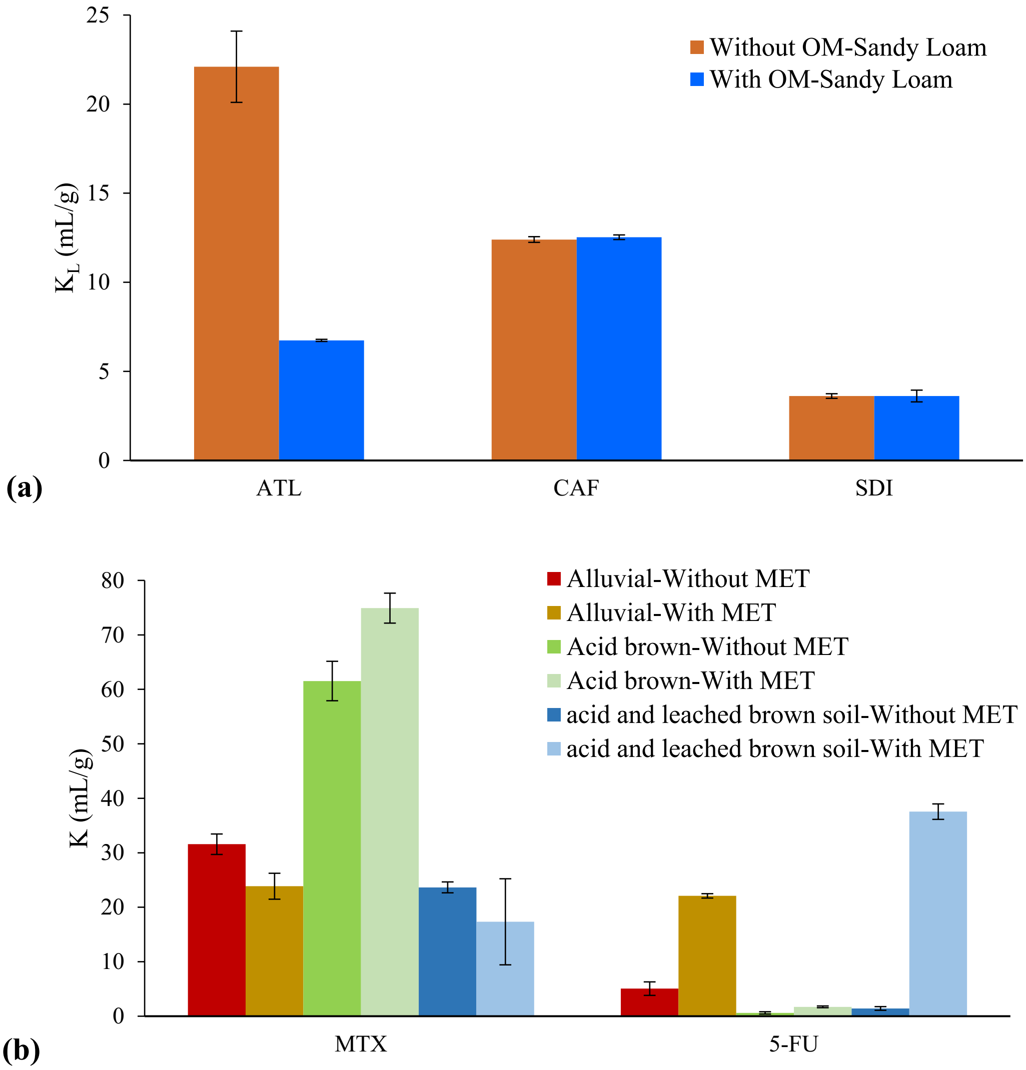

Fig. 5 Competitive/cooperative sorption of PACs (**a**) due to addition of DOM to sandy loam soil (OC = 16.8%, pH = 5.48) (data from Zhang et al. [135]) and (**b**) for MTX and 5-FU in the presence of MET using Alluvial (OC = 10.8%, pH = 7.1), Acid brown (OC = 4.5%, pH = 5.1), Acid and leached brown soil (OC = 2.4%, pH = 5.8) (data from Markiewicz et al. [82]). The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

influenced by the nature of the PACs and the composition of soil or sediment materials [34]. Hydrophobic interaction could be attributed to electron donor–acceptor interaction and/or hydrogen bonding. However, the sorption of hydrophilic PACs is attributed to cation exchange, complexation, or cation bridging [43, 94, 96].

The octanol–water partition coefficient (K_{ow}) measures the hydrophobicity of an organic compound. K_{ow} has been utilized to evaluate the sorption properties of the non-ionizable PACs, where a higher value indicates a greater tendency to sorb to hydrophobic surfaces [14, 34, 57]. Filep et al. [34] focused on the effect of chemical properties by investigating the sorption of nine PACs to three different types of soils and goethite. Their sorption experiments were conducted for 2 h with an S/L ratio of 1:12. The study compared the sorption of hydrophobic and ionizable PACs to different soil materials that vary considerably in OC (Table SM2). The non-ionizable hydrophobic PACs were selected based only on their study. PACs E2, EE2, and E1 (all predominantly neutral as shown in Table SM5) with a pK_{ow} of −4.01, −3.67, and −3.13, respectively, had almost the highest sorption tendency among the investigated PACs (Fig. 6a). The authors suggested that hydrophobic interaction and hydrogen bonding are the main mechanisms involved in the sorption of these compounds. These results align with the findings of Karnjanapiboonwong et al. [57], who tested the sorption of E1, E2, EE2, and TCS in sandy loam and silt loam soils. However, the other hydrophobic PACs investigated by Filep et al. [34] (i.e., LTG, CBZ, and OZP) were generally less sorbed to the three soils. It was suggested that these compounds sorb through π energy of molecules as they form hydrogen bonds.

Kodešová et al. [63] conducted a batch experiment on 13 soils to study the sorption of seven selected PACs. Figure 6b presents the results for eight soils and three PACs based on their work. Sorption results for certain PACs were not reported, so they appear blank in the figure. Their results showed that TMP had the highest sorption to all tested soils compared with CBZ, and CLN (Fig. 6b). This was explained by the dominant electrostatic interaction force. The variation in TMP sorption among the different soils was attributed to the organic carbon content. It could also be due to the higher cationic fraction of TMP in Silt loam 2, Silt loam 3, and Loam 1 soils compared to other tested soils (Table SM5). Finally, CBZ behaved as a non-ionizable compound and its sorption was attributed to hydrogen bonding and van der Waals forces.

The effect of hydrophobicity on the PACs sorption is very complex due to the influence of other factors such as compound type, soil composition, and pH. This is evident from Fig. 6a, b, where a comparison can be made for each PAC with different soils. For example, based on Fig. 6a, b, PAC E1 and TMP showed significant variation in sorption among the studied soils, and in some cases, the sorption was negligible.

Ionization of PACs occurs when a compound loses or gains one or more electrons. The degree of ionization affects the polarity, charge, and hydrophobicity of the PACs, leading to different interactions with the soil and sediment materials [34, 130]. PACs could be cationic,

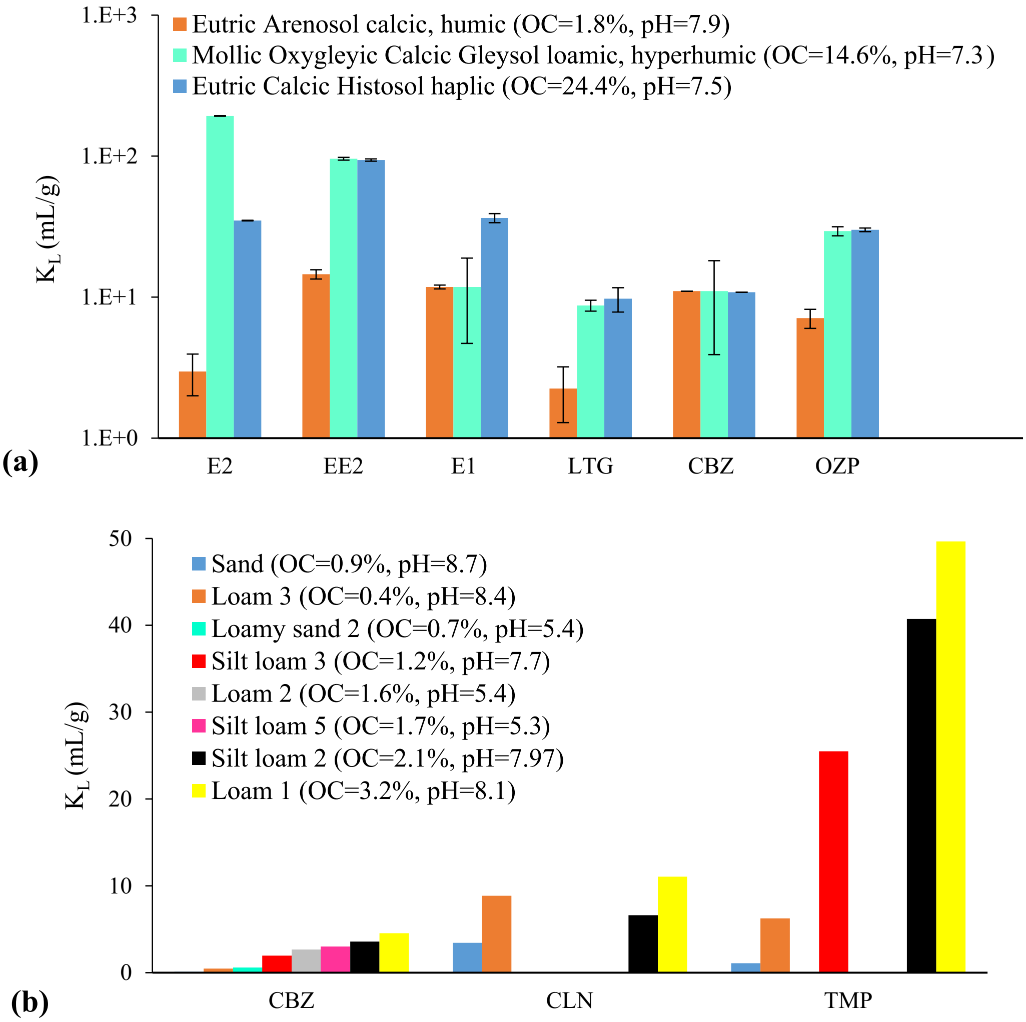

Fig. 6 Sorption of PACs to different soils based on data from (**a**) Filep et al. [34] and (**b**) Kodešová et al. [63]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

anionic, neutral, or zwitterion depending on the degree of ionization, which could be affected by the solution pH and ionic strength [115, 117, 136]. Therefore, ionization has a significant effect on the sorption of PACs to soils [113].

The neutral form of PACs is often less soluble in water and more hydrophobic than their charged form, which leads to greater sorption to soil materials [34, 59]. However, ionic forms of PACs are more soluble and hydrophilic, and they can sorb or penetrate lower soil layers [94, 117]. Soil surfaces are typically predominant by negative charges due to the availability of organic matter. If the PACs are present as cationic species they are expected to have stronger sorption behavior than other forms (anionic and neutral) [84]. Ionic compounds could interact with the soil through cation exchange, cation bridging, and complex formation [34, 94, 96].

Electrostatic interactions, such as cation exchange, electrostatic attraction, and electrostatic repulsion, are noticeable with ionizable PACs due to their interaction with the minerals on the soil surface. Zhang et al. [136] reported that the sorption of the cationic form of SFM to the soil at low pH is due to electrostatic attraction. However, at higher pH, sorption decreases due to the presence of SFM in an anionic form, causing electrostatic repulsion with negatively charged minerals. Martínez-Hernández et al. [84] found a similar trend for cationic CAF and ATL. Cation bridging is another mechanism that can influence the sorption of some PACs, such as OTC with a clay surface [117, 131]. Other mechanisms, such as surface complexation with minerals on the surface could enhance sorption due to the formation of coordinate bonds or ion pairs [83, 131]. π-π and hydrophobic interactions are more dominant mechanisms, especially if the material is rich in organic matter [98, 130]. Hydrogen bonding can occur if the material contains functional groups such as –OH, –COOH, or–NH_2 [73].

