

# Influence of soil properties on <sup>14</sup>C-Saflufenacil behavior: Sorption and mobility study

Fernando S. de Oliveira<sup>a</sup>, Vanessa Takeshita<sup>b</sup>, Kassio F. Mendes<sup>b</sup>, Valdemar Luiz Tornisielo<sup>b</sup>, Taliane Maria da S. Teófilo<sup>a</sup>, Bruno Caio C. Fernandes<sup>a</sup>, Hamurábi A. Lins<sup>a\*</sup>, Daniel V. Silva<sup>a</sup>

<sup>a</sup> Department of Agronomic and Forest Sciences, Universidade Federal Rural do Semi-Árido, Mossoró, RN, Brazil. <sup>b</sup> Nuclear Energy Center at Agriculture, Universidade de São Paulo, Piracicaba, SP, Brazil.

**Abstract: Background:** Knowing the relationships between the soil's physical-chemical properties and herbicide behavior in the soil allows establishing strategies for the efficient control of weeds with less environmental risk. **Objective:** It carried this study to investigate the role of physical-chemical properties of Brazilian soils in the sorption-desorption and mobility of the herbicide saflufenacil. **Methods:** We used nine soils from different regions of Brazil in the study of sorption-desorption and mobility of <sup>14</sup>C-saflufenacil. The herbicide sorption-desorption estimate was performed using the batch equilibrium method and mobility using soil thin-layer chromatography. Principal component analysis (PCA) and clustering were performed to evaluate the impact of soil properties on the sorption-desorption behavior of saflufenacil. **Results:** The results indicated that saflufenacil was weakly sorbed in different types of tropical soils, and the sorption process is reversible, with its mobility varied from mobile ( $R_f = 0.70$ ) to very mobile ( $R_f = 0.99$ ) in the different soils and indicates that the herbicide has leaching potential in these types of soils. The

sorption-desorption capacity and mobility of saflufenacil depend mainly on pH, CEC, clay, and OC content, and therefore it is vital to analyze them to predict the impacts of herbicide application on the environment. The PCA is an essential tool that helps to clarify how the effects of soil properties influence herbicide behavior. **Conclusions:** The OC content in Brazilian soils has a direct role in saflufenacil sorption and desorption. BR3 soil (soil with highest organic carbon; OC = 2,1%) exhibits greater sorption ( $K_d = 1,85 \text{ L kg}^{-1}$ ), value 5.5 times greater than the BR1 (soil with lower sorption; with OC = 0,6%). Therefore, the application of saflufenacil to tropical soils, especially those with low levels of CO (< 1%), may result in a greater potential risk of contamination of surface and groundwater in neighbouring agricultural and non-agricultural areas, particularly those with intensive use and ineffectiveness of saflufenacil. Future investigations could focus on integrating modeling approaches that incorporate soil variability to predict saflufenacil behavior accurately in diverse soil types, aiding in decision-making for sustainable herbicide use.

**Keywords:** Sorption; Herbicide; Transport; Environmental contamination

## Journal Information:

ISSN - 2675-9462

Website: <http://awsjournal.org>

Journal of the Brazilian Weed  
Science Society

**How to cite:** Oliveira FS, Takeshita V, Mendes KF, Tornisielo VL, Teófilo TMS, Fernandes BCC, Lins HA, Silva DV. Influence of soil properties on <sup>14</sup>C-Saflufenacil behavior: Sorption and mobility study. *Adv Weed Sci*. 2024;42:e020240027

<https://doi.org/10.51694/AdvWeedSci/2024.42.00013>

## Approved by:

Editor in Chief: Carlos Eduardo Schaedler

Associate Editor: Mohammad Mehdizadeh

**Conflict of Interest:** The authors declare that there is no conflict of interest regarding the publication of this manuscript.

**Received:** March 19, 2024

**Approved:** June 11, 2024

\* **Corresponding author:**

<hamurabi\_a\_@hotmail.com>



This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided that the original author and source are credited.

**Copyright:** 2022

## 1. Introduction

The sorption-desorption and mobility of herbicides in soils are essential processes that determine environmental behavior, the effectiveness, and the potential for damage to crops, as well as the risk of contamination of the environment (Kah, Brown, 2006; Yavari et al., 2020). The dynamics of these processes depend on multiple factors, such as the physical and chemical properties of herbicides, soil properties and climatic conditions (Kumar et al., 2015; Li et al., 2019a; Zhang et al., 2020). Raimi et al. (2021) highlighted the need for sustainable use of herbicides to minimize their impact on the environment, in line with Sustainable Development Goal 13gest.

Studying the sorption of herbicides is important to predict the environmental fate and establish strategies for the efficient control of weeds, with less environmental and human risk (Mehdizadeh et al., 2021). The sorption-desorption capacity of herbicides in the soil is often measured through of isotherm parameters of retention kinetics, mainly from the Freundlich model (Chagas et al., 2019; Mendes et al., 2019a; Santos et al., 2019). Among the model parameters, the most used are the sorption and desorption coefficients ( $K_{fs}$  and  $K_{fd}$ , respectively), hysteresis index (H), and the isotherm inclination (1/n) of sorption and desorption in different soils (Li et al., 2019b).