Figure 7 shows the average linearized sorption coefficient and the standard deviation for the PACs in the reviewed studies with natural soils (not altered) having a pH of 6–8. PACs within each ionic state have been arranged at an increasing pK_{ow} value. Generally, zwitterion PACs have the highest tendency to sorb to soil, while anionic PACs have the lowest tendency. Some PACs have been reported in multiple categories depending on their pK_a and pH. The average K_L for the PACs ranges between 0.0915 mL/g for SFM and 84725.5 mL/g for NOR. J. Li et al. [72] reported a range up to seven orders of magnitude (from 0.05 to 1,277,873.9 mL/g) based on the reviewed literature in their study.

ter Laak et al. [117] altered the solution pH to investigate the sorption of OCT, SCP, and TYL at different ionic states. Their batch experiments were conducted using clay loam and loamy sand with different S/L ratios depending on the used soil or PACs (Table 3). The values of the sorption coefficient for these PACs are presented in Fig. 8. These PACs are pH-dependent, and their sorption is higher when they are present in a cationic form. The clay loam soil had a higher sorption tendency than the loamy sand, which could be due to the differences in the CEC and organic matter content of the two soils. The overall trend for sorption of the tested PACs in both soils was cationic form > neutral form > anionic form. The cationic forms of PACs had the highest sorption due to electrostatic attraction to negative charges on the soil surface [117]. However, anionic species are more soluble than neutral species and have a higher electrostatic repulsion force with the soil surface, which decreases their sorption interaction. Similar trends for other PACs have been observed by Kodešová et al. [63] and Leal et al. [70].

Solubility

The relation between water solubility (S_w) and sorption was not distinctly addressed in the selected articles. Generally, nonionic organic compounds with lower S_w exhibit an increased tendency for sorption due to the hydrophobic interaction with the soil organic matter. Such behavior may not apply to ionic PACs. For example, ENR and NOR are present in the cationic form (≥ 0.75 cationic mass fraction) in different soils [70]. These PACs have almost similar values for pK_{ow}, pK_{a1} and V_m (Table SM1), while their S_w is 53.9 and 280 mg/L, respectively. Results showed that, generally, there is an increase in sorption of these PACs to soil material with an increase in S_w (Fig. 9). The most dominant sorption mechanism of ENR and NOR was attributed to cation exchange. In addition, sorption of these PACs in Clay 2 and Clay 4 soils was higher than that with the other tested soils due to their higher content of Al and Fe oxyhydroxides. An increase in sorption with Sw is also evident in the work of Boulard et al. [12] for the cationic STL and ATL which have almost similar values for pK_{ow}, pK_{a1} and V_m but significantly vary in their S_w (Table SM2).

Molar volume

Molar volume (V_m) is another factor that could influence the sorption of PACs onto soil materials. Data from J. Li et al. [72] were adopted to demonstrate such an effect. These investigators conducted a batch sorption experiment involving 54 PACs using 13 soils. Cationic APL and VPM (≥ 0.95 cationic mass fraction) and anionic NAP and WFR (≥ 0.93 anionic mass fraction) were selected because each category of these PACs has almost similar characteristics in terms of pK_{ow}, pK_{a1}, and S_w but varies in V_m (Table SM1). Figure 10a shows the K values of

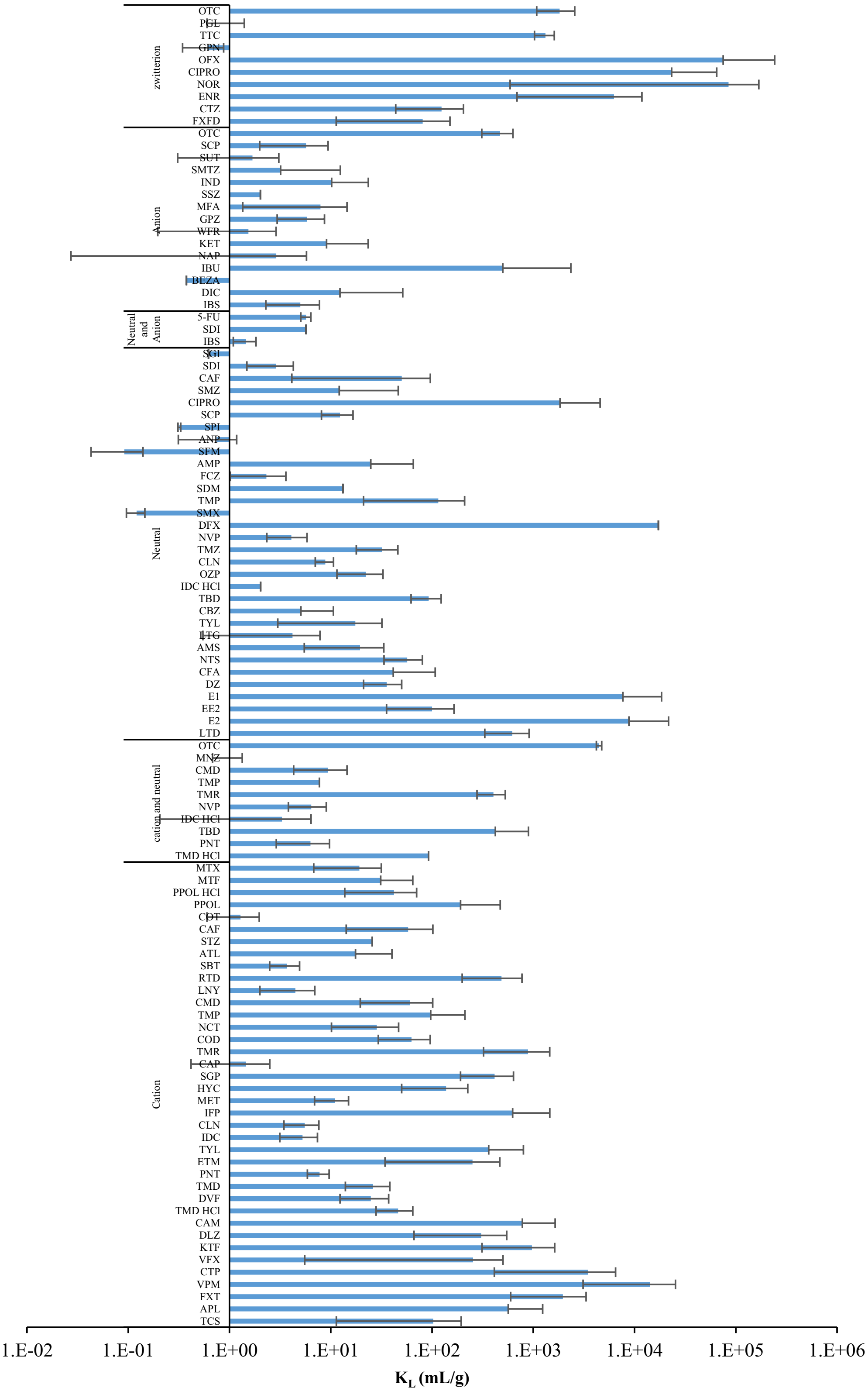

Fig. 7 Linearized sorption coefficient of PACs based on the reviewed articles

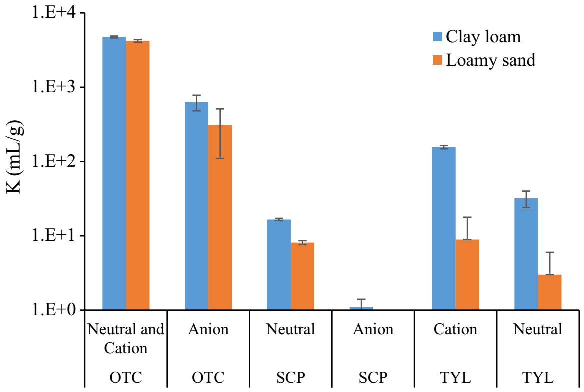

Fig. 8 Sorption of ionic species of PACs to clay loam (OC = 3.1%, pH = 6.8) and loamy sand (OC = 2.2%, pH = 6.6) (based on data from ter Laak et al. [117])

APL (V_m 252.2 cm^3/mol) and VPM (V_m 413.3 cm^3/mol) for nine soils. VPM exhibited higher sorption than APL in all tested soils, probably due to the higher likelihood of the larger cationic VPM sorbing to the negative charge on the soil surface. On the other hand, anionic NAP (V_m 191.9 cm^3/mol) and WFR (V_m 237.2 cm^3/mol) showed an inverse relationship between K and V_m (Fig. 10b). The larger anionic WFR exhibited lower sorption, potentially due to the higher repulsive forces with the negatively charged soil surface. The sorption of anionic BEZA and DIC with Sand 1 in the work of Revitt et al. [101] (data not shown) aligns with the previous findings.

Characteristics of soils

Soil organic carbon

Soil organic carbon significantly affects the sorption of the PACs to soil material [16, 31, 60]. An increase in OC causes an increase in the sorption of the PACs [122]. This can be explained by the enhancement of electrostatic forces and π-π interactions due to the increase of negative charges on the surface of soils, which increases the stability and surface area and hydrophobic partitioning [98]. However, the effect of OC on sorption varies depending on the PACs and soil characteristics such as pH and surface area [60, 131].

Vulava et al. [122] investigated the effect of OC on the sorption of IBU and NAP for soil samples with OC ranging between 0.203% and 5.22% and pH of 4.5 to 6.5 (Table SM2) using the experimental conditions presented in Table 3. NAP experienced more sorption than IBU (Fig. 11a) due to its aromatic moieties, which resulted in more interaction with the aromatic fractions of the soil organic matter. Also, the sorption tendency generally increased as the OC increased. The authors indicated that, at the soil solution pH, part of NAP and IBU was in anionic form and possibly reacted with the protonated amines of the soil organic matter as well as to mineral oxides on the soil surfaces. Figure 11b presents another example using data from Kim et al. [60]. The OC was modified and adjusted for both soils using a fermented rice straw for six months. As shown, the sorption capacity increased with increasing OC for the

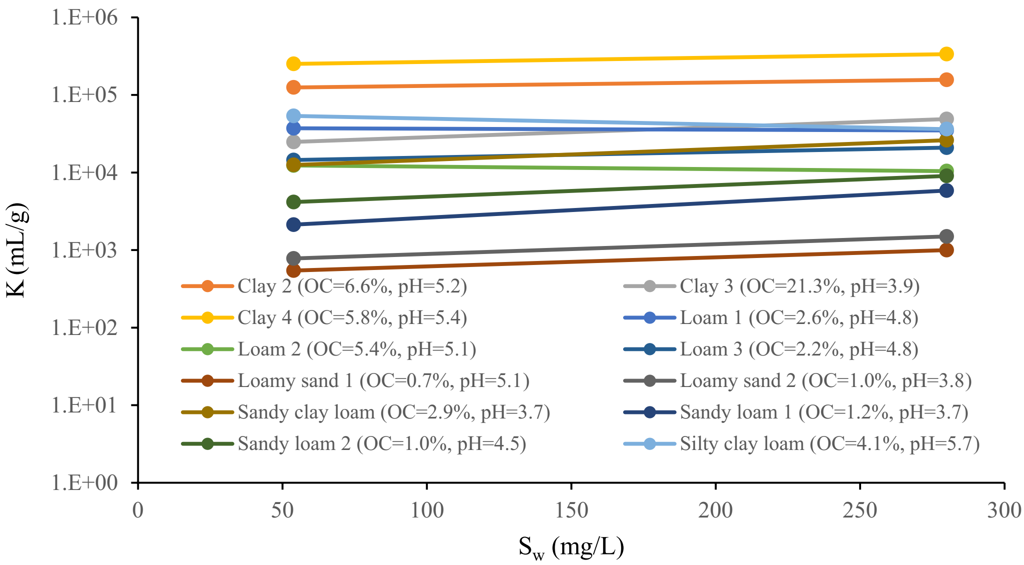

Fig. 9 Sorption of PACs as a function of S_w for cationic ENR (S_w = 53.9 mg/L) and NOR (S_w = 280 mg/L) based on data from Leal et al. [70]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

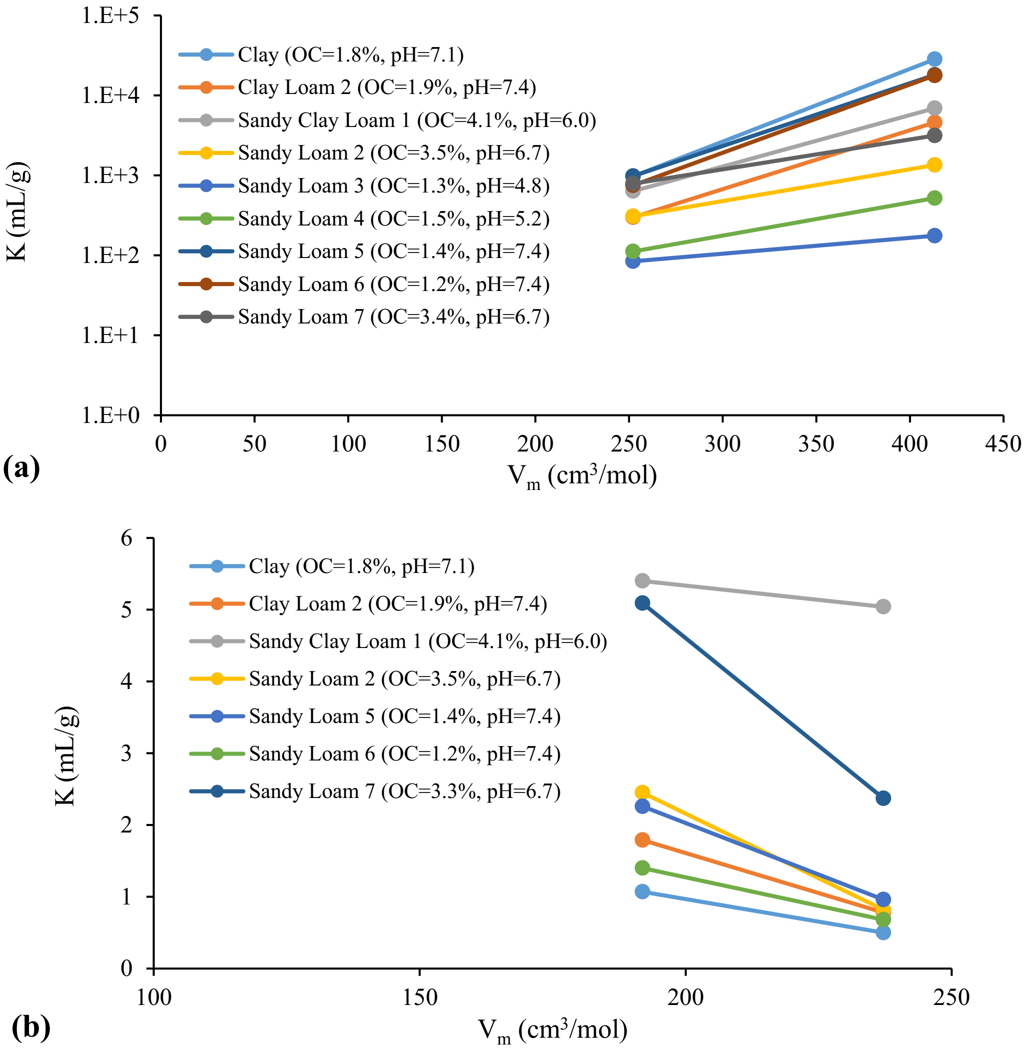

Fig. 10 Sorption of PACs as a function of molar volume for (**a**) cationic APL (V_m 252.2 cm^3/mol) and VPM (V_m 413.3 cm^3/mol) and (**b**) anionic NAP (V_m 191.9 cm^3/mol) and WFR (V_m 237.2 $cm.^3/mol$) (data from [72]). The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

studied PACs. Additionally, OTC had the highest sorption compared with other PACs. For the sandy loam soil (pH 8.13), the PACs predominantly exist in a neutral state since the pH is higher than pK_{a2} (7.32) and they are expected to sorb to the soil through mainly π-π interactions and hydrogen bonding. However, for the silt loam soil (pH 5.64), the PACs exist in a cationic state, and they are expected to sorb to the negative soil surface through mainly electrostatic attraction as well as hydrogen bonding. Other studies have shown a direct relationship between the sorption of PACs and OC [31, 101, 131].

Cation exchange capacity (CEC)

CEC affects the sorption behavior of PACs, and its impact varies based on the type of PAC. In general, CEC is influenced by clay minerals and organic matter in soils, which possess various exchange sites. CEC measures the negative charge sites in soils that neutralize and retain cations via electrostatic forces [56]. The presence of exchangeable cations such as Ca^{2+}, Mg^{2+}, Na^+, and K^+ in soils can affect the sorption ability of certain PACs. Cationic PACs are positively charged, and their sorption can be enhanced by CEC. The impact of CEC is also pH-dependent and works better

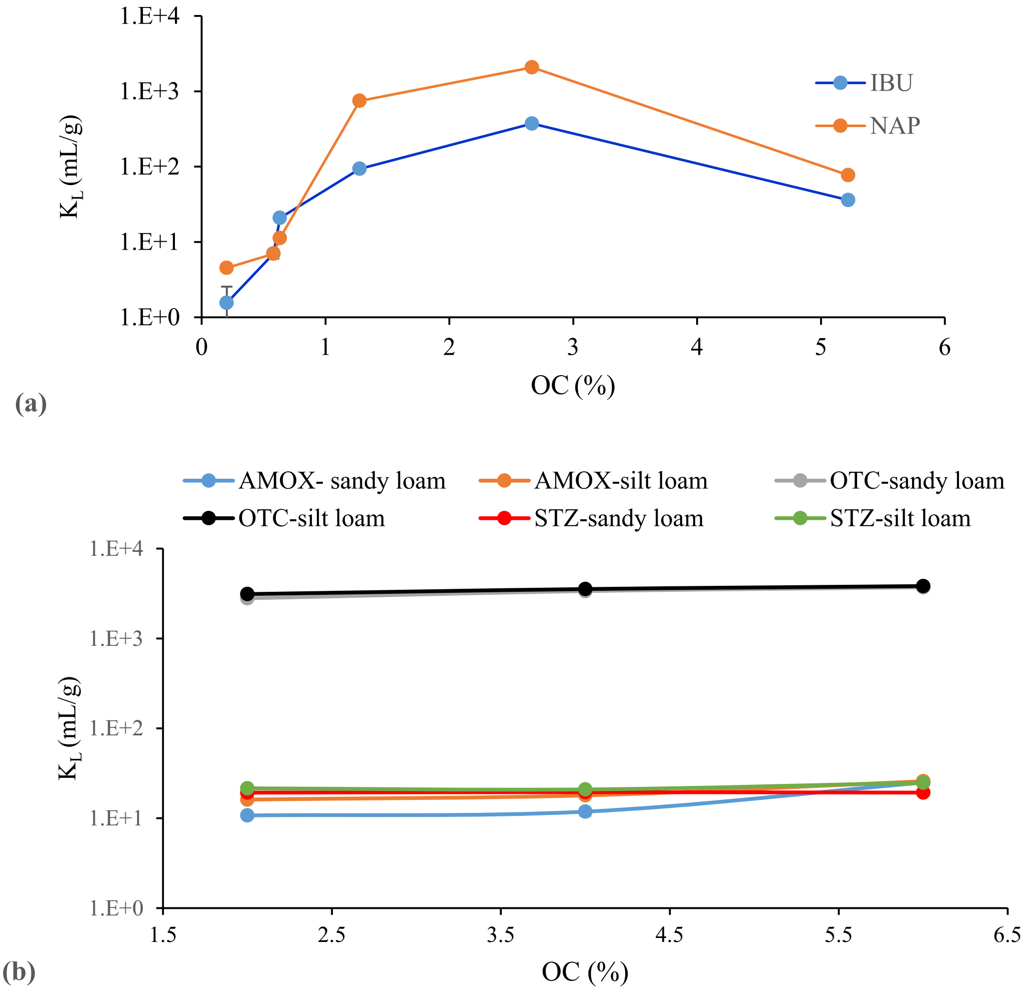

Fig. 11 Sorption of PACs as a function of OC for (**a**) IBU and NAP (based on data from Vulava et al. [122]) and (**b**) AMOX, OTC and STZ to sandy loam (OC = 0.45%, pH = 8.1) and silt loam (OC = 1.1%, pH = 5.6) (based on data from Kim et al. [60]). The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

under acidic conditions, where some PACs are available in cationic forms [70, 121]. As such, an increase in pH can alter the PACs to anionic species, reducing their sorption due to repulsion with the negative charges on the soil surface [62].

Kiecak et al. [59] investigated the effect of CEC on the sorption of selected PACs. The soil properties are listed in Table SM2 and the batch experiments were conducted under the conditions listed in Table 3. Figure 12 presents the sorption results for coarse sand (CEC = 0.07 cmolc/kg) and sandy loam (CEC = 2.48 cmolc/kg) soils only since these soils are almost identical in OC and pH but vary in the CEC. As shown in Fig. 12, PACs with different ionic states showed different levels of increased sorption. Zwitterionic PACs (CIPRO and OFX) experienced the biggest change compared with cationic ATL, neutral CAF, and anionic DIC and SMTZ. It should be noted that the neutral ANP and CBZ and anionic KET showed a slight drop in K_L with an increase in CEC (not shown in Fig. 12).

Surface minerals

The presence of metals or metals oxides in soils can affect sorption of PACs. Al-Khazrajy and Boxall [2] conducted a statistical analysis to correlate sorption of tested PACs (APL, ATL, CMD, DLZ, and MFA) to different exchangeable metals (Al, Fe, Ca, K, Mg, and Na) in tested sediments. The results revealed that these metals were not significant and did not contribute to sorption except for Ca, which correlated with DLZ. However, Figueroa and MacKay [33] studied the sorption of OTC to soil rich in iron oxide. The

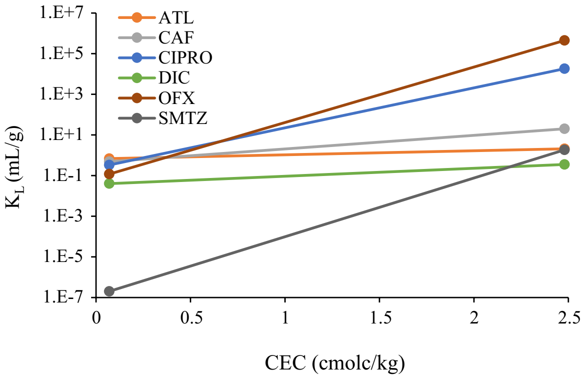

Fig. 12 Sorption of PACs as a function of CEC (based on data from Kiecak et al. [59]). The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

results showed that there was an interaction between OTC ionic species and oxide surface, which caused an enhanced sorption.

ter Laak et al. [118] conducted a sorption experiment on ionizable PACs (OTC, SCP, and TYL) using 11 different soils with varying properties. The authors found that metal oxides, such as Al oxyhydroxide, could explain about 31% of the sorption variation of neutral TYL species due to hydrogen bonding. Furthermore, the authors indicated that Al and Fe oxyhydroxide can cover interlayer adsorption sites, form hydrogen bonds, and engage in surface complexation with numerous organic molecules. Their charge can be either positive or negative depending on the characteristics of the soil solution.

Luo et al. [76] found that the sorption of nalidixic acid (NA) and niflumic acid (NFA) to Swedish soil was higher compared to that of Frensh soil due to the presence of more clay content, and much Al and Fe contents. In addition, the authors reported that the presence of Na ions enhanced the sorption of NFA, while the presence of Ca promoted the sorption of NFA but inhibited the sorption of NA. This difference was ascribed to the formation of Ca^{2+}-NA complex and greater affinity of the anionic form of NFA^{-} towards soil-Ca^{2+} assembly.

Vulava et al. [122] indicated that at pH 5, the predominantly deprotonated NAP and IBU were likely to adsorb more strongly to the amphoteric Fe oxide surfaces compared to the permanently negatively charged clay mineral surfaces. The positive charge on the Fe oxides provided simple ligand exchange sites for NAP and IBU under these conditions. Jones and Brassington [53] reported a ligand complexation between metal oxides (e.g., Al and Fe oxyhydroxides) and weak organic acids. The sorption of the ligand complex increased strongly at lower pH. Sorption of organic anions to metal oxides was influenced to a lesser extent by the presence of metal cations in the solution. Leal et al. [70] observed that sorption of PACs that are related to the fluoroquinolones and sulfonamides classes tends to be higher in soils rich in Al and Fe oxyhydroxides, but no significant correlation was found with K.