Mobility is a process that involves sorption, desorption, and distribution between herbicide-water-soil (Halimah et al., 2016; Li et al., 2019a). Herbicide mobility can be influenced by many factors, including climate, hydrology, physical-chemical properties of herbicides and soils (Liu et al., 2018; Marín-Benito et al., 2018), however, sorption is considered the most crucial factor that controls the mobility of the herbicide in the soil (Flessner et al., 2015; Zhang et al., 2020). Thus, it is expected that in soils with low sorption, herbicides (such as saflufenacil) have high mobility, which becomes a significant concern with the risk of contamination of the environment (Singh, Singh, 2012; Matallo et al., 2014; Azcarate et al., 2015).

Saflufenacil, (2-chloro-4-fluoro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]-N-[methyl (propane-2-yl) sulfamoyl]benzamide), it is a herbicide belonging to the chemical group pyrimidinedione, inhibitor of the enzyme protoporphyrinogen IX oxidase (PROTOX), which is an enzyme involved in

the biosynthesis of chlorophyll and cytochromes (Grossmann et al., 2011). Saflufenacil is used for the pre- or post-emergence control of dicotyledonous weeds (broadleaf) in various crops (for example, sugarcane, corn, soybeans), in the desiccation of crops, and in the management of resistant weeds of glyphosate (Badische Anilin and Soda Fabrik, 2008; Budd et al., 2016). It is a weak acid herbicide, with an acid dissociation constant (pKa) of 4.41, high solubility in water (2,100 mg L<sup>-1</sup> at pH 7.0); low vapor pressure (2.0 × 10<sup>-14</sup> Pa at 25 °C), and moderate octanol-water partition coefficient (log K<sub>ow</sub> of 2.6) (International Union of Pure and Applied Chemistry, 2021). Saflufenacil has a linear sorption coefficient (K<sub>d</sub>) of 0.87 L kg<sup>-1</sup>, sorption coefficient normalized by CO content (K<sub>oc</sub>) of 19.90 and half-life of 43 days in a Brazilian Alfisol with a pH (CaCl<sub>2</sub>) of 5.6, organic carbon (OC) of 4.9% and clay content of 33.2% (Oliveira et al., 2022). Due to the anionic character in most agricultural soils and the high-water solubility, saflufenacil can be a mobile pollutant in the soil profile and of potential risk of contamination of surface and groundwater (Monquero et al., 2012; Papiernik et al., 2012; Matallo et al., 2014). However, the environmental fate of saflufenacil, particularly in tropical soils, are not yet fully understood.

Soil physicochemical properties influence saflufenacil behavior. Several studies have shown that organic matter (OM) is the most frequently reported and essential (but not independent) factor that affects the sorption of saflufenacil in soils (Papiernik et al., 2012; Gannon et al., 2014; Matallo et al., 2014; Barcellos Júnior et al., 2021). However, as saflufenacil is an ionizable herbicide, other factors can influence its sorption, including pH, clay content, and cation exchange capacity (CEC) (Kah et al., 2017; Gámiz et al., 2019; Barbieri et al., 2021). This suggests that application of saflufenacil in Brazilian soils may lead to different results in terms of adsorption and mobility due to large differences in physicochemical properties between soils. For example, an increase in soil pH causes the negatively charged surfaces of soil colloids to repel herbicidal anions (weak acids), thereby limiting sorption and increasing herbicide availability and phytotoxicity (Azcarate et al., 2015; Liu et al., 2018).

By studying the sorption, desorption, and mobility of saflufenacil in a variety of tropical soils, this study fills a knowledge gap in the field of weed science by examining the relationship between saflufenacil and soil properties, providing a basis for understanding its behavior and the destination in the environment. Furthermore, the research findings offer practical implications for developing soil-specific guidelines for saflufenacil application, enhancing weed control efficacy while minimizing environmental risks. Based on this, the hypothesis of this study is that soil properties can limit or increase saflufenacil sorption, influencing the herbicide behavior and application recommendations; and that the use of multivariate analysis, as the main component (PCA) and grouping, can identify

the properties of the soils that most influence sorption and group the soils with similar sorption capacities. In this sense, the present study was developed to investigate the role of physicochemical properties of Brazilian soils in the sorption-desorption and mobility of saflufenacil.

## 2. Material and Methods

### 2.1 Soils

Nine soils from different areas of Brazil were used in the study (Table SF1). The soils were collected in the superficial layer (0–10 cm deep), after the previous cleaning of the vegetable layer, in places without a history of herbicide application. The selection aimed to cover soils with different properties, including soils with high CEC to soils with low CEC, different values of pH, OC and texture, to study the impact of these variations on the sorption and mobility of saflufenacil. After collected, the deformed soil samples were air-dried, ground, sieved through a 2.0 mm sieve, and subjected to physical-chemical characterization.

### 2.2 Radiolabelled herbicide

Saflufenacil [Phenyl-U-<sup>14</sup>C] was supplied by BASF Corporation (Research Triangle Park, NC). The radiolabelled herbicide had a specific activity of 4.65 MBq mg<sup>-1</sup> and radiochemical purity of 99.6%.