Clay and surface area

The presence of clay in soil enhances the sorption of some PACs due to an increase in the surface area and CEC, leading to more active sites for sorption. Figure 13a, b compare two different soils with different clay content (Table SM2) and specific surface area (SSA). Both results support the conjecture that increasing the clay/SSA in soil generally enhances the sorption of PACs. CIPRO, DFX, ENR, and NOR had higher sorption than the other tested PACs due to their predominant cationic nature in both tested soils (Table SM5) which were affected more by cation exchange. This trend is more evident in the work of Leal et al. [70] (Fig. 13a) than that of Kodešová et al. [63] (Fig. 13b) due to the higher differences in the SSA between the compared soils. Furthermore, the effect of clay content and SSA may not be noticeable for compounds with low sorption tendency, such as CBZ, CLN, and SMTZ in the work of Kodešová et al. [63]. Enhanced sorption by clay minerals is also evident for the cationic ENR in the work of Nowara et al. [93].

pH

The sorption of PACs could change with the solution pH [35, 90, 115, 131]. Soil pH affects the charges and forms of the PACs, making them available as cationic, neutral, or anionic species, which ultimately affect sorption [10, 60, 124]. At low pH, carboxylic groups of the soil organic matter exist mainly in a non-dissociated form and weak acids PACs are also present in a large extent in neutral forms which results in higher sorption by hydrogen bonding, π-π interactions, or Van der Waals forces, depending on the structure of the compound. Moreover, the solubility of PACs can be affected by changes in pH [67].

Figure 14a illustrates the effect of pH on the sorption of PACs with different soils based on five of the reviewed articles [10, 35, 60, 115, 131]. Solution pH in these studies was adjusted by adding HCl or NaOH. The soil properties and experimental conditions are listed in Tables SM2 and 3, respectively. Kim et al. [60] found that the sorption of AMOX, OTC, and STZ decreased as the pH increased. This could be due to the presence of AMOX and OTC in a cationic form under acidic conditions, enhancing

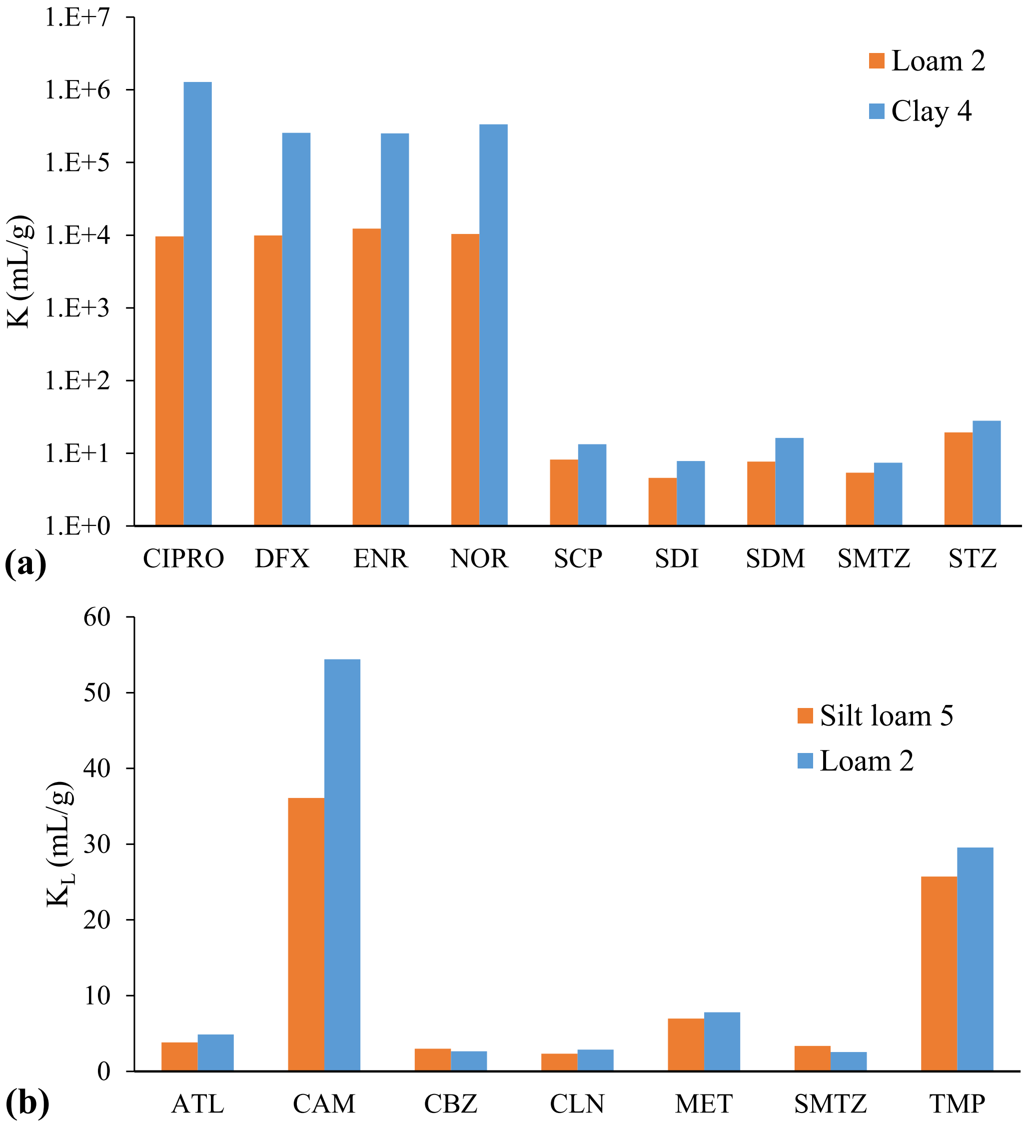

Fig. 13 Sorption of PACs as a function of surface area based on data from (**a**) Leal et al. [70] for Loam 2 (OC = 5.4%, pH = 5.1) and Clay 4 (OC = 5.8%, pH = 5.4), with SSA of 103 and 163 m^2/g, respectively and (**b**) Kodešová et al. [63] for Silt loam 5 (OC = 1.7%, pH = 5.3) and Loam 2 (OC = 1.6%, pH = 5.4) with SSA of 16.6 and 23 m.^{2}/g, respectively. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

their attraction to negative charges on the soil surface. OTC had the highest sorption at low pH due to the cationic exchange interaction and its ability to form a metal complex with divalent metals, leading to more sorption to clay minerals. The findings of Yao et al. [131] for OTC sorption on two tested soils were consistent with those of Kim et al. [60] for the same compound. Srinivasan et al. [115] also observed a drop in SMTZ sorption with increased pH. The authors attributed the higher sorption at lower pH to the presence of the compound in part in a cationic form that is electrostatically attracted to negatively charged soil surfaces. However, when the pH > pK_{a2} (= 5.7), the anionic species of SMTZ seemed to dominate, and its sorption affinity to the soil surface dropped. Białk-Bielińska et al. [10] noticed a similar behavior for SMX and SDI. They attributed this to the electrostatic repulsion forces between the anionic forms of these compounds and the negatively charged soil surface. However, a study by Foolad et al. [35] revealed that CBZ (pK_{a2} = 13.9) and AMP (pK_{a1} = 9.38) are slightly affected by changing the pH due to the higher pK_a values of the compounds, making them nonionizable with predominant neutral mass fraction (Table SM5) in the tested soils.

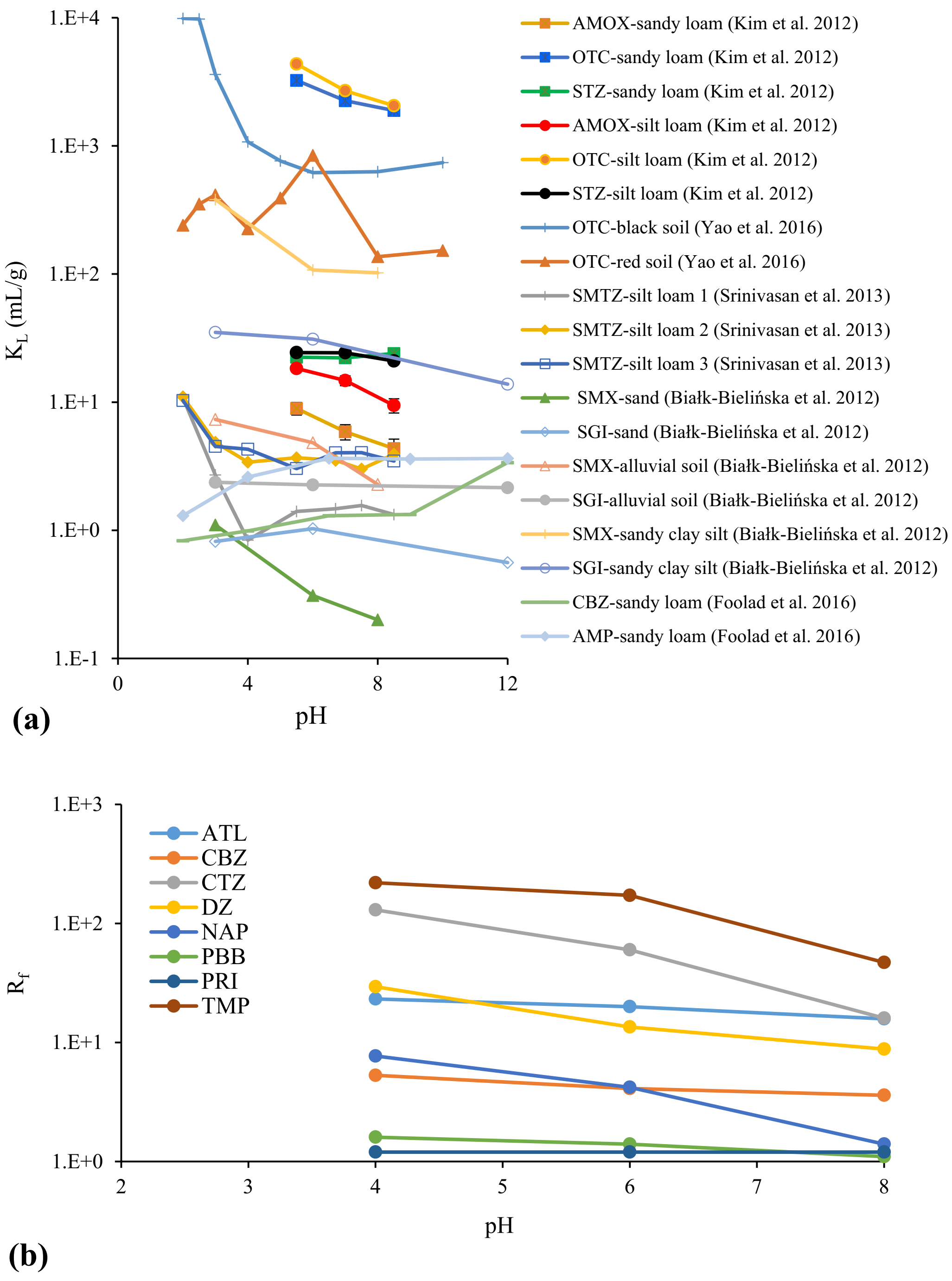

Fig. 14 Effect of pH on (**a**) K_L based on different studies and (**b**) R_f based on data from Schaffer et al. [105]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

Schaffer et al. [105] investigated the effect of pH on R_f of eight pH-dependent PACs while conducting a saturated column experiment on sand (Table 4). As shown in Fig. 14b, R_f decreased for all PACs with increasing pH. The authors attributed this decrease to the change in the ionic states of the studied PACs with the increase in pH. PBB and NAP deprotonated more with increasing pH and formed more anionic species. These species are more polar and hydrophilic, which makes them more mobile. Conversely, hydrophobic interactions decreased for neutral PACs (CBZ and PRI) with increasing pH. ATL, DZ, and TMP had the strongest retardation among the studied PACs. These compounds shifted from cationic to neutral state with increasing pH causing less retardation. In addition, retardation for the zwitterion CTZ decreased with increasing pH due to a decrease in the number of interactions with the negative charges on the soil surface.