The initial concentration of <sup>14</sup>C-saflufenacil was determined from the stock solution, with aliquots of 500 µL, in duplicate, pipetted into scintillation vials containing 10 mL of scintillator solution and analyzed in liquid scintillation spectrometry (LSS) (Tri-Carb 2910 TR LSA, LSA PerkinElmer, Waltham, MA, USA) for 5 min. Then, <sup>14</sup>C-saflufenacil was carefully mixed in acetone and diluted with a 0.01 mol L<sup>-1</sup> CaCl<sub>2</sub> solution at five different concentrations (0.037; 0.052; 0.065; 0.071 and 0.1 µg mL<sup>-1</sup>) to obtain the solutions of work for the study. In the same order, these concentrations corresponded to doses of 44, 61, 78, 84, and 120 g a.i. ha<sup>-1</sup>.

### 2.3 Sorption-desorption studies

The saflufenacil sorption-desorption study was determined by the Batch Equilibrium method, and the procedures were performed according to the OECD-106 guidelines, “Adsorption-desorption using a batch equilibrium method,” established by the Organization for Economic Cooperation and Development (OECD, 2000).

A 10 mL aliquot of the aqueous solutions was transferred to 50 mL screw cap Teflon flasks containing the soil samples (10 g) in duplicate, resulting in a 1:1 (m v<sup>-1</sup>) soil: solution ratio. The Teflon flasks were shaken on a horizontal pendulum table (Tecnal *Equipamentos Científicos*, model I-240, Piracicaba, SP, Brazil) at 38 g for 24 h in a dark room (20 ± 2 °C), to achieve equilibrium concentration (Matallo et al., 2014). After that, the tubes were centrifuged

at 760 g for 10 min (Hitachi CF16RXII, Hitachi Koki Co., Ltd., Indaiatuba, SP, Brazil), and a 1 ml aliquot of the supernatant from each tube was transferred to scintillation vials containing 10 mL of scintillating solution and analysed in LSS for 5 min, to determine the concentration of  $^{14}\text{C}$ -saflufenacil in equilibrium in the solution ( $C_e$ ). The sorbed herbicide ( $C_s$ ) concentration was determined by the difference between the initial concentration and the final concentration in the supernatant after equilibration.

After determining the herbicide concentration in the sorption study, the desorption study was carried out using the same Teflon tubes with the soils analysed in the sorption test. The remaining  $\text{CaCl}_2$  solution was removed entirely, and 10 mL of a new  $\text{CaCl}_2$  solution ( $0.01 \text{ mol L}^{-1}$ ), without the herbicide, was added to the Teflon tubes, which were stirred for 24 h under the same conditions as the sorption study until achieve the reequilibrium concentration. Afterward, the tubes were again centrifuged (760 g; 10 min) and two aliquots of 1 ml of the supernatant from each tube were transferred to scintillation vials containing 10 ml of the scintillation solution and analysed in LSS for 5 min. The amount of herbicide desorbed was determined from the difference between the concentration sorbed in the soil and the remaining supernatant.

#### 2.4 Sorption-desorption model

The sorption-desorption data were adjusted to the Freundlich equation:  $C_s = K_f \times C_e^{1/n}$ , where  $C_s$  is the concentration ( $\text{mg kg}^{-1}$ ) of the herbicide sorbed in the soil;  $K_f$  is the Freundlich sorption coefficient ( $\text{mg}^{1-1/n} \text{ kg}^{-1} \text{ L}^{1/n}$ );  $C_e$  is the concentration of the herbicide ( $\text{mg L}^{-1}$ ) after equilibrium, and  $1/n$  is a constant that characterizes the non-linearity of the isotherm. The  $K_f$  values were normalized to the OC content in the soil using the following formula:  $K_{foc} = (K_f / (\% \text{ OC})) \times 100$ . The linear sorption distribution coefficient ( $K_{ds}$ ) and linear sorption coefficient normalized by organic carbon content ( $K_{soc}$ ), in  $\text{L kg}^{-1}$ , were calculated using the following formulas:  $K_d = C_s / C_e$ ;  $K_{oc} = (K_d / (\% \text{ OC})) \times 100$ . The hysteresis coefficient (H) for the sorption-desorption isotherms was calculated according to the formula:  $H = (1/n_{\text{desorption}}) / (1/n_{\text{sorption}})$ .

#### 2.5 Mobility studies in soil thin layer chromatography (TLC)

The mobility of  $^{14}\text{C}$ -saflufenacil in soils was studied in duplicate on TLC plates, according to the technical recommendations of the Environmental Protection Agency OPPTS 835.12.10 (Environmental Protection Agency, 1998) and Takeshita et al. (2021). The glass plates ( $0.15 \times 0.09 \times 0.005 \text{ m}$ ) were coated with moist soil of 0.005 m, which was prepared with a mixture of 100 g of soil and deionized water on acrylic support ( $0.3 \times 0.12 \times 0.028 \text{ m}$ ). Afterward, the plates were air-dried, and a strip of the soil of 0.005 m was removed 0.12 m above the base to prevent the elution of water by capillarity from exceeding this height.

In each soil TLC plate, with the aid of a micro syringe, 2  $\mu\text{L}$  of  $^{14}\text{C}$ -saflufenacil solution ( $333.33 \text{ Bq } \mu\text{L}^{-1}$ ) was supplied at a single point 0.02 m from the base of the plate, in duplicate. Then, the plates were placed in an upright position in a closed glass vat, containing 0.1 L of deionized water as eluent. To keep the atmosphere saturated with water in the glass vat, a sheet of filter paper was fixed up to 0.02 m above the plate, leading to a uniform elution flow. After the water reached 0.1 m above the application point (elution limit line), TLC soil plates were removed, air-dried ( $23 \pm 5 \text{ }^\circ\text{C}$ ), and placed in contact with phosphorescent image plates, for 12 h, for sensitization and obtaining autoradiographic images.

Subsequently, an autoradiogram was found by reading the image plate on a Cyclone® Plus radio scanner (model C431200, PerkinElmer, Inc., Shelton, CT, USA). Chromatograms with colour intensity levels were generated for visual interpretation of radioactivity in autoradiograms. Areas with a blue colour indicate low levels of radioactivity, while red colour indicates higher levels of radioactivity. The values of the mobility retention factor ( $R_f$ ) were measured by the equipment from the autoradiograms manufactured from the soil TLC plates, using the following formula:  $R_f = D_p/D_a$ , where  $D_p$  is the frontal distance covered by the herbicide, and  $D_a$  is the distance travelled by the water solvent, which moves through capillarity in the same period. The values of  $R_f$  were classified according to the classification system of mobility classes proposed by Helling and Turner (1968): class 1, 0-0.09 (immobile); class 2, 0.10 to 0.34 (little mobile); class 3, 0.35 to 0.64 (moderately mobile); class 4, 0.65-0.89 (mobile); and class 5, 0.90-1.00 (very mobile).

#### 2.6 Statistical analysis

Before proceeding with statistical analyses, all data were normalized to standardize variables with different measurement units, subtracting their means and dividing by their standard deviations. Saflufenacil sorption, desorption, and mobility data were expressed as mean and confidence intervals of the mean or standard deviation ( $n = 2$ ). Principal component analysis (PCA) and clustering were performed to evaluate the influence of soil properties on saflufenacil sorption-desorption. Statistical analyses were performed using R software (R Development Core Team, Vienna, Austria). The figures were plotted using Sigma Plot® (Version 12.0 for Windows, Systat Software Inc., Point Richmond, CA, USA).

### 3. Results and Discussion

#### 3.1 Soil properties

To have greater representation in this study, the selected soils had high variability in their origins and physicochemical characteristics (Table S1 and Table 1). The pH of the soils ranged from 4.4 (very high acidity) to 6.5 (weak acidity), this

in Ultisol Rhodic Paleudult (BR6) and Inceptisol Ochrept (BR4), respectively. The values of potential acidity (H + Al) of the soils ranged from 10 (Ultisol Typic Hapludult - BR1 and Quartzipsamments - BR2) to 57.8 mmol<sub>c</sub> kg<sup>-1</sup> (Typic Plinthustalfs - BR8), reflecting the great variation of the soil acidity. The CEC also showed great variations, with the highest value found in BR8 (104.7 mmol<sub>c</sub> kg<sup>-1</sup>) and the lowest in BR2 (14.6 mmol<sub>c</sub> kg<sup>-1</sup>). As for base saturation (V), the highest value (78%) was found in BR1, and the lowest (28%) in Oxisol Typic Hapludox (BR7).

Regarding the concentration of organic carbon (OC), except for the OC content of the Alfisol Aqualf (BR3), which was 2.1%, the OC content of the studied soils was less than 1%. There was a wide variation in sand content, with the lowest values (21%) in BR6 and the highest (94.2%) in BR2. The clay content ranged from 2 to 59%, these extremes being represented by Quartzipsamments (BR9) and BR6, respectively.

The considerable variation in soil properties in the present study was expected and is related to the different paedogenetic processes of soil formation in the places of origin. In Brazil, the registration of herbicides requires research on environmental behaviour in at least three types of national soils, according to the Brazilian Institute for the Environment and Renewable Natural Resources (Ibama). In addition, the recommendations for the use of herbicides in pre-emergence only consider the texture and OM content of the soil. However, other soil attributes can also influence the sorption of herbicides, such as herbicides with essential characteristics (such as hexazinone), which can change their behaviour in the soil due to changes in soil pH (Azcarate et al., 2015). Studies have reported that increasing soil pH reduced sorption and increased desorption of atrazine (herbicide with basic character) in different soils (Yue et al., 2017; Martins et al., 2018).

However, on acidic herbicides like the one in this study, more research is needed.

Other chemical attributes can have indirect effects, such as contributing to the stability of soil OM. In addition to the organic material supply, cations are also essential for the maintenance of soil OM (Marinho et al., 2016). Therefore, it is understood that understanding the environmental behaviour and fate of herbicides in a more significant number of soil samples and with different properties can generate more effective and safer recommendations, thus avoiding possible soil and water contamination (Chagas et al., 2019; Santos et al., 2019).

### 3.2 Saflufenacil sorption

The Freundlich model was applied to find the isotherms and estimate the sorption parameters of saflufenacil in soils (Figure 1 and Table 2). The Freundlich model equation fitted the sorption isotherms with high coefficients of determination ( $R^2 \geq 0.99$ ), which indicates that this model is adequate to describe the results of saflufenacil sorption in all studied soils.

The saflufenacil sorption isotherms were type C (Limousin et al., 2007). There was a practically linear increase in sorption with the increase in the concentration of saflufenacil, indicating that the number of adsorption sites remains almost constant regardless of solute concentrations (Mendes et al., 2019b). The sorption linearity is even more evident by the slope values (1/n), which ranged from 0.87-1.05 (Table 2). These results are consistent with Matallo et al. (2014), who also observed the same type of sorption isotherm of saflufenacil in two Brazilian soils.