Characteristics of solution

Ionic strength

Ionic strength is related to the concentration of ions in solution and increases as the ion concentrations increase [10, 115]. The adsorption of PACs to soils can be promoted or inhibited due to ionic strength since some PACs are available in an ionic form and interact with the surface charge of soils [115, 124].

Based on the reviewed papers, the studied sorption behavior of different PACs at different ionic strengths is presented in Fig. 15. In these studies, the ionic strength was adjusted by changing the concentration of $CaCl_2$ in the solution. The equilibrium time was 24 h for all studies except for Mutavdžić Pavlović et al. [91] which was 4 h. The soil properties and experimental conditions varied between these studies, as listed in Tables SM2 and 3, respectively. Linear sorption isotherm was reported by Białk-Bielińska et al. [10], but isotherms followed the Freundlich model for the other studies. Data for Mutavdžić Pavlović et al. [90] showed an increase in the sorption of SMZ with increasing ionic strength up to a certain point, after which sorption decreased at higher ionic strengths due to the decrease in the thickness of the electrical double layer of the charged surface. Thus, the surface charge decreased, and less interaction occurred between protonated SMZ and the soil surface. However, when Mutavdžić Pavlović et al. [91] investigated the effect of ionic strength on CIPRO, a decrease in sorption in all studied soils was observed. This could be due to the increase of Ca^{2+}, which instead binds electrostatically with the negatively charged soil surface. Therefore, Ca^{2+} cations compete and block COOH or OH sites, causing less sorption. Białk-Bielińska et al. [10] found a decrease in sorption for selected PACs. The authors related this to a decrease in the thickness of the electrical double layer and suggested a cation exchange mechanism as the main sorption mechanism between SMZ and the mineral surface. Competition has also been noticed by ter Laak et al. [117] when the cationic forms of TYL and OTC were studied at different ionic strengths. On the other hand, Srinivasan et al. [115] found an increase in the sorption of SMTZ with one of the studied soils. This was attributed to either cation bridging between SMTZ and Ca^{2+} cations or salting out (decrease in solubility) of SMTZ, leading to precipitates and sorption to the soil.

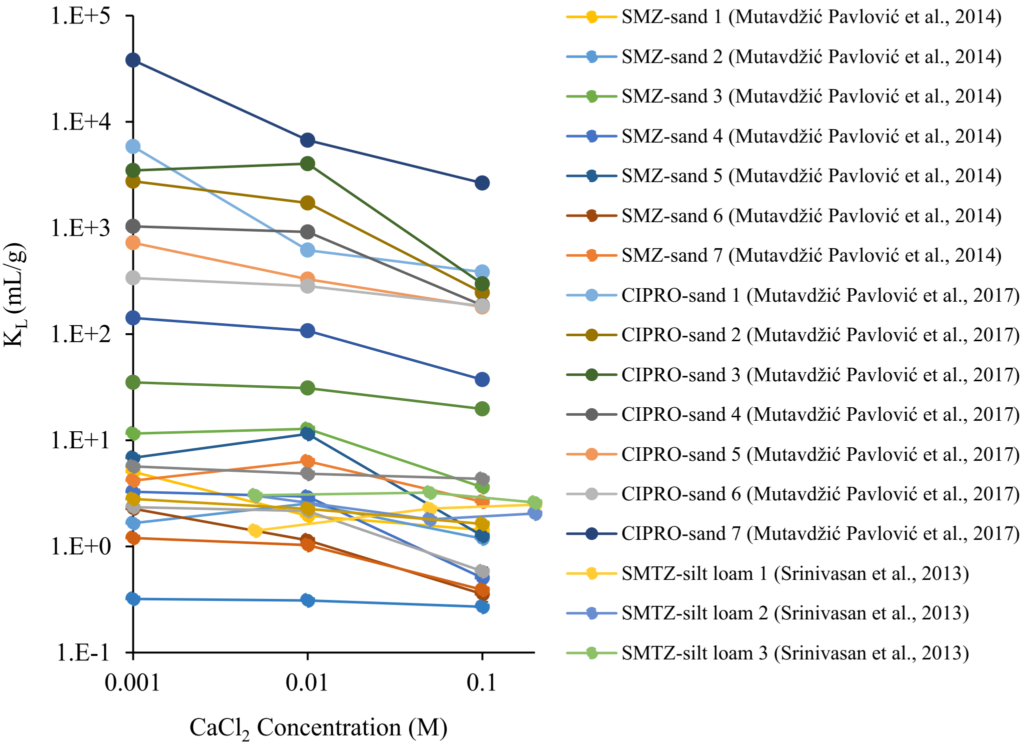

Fig. 15 Sorption of PACs as a function of ionic strength. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

Dissolved organic matter (DOM)

The DOM is a complex mixture of organic compounds and is introduced into soils through various sources such as irrigation of reclaimed wastewater [95] or by using animal manure [40, 99]. Its presence in the soil affects the sorption of PACs through different mechanisms, such as competition for sorption sites [48, 136], alteration of the soil's surface charge [20, 77], and formation of complexes with certain PACs [125].

DOM has an impact on the sorption of PACs in several ways. It enhances the solubility of hydrophobic PACs, leading to less sorption and more mobility in soils [77, 92]. In addition, most DOM contains hydroxyl and carboxylic functional groups, leading to an increase in binding sites with PACs. Rizzuto et al. [103] studied the binding of six PACs to DOM at two different pH (6.5, and 8) through equilibrium dialysis. Partial binding was observed for hydrophobic PACs (BEZA and DIC) at higher pH. The authors attributed this to the presence of a carboxylic group of the PACs or a shift of DOM structure at high pH, making it more suitable to bind with some PACs. The authors found a nonlinear binding behavior as the DOM concentration increased.

Figure 16a, b illustrate the impact of introducing DOM on sorption of the PACs to different soils, based on two reviewed articles [20, 125]. The soil properties and experimental conditions are listed in Tables SM2 and 3, respectively. In the work of Wang et al. [125], the sorption of OTC increased when plant-derived DOM (PDOM) was added to three soils, however, a decrease in OTC sorption was noticed when chicken manure-derived DOM (MDOM) was added (Fig. 16a). This is because PDOM is a humus-like substance containing higher aromaticity, low hydrophilicity, and polarity, making it easier to combine with soil and provide more binding sites for OTC. Conversely, MDOM is a protein-like substance that enhances the dissolution and mobility of OTC. Foolad et al. [35] and Haham et al. [48] also reported a decrease in AMP, CBZ and SPI sorption when DOM was added to soil, due to competition for the same sorption sites. Similarly, Zhang et al. [136] reported a decrease in the sorption of SFM, SMX, SPI, and TMP when TSE was used as opposed to using 0.01 M $CaCl_2$ solution (Fig. 16b). This could be due to competitive sorption or the formation of complexes between these PACs and DOM. The effect of DOM in the TSE on the sorption of PACs appears to be influenced by the ionic state of the compounds. The drop in K for the anionic SFM and SMX is more pronounced compared to that for neutral SPI and neutral/cationic TMP (see fraction of PACs in Table SM5).

S/L ratio

The S/L ratio used in the reviewed studies varies from 1:1 [24, 29] to 1:1000 [122]. The S/L ratio is usually selected so that there is an appreciable drop in the liquid concentration while still being detected. Few studies have explored the effect of the S/L ratio on the sorption of PACs. Estevez et al. [29] investigated the effect of the S/L ratio on the sorption of IBU to four different soils (Fig. 17a). An S/L ratio of 1:5 resulted in almost doubled K_L for IBU compared with a 1:1 ratio, independent of the soil type. An increase in K for PACs at a lower S/L ratio was also observed in Boulard et al. [12]. These authors performed sorption experiments for 27 PACs at an S/L ratio of 1:25 and 1:5 (Fig. 17b). Results showed higher sorption at an S/L ratio of 1:25 for almost all PACs than at a 1:5 ratio. Changes in the S/L ratio could alter the solution chemistry in terms of salinity and pH which could affect the sorption behavior of PACs and cause a change in the value of K or K_L.

Temperature

The sorption of PACs to soils is influenced by temperature in two different ways. If the sorption reaction is endothermic, raising the temperature will increase the extent of sorption [129], while for exothermic reactions, an opposite behavior is observed due to an increase in the compound solubility [50, 85, 91]. For example, Maszkowska et al. [85] showed an increase in the sorption of the neutral SGI and anionic SSZ and a decrease in the sorption of the cationic PPOL-HCl with an increase in temperature (Fig. 18a). Mutavdžić Pavlović et al. [91] noticed a decrease in the sorption of CIPRO with an increase in temperature (Fig. 18b). Hiller and Šebesta. [50] also observed a similar behavior for the sorption of IBU.

Sorption in packed soil columns

Pore water velocity

The effect of v_o on R_f for PACs was reported by Kiecak et al. [58] and Schübl et al. [109] subject to the experimental conditions presented in Table 4. Both investigators assumed linear sorption in fitting the column breakthrough data. Kiecak et al. [58] used different v_o based on the soils used (Table 4). Variations of R_f with v_o are shown in Fig. 19. Only ATL showed an increase in R_f with v_o for medium sand and sandy loam. However, R_f was almost the same for the other studied PACs for the same soil, independent of v_o. The authors concluded that the transport of these PACs is not affected by changing v_o. Schübl et al. [109] investigated the transport of ANP, ATL, CAF, CBZ, and SMTZ using two values of v_o for two different soils (Tables 3 and 5). The results (data not shown) also showed that the studied PACs were unaffected by v_o.

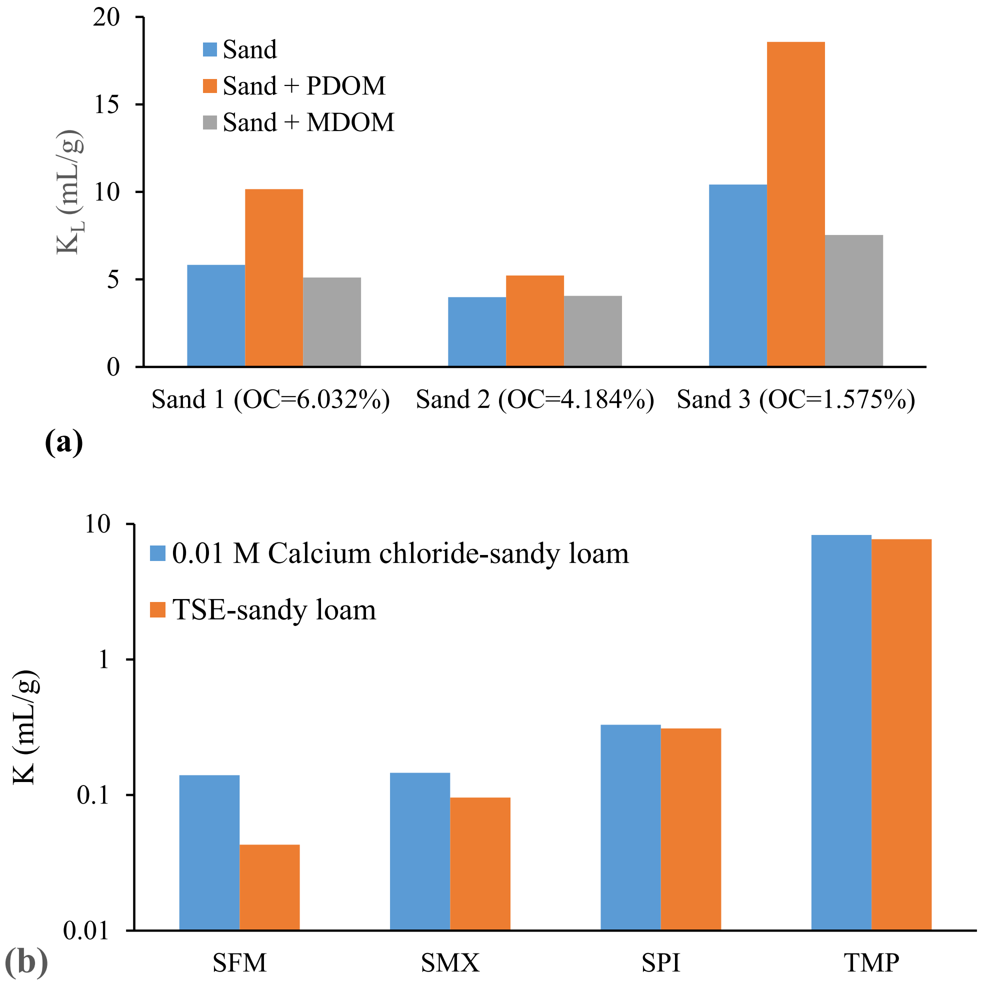

Fig. 16 Sorption of (**a**) OTC as a function of the type of DOM based on data from Wang et al. [125] and (**b**) PACs as a function of solution type for Sandy loam soil (OC = 1.3%, pH = 7.1) based on data from Zhang et al. [136]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

Variations of experimental conditions

One of the challenges encountered in comparing the extent of sorption of PACs to soil is attributed to variations in the experimental conditions. For batch reactors, variations occur in the range of the initial concentration applied in the isotherm experiments, number of tested PACs, S/L ratio, mixing time, bio-inhibition method, and type of solution (Table 3). For column reactors, variations occur in the injected initial concentration, injection type, column dimensions, average-flow velocity, number of tested PACs**,** bio-inhibition method, and method of determination of R_f (Table 4). While variations of the experimental conditions are necessary to assess the impact of certain parameters, the experimental setup should be designed to closely resemble the conditions in the field if laboratory-based data are to be utilized for field assessment.

Differences in the experimental settings could affect the extent of sorption as well as the sorption behavior. For example, an increase in the S/L ratio generally causes a drop in K_L as discussed earlier (Fig. 17). Testing sorption at short mixing times underestimates K or K_L in case true sorption equilibrium is not reached. Additionally, isotherms constructed with different values of maximum initial concentration, will lead to different K_L values in case of nonlinear sorption [48, 92]. Meanwhile, application of different bio-inhibition methods may result in different K (or K_L) values for the same PAC/soil combination due either to alteration of the soil material in case of autoclaving or gamma radiation [7, 9] or due to

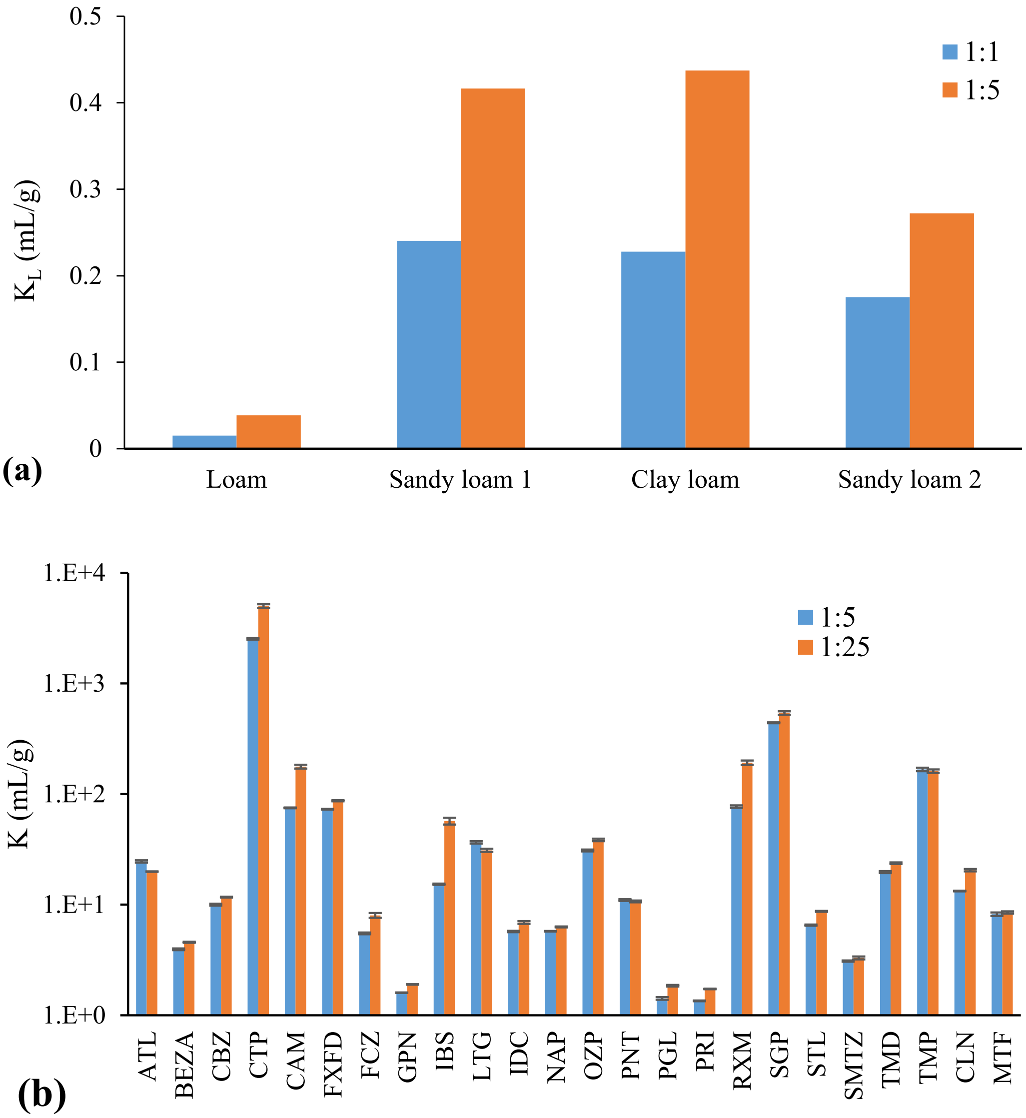

Fig. 17 Sorption as a function of S/L ratio for (**a**) IBU based on data from Estevez et al. [29] and (**b**) other PACs based on data from Boulard et al. [12]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

interaction of chemical inhibitors (like NaN_3 and mercury chloride) with the tested contaminants [21, 49].

Comparison between batch- and column-determined sorption distribution coefficients

A comparison between the values of the sorption distribution coefficients determined by the batch (K_{batch}) and column (K_{column}) techniques was conducted in this study based on available data from the reviewed studies [20, 27, 31, 58, 59, 107, 109]. The experimental conditions of the batch and the column studies are presented in Table 3 and 4, respectively. The values of K_{column}, if not directly reported by the investigator, were determined from the reported R_f values (Table 4) using Eq. (9) along with the values of ρ_b and θ associated with the column experiment. An exception is that of Chefetz et al. [20] who did not report ρ_b and θ of their column experiments. In this case, typical values for packed soil columns operated under saturated conditions of ρ_b (1.7 g/cm^3) and θ (0.35) were used [80]. For the study of Kiecak et al. [58], the values of K_{column} for the same PAC at different v_o values were averaged. For the studies of Kiecak et al. [58], and Schübl et al. [109], the values of K_{column} obtained under biotic conditions were not considered since no batch data were reported by Kiecak et al. [59] under the same conditions. Also, the values of K_{column} for the course quartz

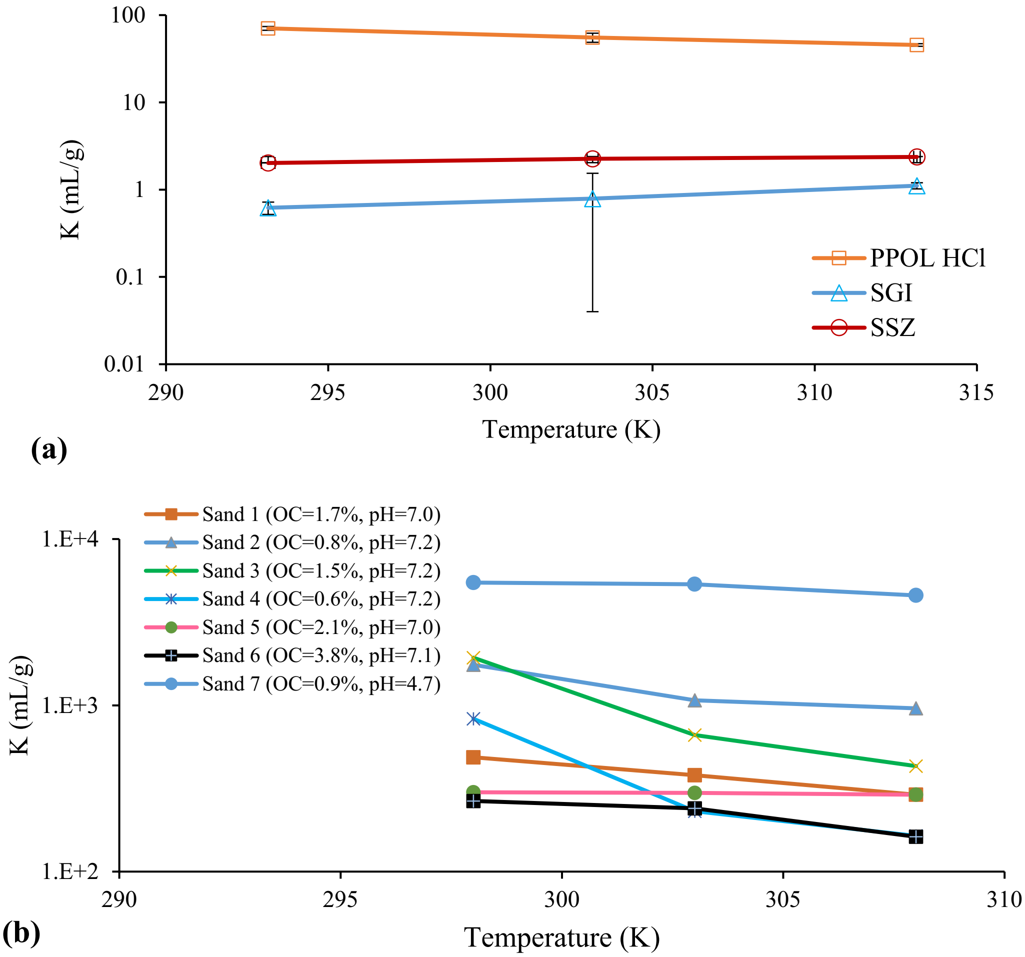

Fig. 18 Effect of temperature on the sorption of (**a**) SGI, SSZ, and PPOL HCl based on data from Maszkowska et al. [85] and (**b**) CIPRO based on data from Mutavdžić Pavlović et al. [91]. The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

sand reported by the authors were not considered since the R_f values of the investigated PACs using this material are approximately 1.0 (i.e., no retardation). Figure 20 compares the values of K_{batch} and K_{column} obtained from the above studies. The figure depicts that K_{batch} for PACs is generally higher than their K_{column} counterparts. The ratio of K_{batch} to K_{column} (an indication of the variation between the two values) averages 26 for the investigated PACs in the mentioned studies. However, the ratio reaches approximately 50 in the work of Kiecak et al. [58, 59] and Fan et al. [31], 8 in Chefetz et al. [20], 5 in Durán–Álvarez et al. [27], and dropped to 2 in Scheytt et al. [107]. For Schübl et al. [109], the ratio was 2 for ATL and 4.4 for CAF but reached 53 for CBZ.