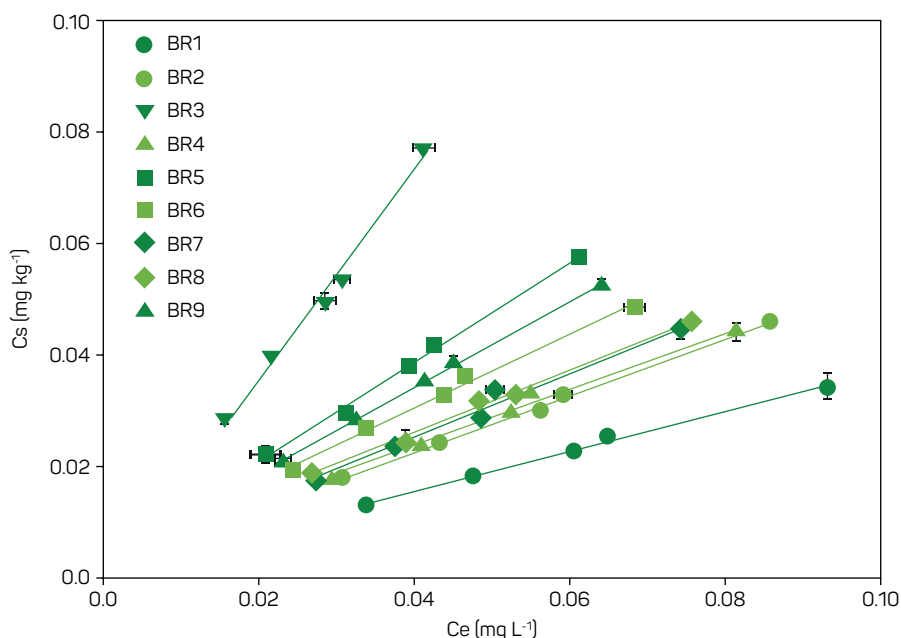
The Freundlich sorption distribution coefficient ( $K_f$ ) of saflufenacil in soils was low, with values ranging between 0.32 and 2.09 mg<sup>-1-1/n</sup> kg<sup>-1</sup> L<sup>1/n</sup> (Table 2). These low

**Table 1-** Physical and chemical properties of soils used in sorption, desorption, and mobility studies

Soils	pH	P	K <sup>+</sup>	Ca <sup>2+</sup>	Mg <sup>2+</sup>	H + Al	SB	CEC	V	OC	Sand	Silt	Clay	Texture class
	H <sub>2</sub> O	mg kg <sup>-1</sup>		mmol <sub>c</sub> kg <sup>-1</sup>							%			
BR1	5.9	15	1.4	22	12	10	35.4	45.4	78	0.6	88.8	7.5	3.7	Sand
BR2	4.5	4	0.8	2	1	10	4.6	14.6	32	0.2	94.2	2.4	3.4	Sand
BR3	4.9	7	2.4	15	5	20	22.4	42.4	53	2.1	66.4	29.1	4.5	Sandy Loam
BR4	6.5	2.3	2.5	54.3	29.4	49.5	86.2	135.7	63.5	0.9	48	15	37	Sandy Clay
BR5	5.9	4.7	2.8	18.9	17.6	47.9	39.3	87.2	45.1	0.7	72	14	14	Sandy Loam
BR6	4.4	0.1	0.6	5	13.7	41.3	19.3	60.6	31.8	0.3	21	20	59	Clay
BR7	4.6	0.3	0.7	8.6	8.5	54.5	17.8	72.3	28	0.4	77.6	2.4	20	Sandy Clay Loam
BR8	5.1	1.7	1.6	35	6.4	57.8	43.0	100.8	45	0.8	86.7	4.3	9.0	Loamy Sand
BR9	5.6	2.6	2.8	14.4	12.9	39.6	30.1	69.7	45.6	0.5	93	5.0	2.0	Sand

BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments; pH: hydrogen potential; P: phosphorus; K<sup>+</sup>: potassium; Ca<sup>2+</sup>: calcium; Mg<sup>2+</sup>: magnesium; H + Al: potential acidity; SB: sum of bases; CEC: cation exchange capacity; V: base saturation; OC: organic carbon.





BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodar Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9= Quartzipsamments. The vertical and horizontal bars represent the standard deviation of the means (*n* = 2) of Ce (concentration in equilibrium) and Cs (concentration in soil), respectively. Symbols can cover the bars.

**Figure 1** - Freundlich isotherms of <sup>14</sup>C-saflufenacil sorption in nine Brazilian soils.

Soils	$K_{ds}$	$K_{soc}$	$K_{fs}$	$K_{foc}$	1/ <i>n</i>	R <sup>2</sup>	Sorption (%)
	(L kg <sup>-1</sup> )		(mg <sup>-1/n</sup> kg <sup>-1</sup> L <sup>1/n</sup> )				
BR1	0.36 (0.33-0.39) <sup>a</sup>	61.81 (57.06-66.57)	0.32 (0.27-0.37)	55.43 (47.26-63.60)	0.94 ± 0.04 <sup>b</sup>	1.0	35.46 ± 2.31
BR2	0.51 (0.49-0.52)	220.87 (213.49-228.25)	0.45 (0.41-0.48)	194.35 (179.59-209.10)	0.93 ± 0.02	1.0	46.97 ± 0.89
BR3	1.85 (1.71-1.99)	86.0 (79.36-92.64)	2.09 (1.59-2.59)	96.88 (73.53-120.23)	1.04 ± 0.06	0.99	76.92 ± 1.07
BR4	0.51 (0.46-0.55)	57.56 (52.66-62.46)	0.40 (0.32-0.48)	45.85 (37.09-54.61)	0.88 ± 0.06	0.99	46.26 ± 1.63
BR5	0.89 (0.82-0.97)	125.77 (114.82-136.73)	0.76 (0.58-0.93)	107.61 (82.51-132.70)	0.92 ± 0.08	1.0	58.77 ± 1.64
BR6	0.66 (0.63-0.69)	194.85 (186.74-202.96)	0.51 (0.46-0.56)	149.71 (134.32-165.10)	0.87 ± 0.03	1.0	50.88 ± 1.32
BR7	0.58 (0.54-0.61)	134.30 (125.59-143.02)	0.49 (0.41-0.57)	115.12 (95.71-134.52)	0.92 ± 0.05	0.99	46.04 ± 1.28
BR8	0.56 (0.53-0.58)	71.28 (68.20-74.36)	0.44 (0.37-0.51)	56.28 (47.40-65.17)	0.87 ± 0.06	1.0	48.22 ± 2.05
BR9	0.78 (0.74-0.82)	173.22 (164.27-182.18)	0.64 (0.53-0.75)	143.44 (118.46-168.43)	0.91 ± 0.06	1.0	54.71 ± 1.34

BR: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments.  $K_{ds}$ : linear sorption distribution coefficient;  $K_{soc}$ : linear sorption coefficient normalized by organic carbon content;  $K_{fs}$ : Freundlich sorption distribution coefficient;  $K_{foc}$ : Freundlich sorption coefficient normalized by organic carbon content. <sup>a</sup> Average ( $K_{ds}$ ,  $K_{soc}$ ,  $K_{fs}$  e  $K_{foc}$ ) followed by the number in parentheses is the confidence intervals of the average (*n* = 2). <sup>b</sup> Average (1/*n* and sorption) followed by the average standard deviation (*n* = 2).

$K_{fs}$  values in soils are consistent with the results found by Papiernik et al. (2012), and Matallo et al. (2014). The highest  $K_{fs}$ , found in BR3 was 5.5 times greater than the lowest  $K_{fs}$  reported in BR1. The studied soils presented linear sorption distribution coefficient ( $K_{ds}$ ) < 1.0 L kg<sup>-1</sup>, except for BR3, which had 1.85 L kg<sup>-1</sup>. The highest sorption coefficients ( $K_{fs}$  and  $K_{foc}$ ) in BR3 are attributed to the higher OC content, which is generally reported as one of the main controllers of saflufenacil sorption

(Papiernik et al., 2012; Matallo et al., 2014; Barcellos Júnior et al., 2021).

In general, the pH of the studied soils was close to or higher than the pKa of saflufenacil, with 4.41 (International Union of Pure and Applied Chemistry, 2021). In soils with a pH close to or equal to the herbicide pKa, as in BR6 (pH 4.4), the molecular (neutral) and dissociated (anionic) species are approximately equal (50% of each). On the other hand, in soils with a pH greater than the herbicide

pKa, such as BR4 (pH 6.5), the dissociated/anionic form of the herbicide predominates over the molecular form (Gannon, 2011). Saflufenacil has high solubility at pH values close to pH 7.0 (International Union of Pure and Applied Chemistry, 2021). In this case, saflufenacil is completely deprotonated and retains only the anionic form, with lower sorption strength in negatively charged soils (electrostatic repulsion) and high affinity for the soil solution, suggesting that the herbicide is more mobile in the soil profile (Singh, Singh, 2012; Azcarate et al., 2015). In a recent study, Gámiz et al. (2019) observed that sorption of picloram and imazamox, weak acid herbicides such as saflufenacil, exhibited similar behaviour in unamended and amended soils with biochar, which the authors attributed to their anionic character.

The Freundlich sorption coefficient normalized by OC content ( $K_{f_{soc}}$ ) is indicative of the strength of hydrophobic bonds of soil OM in herbicide sorption. The soils presented low  $K_{f_{soc}}$  values in this study, ranging from 45.85 to 194.35  $\text{mg}^{-1-1/n} \text{kg}^{-1} \text{L}^{1/n}$ , in BR4 and BR2 soils, respectively. As for  $K_{f_{soc}}$ , there were low values of the linear sorption coefficient normalized by the OC content ( $K_{soc}$ ), which ranged from 57.56  $\text{L kg}^{-1}$  (BR4) to 220.87  $\text{L kg}^{-1}$  (BR2).

In general, herbicide molecules with a hydrophobic character have a greater affinity to form strong hydrophobic bonds with soil OM, making the  $K_{f_{soc}}$  of this molecule relatively constant in many soils (Li et al., 2019b). However, this is not the case for saflufenacil in the present study, indicating that hydrophobic interactions with OM were not the only determining factor for saflufenacil sorption. Thus, the sorption of herbicides with an ionizable functional group (which undergoes dissociation) such as saflufenacil may be related to weak energy interactions in solution or the solid-liquid interface, such as electrostatic

interactions (anionic exchange, anionic repulsion), binding of hydrogen, and Van der Waals forces (Kah et al., 2017; Gámiz et al., 2019).