Deviations between K_{batch} and K_{column} of PACs raises a concern about the validity of using K_{batch} in simulating the transport of these compounds in aquifers. While the batch experiment is easier to conduct, the column experiment is more representative of the transport process in aquifers. The cause of this discrepancy has not been addressed in the reviewed cases. Nonetheless, the discrepancy between the K values determined by the batch and column techniques has been reported for other organic compounds, with the batch-determined values being higher than their column counterparts [79]. It was further suggested that the discrepancy could stem from fundamental differences between the two techniques, improper interpretation of transport behavior, inability to account for some transfer/transform mechanisms, and/or experimental artifacts [79]. Improper interpretation of transport behavior could be attributed to failure to account for nonideal sorption behavior including sorption nonlinearity, hysteresis, and nonequilibrium. For example, it was suggested that a major potential cause of the reported discrepancy between the two techniques could be due to the assumption of a single-rate sorption

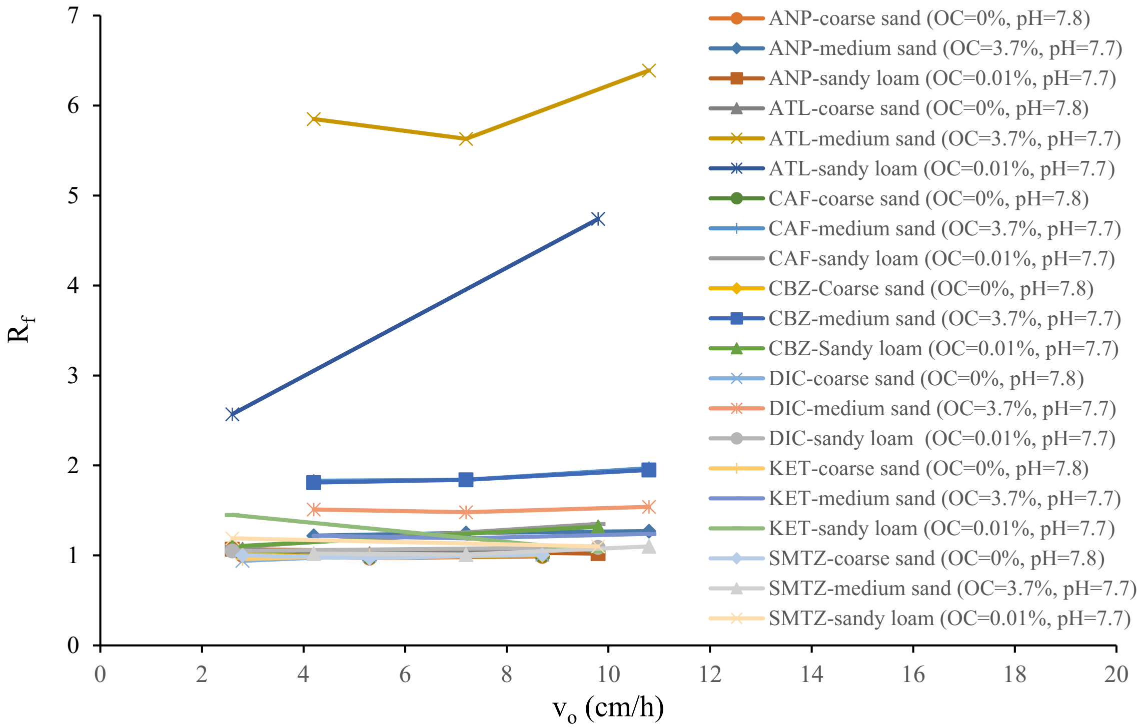

Fig. 19 Retardation of PACs as a function of pore water velocity (based on data from Kiecak et al. [58]). The distribution of each PAC based on its ionic states under the applied experimental conditions is listed in Table SM5

reaction for systems with multi-rate sorption behavior [80].

Among the above-reviewed batch and column studies of PACs, it is noted that the highest and intermediate discrepancies between batch and column K values occurred in studies that employed a short hydraulic residence time in the column ($t_{column} = L/v_o$) relative to the batch equilibrium time (t_{batch}). For example, in the work of Fan et al. [31], the t_{column} was less than 1 h compared with a t_{batch} of 168 h. Conversely, the deviation between t_{batch} and t_{column} is within a factor of 3 for the studies with the least discrepancy. Hence, a possible cause for the observed higher values of K_{batch} relative to their column counterparts for the PACs in the reviewed studies could be due to the inability to accurately account for sorption nonequilibrium during the column study. It was also observed that, for any of the studies that involved more than one soil material [20, 27, 31, 58, 59], the soil with the higher OC resulted in a higher discrepancy between K_{batch} and K_{column}. This also supports the conjecture that sorption nonequilibrium could be the reason for the discrepancy since an increase in OC will likely result in slower mass transfer to the sorption sites. Given that the extent of PAC sorption is positively influenced by the soil organic matter, compounds with higher K values are expected to experience a higher discrepancy if nonequilibrium is not properly considered. This is supported by the apparent increase in the level of variations between the two K values (K_{batch}/K_{column}) with the increase in the product of the relative retention time in the two reactors (t_{batch}/t_{column}) and K_{batch} as shown in Fig. 21.

Development of predictive relationships

Development of models for prediction of sorption distribution coefficient of PACs to soil could be invaluable for those involved in environmental exposure and risk assessment with less dependence on expensive laboratory testing [8, 72]. Two main approaches have been explored in the development of predictive models: regression analysis and machine learning. In both approaches, investigators considered compound and soil characteristics as input descriptors for predicting K values for PACs. Table 5 lists some of the developed regression equations for the sorption of PACs to soil materials. ter Laak et al. [118] developed a partial least-squares regression model (Eq. 10) to estimate the K of selected PACs. The authors utilized experimental data encompassing 146, 114, and 99 points for OTC, TYL, and SCP, respectively, across 11 soils. The developed model accounted for 69%, 68%, and 78% of the variations for OTC, TYL, and SCP,

Table 5 Reported regression equations for sorption of PACs to soils [a]

Reference	Class	Equation	Eq	n	R^2
ter Laak et al. [118]	Ionizable	$K = c_1\alpha + c_2 \log OC + c_3 \log clay + c_4 \log CEC + c_5 \log FeOx + c_6 \log AlOx + C$	10	99–146	0.68–0.78
Franco and Trapp [37]	Neutrals	$\log K_{oc} = 0.5\log K_{ow} + 1.13$	11	22	0.8
	Weak acids ($pK_a > 7.5$)	$\log K_{oc} = 0.54\log K_{ow} + 1.11$	12	11	0.81
	Strong acids ($pK_a < 4$)	$\log K_{oc} = 0.11\log K_{ow} + 1.54$	13	29	0.04
	Weak bases ($pK_a < 3.5$)	$\log K_{oc} = 0.42\log K_{ow} + 1.34$	14	11	0.83
	Strong bases ($pK_a > 7.5$)	$\log K_{oc} = 0.47\log K_{ow} + 1.95$	15	13	0.75
	Combined acids	$\log K_{oc} = \log\left(\Phi_n 10^{0.54\log K_{ow}+1.11} + \Phi_{ion} 10^{0.11\log K_{ow}+1.54}\right)$	16	62	0.54
	Combined bases	$\log K_{oc} = \log\left(\Phi_n 10^{0.37\log K_{ow}+1.70} + \Phi_{ion} 10^{pK_a^{0.65}} f^{0.14}\right.$	17	43	0.76
Franco et al. [36]	Acids	$K_{oc} = \frac{K_{oc,n}}{1+10^{a(pH+\delta-pK_a)}} + \frac{K_{oc,ion}}{1+10^{a(pK_a-(pH+\delta))}}$	18	5–88	0.27[b]
Droge and Goss [26]	Organic cations	$K = K_{CEC,\,clay}(CEC_{soil} - 3.4OC) + OCD_{oc,IE}$	19	21–22	0.83–0.93
Jolin et al. [52]	Cations	$K = K_{PTMA}\ S_{soil}$ where $S_{soil} = S_{clay}(CEC - \sigma OC) - S_{oc}OC$ $\log S_{clay} = 1.22\left(V_m - V_{m_{PTMA}}\right) - 0.22Na_i \pm CF_{clay}$ $\log S_{oc} = 1.52\left(V_m - V_{m_{PTMA}}\right) + 0.32Na_i \pm COC$	20	30	0.8 (TMD) 0.75 (DES)
Li et al. [71]	Neutrals ($\log K_{ow} > 0.85$)	$\log K = 0.779\log K_{ow} + 0.211\ OC - 1.729$	21	15	0.921
	Bases ($pK_a > 8$)	$\log K = 0.315\log D_{ow} + 0.188f_{oc} + 0.585$	22	30	0.733
	Bases ($pK_a > 8$)	$\log K = 0.312\log D_{ow} + 0.171\ OC + 4.164\ ExNa + 0.336$	23	30	0.815
	Weak bases ($pK_a < 8$)	$\log K = \log\left(\Phi_n 10^{0.021MW-1.70} + \Phi_{ion} 10^{-0.535\ HF+0.345\ Nai+0.145\ OC+1.559}\right.$	24	25	0.895
	Weak bases ($pK_a < 8$)	$\log K = \log\left(\Phi_n 10^{0.021MW-4.979} + \Phi_{ion} 10^{-0.54\ HF+0.331\ Nai+3.208\ ExNa+0.139\ OC+1.389}\right.$	25	25	0.922
	Acids ($6.8 > pK_a > 3.2$	$\log K = \log\left(\Phi_n 10^{-0.313\ HF+0.191\ OC+0.417} + \Phi_{ion} 10^{-0.0083\ MW-0.038\ CEC+0.301\ OC-2.36}\right.$	26	30	0.886

[a] n is the number of data point, R^2 is the coefficient of determination, Φ_n is neutral fraction, Φ_{ion} is ionic fraction, f is $K_{ow}/(K_{ow}+1)$, $\log D_{oc,IE} = 1.53V_x + 0.32Nai - 0.27$, $\log D_{CEC,\,clay} = 1.22V_x - 0.22Nai + 1.09$, $D_{oc,IE}$ is isolated natural organic matter, $K_{CEC,\,clay}$ is cation exchange capacity attributed to clay minerals, V_x is McGowan Volumes, $K_{oc,n}$ is normalized organic carbon for neutral fraction, $K_{oc,ion}$ is normalized organic carbon for ionic fraction, a is 1 for acids and -1 for bases, $(pH + \delta)$ is a soil pH corrective factor, α is fraction of species under acidic conditions, FeOx is iron oxyhydroxide concentration, AlOx is aluminum oxyhydroxide concentration, C is a regression constant, c_1 to c_6 are coefficients. σ is number of moles of negative charge sites per gram of organic carbon, CF_{clay} is a correction factor for compound structural moieties specific to inorganic cation exchange sites, COC is a correction factor for structural moieties specific to organic carbon cation exchange sites

[b] Average root mean square deviations value for 9 data sets of acids

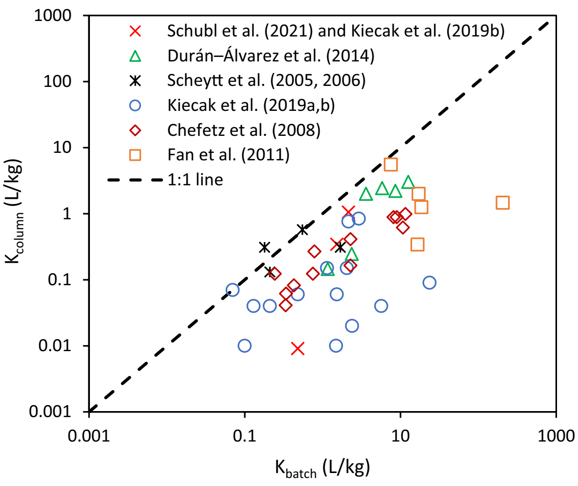

Fig. 20 Comparison of batch- and column-determined sorption distribution coefficients of PACs

respectively. The model predicted K by a factor of six for OTC and TYL and a factor of three for SCP.

Franco and Trapp [37] compiled a database from the literature for 164 organic compounds including five basic PACs. Regression equations were developed to predict the normalized organic carbon coefficient ($K_{oc} = K/OC$) for each ionic state separately and for all ionic states together. Equations 11 to 15 assume no dissociation for weak acids ($pK_a > 7.5$) and weak bases ($pK_a < 3.5$), while complete dissociation was assumed for strong acids ($pK_a < 4$) and strong bases ($pK_a > 7.5$). The authors developed Eqs. 16 and 17 to account for variation in soil pH as it affects the fraction of ionized PACs. Strong bases exhibited the highest sorption among all tested compounds, and they were highly correlated to log K_{ow}. Franco et al. [36] considered the influence of soil pH with a corrective factor (Eq. 18). The regression considers the

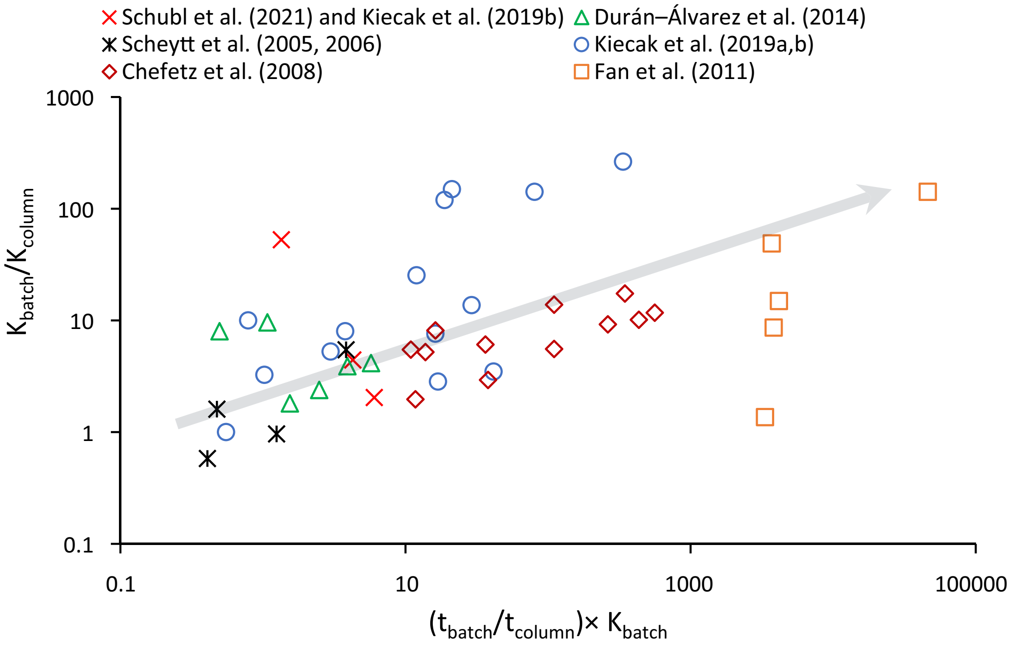

Fig. 21 Variations between batch and column K of PACs as influenced by the batch sorption coefficient multiplied by the residence time in the batch reactor relative to that in the column reactor

influence of pH on the distribution of chemical species and the specific partition coefficients of each species, which are determined by their pK_a and log K_{ow} when in a neutral state. Recognizing that the pH of the soil enables the calculation of the proportions of neutral and ionic molecules present, it enhanced the current regression model for acidic compounds. However, applying the same methodology to bases did not yield successful results.

Droge and Goss [26] developed a model (Eq. 19) that correlates the sorption of organic cations, including PACs to the soil. The model was tested using 29 strong bases, focusing on the contributions of organic matter and clay minerals. The derived model was applied to one reference organic matter and one clay mineral. The results indicated its particular suitability for clayey soils. The model demonstrated that the sorption of organic cations to clay minerals accounts for more than 90% of the overall affinity.

Jolin et al. [52] employed a predictive model (Eq. 20) to estimate the sorption of organic cations using a probe molecule. Phenyltrimethylammonium (PTMA) and benzylamine were employed as probe molecules, but the former demonstrated superior performance. The model assumes that the K of an organic cation is related to the K of PTMA (K_{PTMA}) multiplied by a structural scaling factor (S_{soil}) that accounts for free energy differences in sorption between the target organic cation and PTMA. S_{soil} is assumed to consists of two components: one related to CEC and the other to OC. The authors tested their model for sorption of two cationic PACs (desipramine (DES) and TMD) using 30 soils. They found that predicted values of K for the two tested PACs were within an order of magnitude of their measured values.

Li et al. [71] generated a database for the sorption of 21 ionizable PACs to five types of soil and used the dataset to evaluate the performance of previously developed models by Droge and Goss [26], Franco et al. [36], Franco and Trapp [37], and Kah and Brown [55]. The authors found that the evaluated models were unable to adequately predict K. They developed new models for each PAC class (Eq. 21–26). For basic PACs, the inclusion of the pH-adjusted lipophilicity (D_{ow}) and OC accounted for 73.3% of the variations in the experimental K values (Eq. 22). The addition of exchangeable Na^+ (ExNa) resulted in a higher R^2 of 0.815 (Eq. 23). The sorption of weak bases was influenced by the hydrophilic factor (HF), molecular weight (MW), number of hydrogens bound by the charged nitrogen (Nai), and OC (Eq. 24). The addition of ExNa to Eq. 24 improved the model further (Eq. 25).

Carter et al. [19] used a database of measured K for 83 PACs ($-4.13 < \log K_{ow} < 7.59$) with various soil types to evaluate several existing models that were developed to estimate K of organic compounds to soil material. Their evaluation included the models developed by Droge and Goss [26], Franco et al. [36], and Franco and Trapp [37]. In addition, they evaluated models developed for organic compounds other than PACs including those of Binetin and Devillers [11], Kah and Brown [55], and Sabljic [104]. The authors found that the model of Franco et al. [36] best predicted the sorption of soils for PACs that contain a single acidic functional group, whereas that of Droge and Goss [26] led to the best performance for PACs with a basic functional group. However, all evaluated models resulted in poor prediction ($R^2 < 0.29$) when applied to the tested dataset. The authors concluded that models that included PACs within their training set performed better than those developed for general group organic chemicals. Moreover, models that consider chemical charge in combination with information about soil properties perform better than those that are solely based on K_{ow}. This is also echoed by Sigmund et al. [113] who indicated that models that are based on the K_{ow} and D_{ow} approaches will fail to adequately estimate the sorption of ionized organic compounds if the charged species interact with the soil constituents.

Meta-analysis and machine learning approaches have been explored to estimate the sorption behavior of PACs. For example, Barron et al. [8] proposed an artificial neural network model that used 37 molecular descriptors as input variables to estimate K of PACs. Molecular descriptors include K_{ow}, K_a, molar refractivity, aromatic ratio, hydrophilic factor, and topological surface area. The model showed a high correlation between the experimental and predicted K values ($R^2 > 0.88$). Also, the model could predict K within a factor of two for four PACs (meclofenamic acid, mefenamic acid, ibuprofen and furosemide) which had not been included in the training set.

Garduño-Jiménez et al. [38] utilized principal component analysis and partial least squares to develop machine learning models to quantitatively identify the factors influencing K for PACs. Their data set included 82 data points from 13 references. The tested factors included properties of PACs, soil characteristics, and experimental conditions. The authors concluded that the factors that are significantly important in predicting K include the solubility of the PAC, the soil/liquid equilibration time prior to adding the PAC, the OC, and the soil sterilization method.

J. Li et al. [72] generated a dataset for the sorption of 54 PACs onto 13 soils and sediments. They utilized the dataset to develop new models to predict K using linear regression and machine learning approaches (artificial neural network, random forest, and support vector machine). The authors found that models accounting for solid and molecular descriptors generated from each approach outperformed those incorporating only molecular descriptors. Among the developed models, the one based on the random forest approach with chemical and solid descriptors performed the best. Such a model could predict K of an independent data set to within a factor of 10. The authors also found that the molar volume of a PAC is the most important descriptor for estimating K. Other top contributing molecular descriptors included unsaturation index, molecular charge fraction, solubility, D_{ow}, K_{ow} and K_a. On the other hand, solid descriptors generally showed less influence on K prediction than molecular descriptors, with the highest contributing solid descriptors being OC and the fragment-based polar surface area. Soil/sediment pH also appeared to affect the prediction of K.

Wang et al. [123] used three machine learning approaches (random forest, extreme gradient boosting, and gradient boosting decision tree) for developing predictive models for soil sorption of three classes of antibiotics: sulfonamides (SUL), tetracyclines (TET), and fluoroquinolones (FLU). A dataset of 2203 data points of 17 antibiotics with 255 soils was used including 1118, 736, and 349 data points for SLU, TET, and FLU, respectively. Soil characteristics, antibiotic properties, and reaction conditions (solution pH, S/L ratio, and compound equilibrium concentration) were selected as feature variables that could influence soil sorption capacity. The optimal independent models resulted in an excellent predictive performance with an R^2 of 0.942—0.977 and root mean square error of 0.051 to 0.210 on test sets compared with the combined models. Prediction by the optimal independent models indicated that soil has the highest sorption potential for SUL, followed by TET and FLU. This was attributed mainly to differences in the functional groups associated with the antibiotics. The authors employed the Shapley additive interpretation method to assess the relative contribution of each influencing factor toward soil sorption capacity. Results indicated that reaction conditions had the highest contribution with mean absolute Shapley of 52.1%, 63.5%, and 54.1% for SUL, TET, and FLU, respectively.

Conclusion and prospects

Sorption of the PACs to soil materials is a complex process influenced by the properties of PACs, soils, and solutions. In general, the sorption of PACs based on their ionic states can be arranged as zwitterion > cation > neutral > anion. Increasing S_w, OC, CEC, S/L ratio, and soil surface area while decreasing pH, ionic strength, and temperature generally result in an increase in the extent of sorption of PACs. In some cases, the interaction of the PACs with soil material could experience nonideal behavior in terms of sorption competition, nonlinearity, nonequilibrium, and hysteresis. Competition occurs due to the presence of more than one PAC in the solution or due to the presence of DOM. While many of the PACs exhibit linear sorption behavior, some may deviate from linearity. The reaction rate of PACs to soil material in batch reactors is characterized by a fast reaction at the initial stages followed by a slow approach to equilibrium. Comparison between sorption equilibrium coefficients of PACs determined by batch- and column- techniques revealed that the former method results in higher values. Further analysis of the data indicates that the discrepancy between the two techniques could be attributed to variations in the residence times of the two systems. Regression analysis and machine learning approaches have been explored in the development of models for the prediction of the sorption of PACs to soil materials. These models incorporate molecular and soil descriptors. While some of these models have been validated, their robustness requires validation using broader external datasets.

Limited work has been done to assess the sorption of PACs to soil materials in arid and semi-arid regions. The lack of freshwater resources in these regions promotes the utilization of TSE either directly for irrigation purposes or through aquifer recharge, which poses a risk of soil and groundwater contamination. Thus, there is a need to investigate the sorption behavior of PACs to soil materials in these regions. Most of the work done on assessing the sorption of PACs to soils was limited to artificially made aqueous solutions. Limited work has been done on using real water samples. Future work should consider the utilization of real groundwater, surface water or TSE samples since the solution composition could have an impact on the sorption of these compounds [123]. In addition, applied experimental conditions should closely resemble the environmental conditions. It is also necessary to follow standardized experimental protocols to avoid inconsistencies arising from deviations in the experimental procedure among different investigators.

There is more focus in the literature on using batch reactors to assess the sorption behavior of PACs to soil material than on column studies. Batch systems are informative but do not closely resemble the transport of PACs through soils and aquifer material. Future studies should consider more column investigations focusing on changes in the pore-water velocity, groundwater characteristics, and soil heterogeneity. The applied experimental conditions of the column studies should closely resemble the environmental conditions, especially the input concentration, the pore-water velocity, and the retention time in the reactor. The observed discrepancy between batch- and column-determined sorption distribution coefficients of PACs in the literature data requires further work to elucidate the reason(s) behind this discrepancy. Modeling the transport of PACs through packed soil columns should account for possible nonlinear sorption behavior and should consider a more advanced treatment of the mass transfer process as it could have a significant impact on the transport of these compounds.

Mechanistic understanding of the sorption of PACs to soil materials requires thorough knowledge of the physicochemical properties of the components of the system (i.e., compounds, soils, and solutions). Meanwhile, the coverage of the sorption experiments should be broadened to include more types of soils and PACs. Such effort will greatly assist in improving the development of robust predictive models which could be utilized to carry on risk assessment and support environmental decision-making. While simple predictive models are preferable in the implementation of risk assessment, the current practices which are based on the K_{ow} and D_{ow} approaches need to be updated to account for the complexities of the interactions between the PACs and the soil material [19].

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s12302-024-00984-9.

Additional file 1.

Author contributions

Ahmad M. Alhalabi: Conceptualization, data extraction, data analysis, drafting and revising of manuscript. Mohammed A. Meetani: Conceptualization and review of manuscript. Ahmad Shabib: Bibliometric analysis and review of revised manuscript. Munjed A. Maraqa: Conceptualization, drafting of manuscript, and review of revised manuscript.

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Availability of data and materials

No datasets were generated or analysed during the current study.

Code availability

Not applicable.

Declarations

Ethics approval and consent to participate

The authors have approved the final draft of the manuscript.

Consent for publication

Not applicable.

Competing interests

The authors declare no competing interests.

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