The percentage of saflufenacil sorption in different soils showed characteristic behavior of  $K_{fs}$  and  $K_{ds}$  values because the soils that presented the highest  $K_{fs}$  and  $K_{ds}$  had the highest percentages of herbicide sorption. The following descending order of sorption was observed: BR3 > BR5 > BR9 > BR6 > BR8 > BR2 > BR4 > BR7 > BR1. In percentage data, in the soil with greater saflufenacil sorption (BR3), almost 77% of the herbicide was sorbed, while the soil with less sorption (BR1) had 35.46% herbicide sorption, concerning the initial concentration.

### 3.3 Saflufenacil desorption

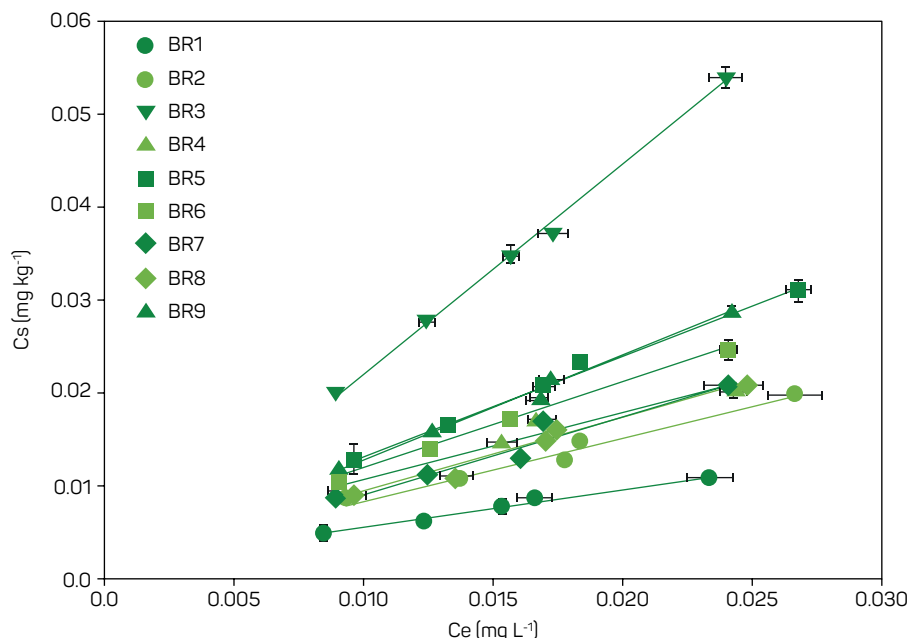
The Freundlich isotherm equations also provided a good description of saflufenacil desorption data for all soils (Table 3 and Figure 2), as observed in the high coefficients of determination ( $R^2 \geq 0.96$ ). The desorption isotherms were like those of the sorption study, indicating reversibility of saflufenacil in the studied soils (Bakhtiary et al., 2013). Isotherms with linear trends and a type C curve were observed (Limousin et al., 2007).

The hysteresis index (H) values were close to 1 in the studied soils (Table 3), indicating that the desorption of saflufenacil occurred at practically the same intensity as the sorption and, therefore, that the desorption was not hysterical. This result may reflect the weak sorption of saflufenacil in soil and its relatively high solubility in water (Hiller et al., 2012). These results agree with those reported by Matallo et al. (2014), who also reported H values close to 1 for saflufenacil in two Brazilian soils.

**Table 3** - Freundlich desorption parameters, linear distribution coefficients, and desorption percentage of  $^{14}\text{C}$ -saflufenacil in nine Brazilian soils

Soils	$K_{dd}$	$K_{doc}$	$K_{fd}$	$K_{fdoc}$	1/n	$R^2$	H	Desorption (%)
	( $\text{L kg}^{-1}$ )	( $\text{L kg}^{-1}$ )	( $\text{mg}^{-1-1/n} \text{kg}^{-1} \text{L}^{1/n}$ )	( $\text{mg}^{-1-1/n} \text{kg}^{-1} \text{L}^{1/n}$ )				
BR1	0.42 (0.42-0.42) <sup>a</sup>	72.24 (72.0-72.49)	0.24 (0.24-0.25)	41.38 (40.40-42.35)	0.82 ± 0.01 <sup>b</sup>	0.98	0.87	65.65 ± 2.31
BR2	0.67 (0.65-0.69)	290 (282-298)	0.45 (0.39-0.51)	194.35 (167.91-220.79)	0.86 ± 0.03	0.98	0.93	55.38 ± 1.95
BR3	2.21 (2.09-2.34)	102.98 (96.99-108.96)	2.27 (1.80-2.74)	105.28 (83.34-127.22)	1.0 ± 0.05	1.0	0.96	27.95 ± 3.26
BR4	0.74 (0.70-0.77)	83.81 (79.55-88.07)	0.37 (0.30-0.44)	42.56 (34.60-50.51)	0.78 ± 0.05	0.96	0.89	50.55 ± 2.08
BR5	1.06 (0.90-1.23)	149.72 (126.61-172.82)	0.73 (0.39-1.08)	103.38 (54.38-152.38)	0.86 ± 0.12	0.99	0.93	44.27 ± 1.92
BR6	0.95 (0.87-1.03)	279.71 (255.17-304.25)	0.59 (0.41-0.78)	179.26 (124.15-234.38)	0.85 ± 0.07	0.98	0.97	46.96 ± 1.42
BR7	0.82 (0.78-0.87)	190.93 (180.41-201.45)	0.61 (0.50-0.72)	143.95 (118.63-169.28)	0.91 ± 0.04	0.96	0.98	52.10 ± 1.81
BR8	0.82 (0.73-0.91)	105.64 (94.22-117.06)	0.68 (0.44-0.91)	90.32 (59.77-120.87)	0.94 ± 0.08	0.98	1.07	53.20 ± 1.86
BR9	1.11 (1.08-1.15)	247.67 (239.02-256.31)	0.87 (0.73-1.0)	192.67 (162.18-223.15)	0.92 ± 0.04	0.99	1.01	48.32 ± 5.89

BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments.  $K_{dd}$ : linear desorption distribution coefficient;  $K_{doc}$ : linear desorption coefficient normalized by organic carbon content;  $K_{fd}$ : Freundlich desorption distribution coefficient;  $K_{fdoc}$ : Freundlich desorption coefficient normalized by organic carbon content. <sup>a</sup> Number in parentheses are confidence intervals of the average ( $K_{dd}$ ,  $K_{doc}$ ,  $K_{fd}$  and  $K_{fdoc}$ ),  $n = 2$ . <sup>b</sup> Standard deviation from the mean (1/n and desorption).



BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments. The vertical and horizontal bars represent the standard deviation of the means ( $n = 2$ ) of  $C_e$  (concentration in equilibrium) and  $C_s$  (concentration in soil), respectively. Symbols can cover the bars.

**Figure 2** - Freundlich isotherms of  $^{14}\text{C}$ -saflufenacil desorption in nine Brazilian soils

In general, soils with  $H$  indices less than 1 indicate lower reversibility of sorption and, therefore, that positive hysteresis occurs, while those with indices greater than 1 have negative hysteresis, with more significant potential for desorption and, consequently, increased risk of herbicide leaching in the soil profile (Singh, Singh, 2012). Although higher  $H$  indices represent a greater desorption potential of the herbicide, this was not reflected in the decreasing order of desorption of saflufenacil in the studied soils, indicating that desorption does not depend only on  $K_{fs}$  and  $K_{ds}$  but on how the herbicide interacts on the surface of the soil. Furthermore, the mechanisms that control sorption are likely to differ for soils (Matallo et al., 2014; Paszko et al., 2016).

As for the Freundlich desorption coefficients ( $K_{fd}$ ) (Table 3), similarly to sorption, the soil with the highest OC content (BR3) had the highest value, with  $2.27 \text{ mg}^{1-1/n} \text{ kg}^{-1} \text{ L}^{1/n}$ , which represents 9.4 times more than the lowest value reported in BR1, with  $0.24 \text{ mg}^{1-1/n} \text{ kg}^{-1} \text{ L}^{1/n}$ . This behavior was maintained for  $K_d$  values, ranging from 0.42 (BR1) to  $2.21 \text{ L kg}^{-1}$  (BR3). The higher values of  $K_{fd}$  and  $K_{dd}$  in BR3 suggest a greater binding or slower release of saflufenacil from soil organic colloids and are consistent, who when evaluating the sorption and desorption of saflufenacil in six American soils, verified higher  $K_{fs}$  and  $K_{fd}$  in soil with higher OM content.

As in sorption, the values of  $K_{fdoc}$  and  $K_{doc}$  had a wide variation, in which the sand soil (BR2) (Table 1) presented the highest values, which corresponded, respectively, to 4.7 and 4.0 times more than those found in BR1, with the lowest values in the present study. In general, high concentrations

of saflufenacil, especially in soils with low sorption energy, can mean a faster return of saflufenacil to the soil solution, increasing the amount of herbicide desorbed.

The averages of the desorption percentages presented in Table 3 represent the percentage of saflufenacil desorbed (24 h after sorption) compared to the total amount sorbed in each soil type. In general, the highest percentages of saflufenacil desorption were found in soils that had the lowest sorption, with a variation of approximately between 28 and 66%. The desorption order was: BR1 > BR2 > BR8 > BR7 > BR4 > BR9 > BR6 > BR5 > BR3.

### 3.4 Mobility of saflufenacil

The  $R_f$  values were high, ranging from 0.703 (BR9) to 0.994 (BR1) (Table 4), indicating that saflufenacil has a high potential for mobility in soils, according to the classification proposed by Helling and Turner (1968), in that these authors proposed a classification system for the mobility of herbicides in soil based on the movement of 40 pesticides, using the soil TLC technique. Based on this classification, saflufenacil in BR3, BR5, BR6, and BR9 soils was classified as mobile (0.65-0.89) and BR1, BR2, BR4, BR7 BR8 soils, as very mobile (0.9-1.0).

The high  $R_f$  values between soils result from the weak sorption and high desorption of saflufenacil in the soil colloids (Tables 3 and 4). In general, the weaker the soil sorption capacity, the stronger the herbicide desorption and mobility capacity (Li et al., 2019a; Zhang et al., 2020). Polar herbicides, such as saflufenacil, have a greater affinity for the aqueous phase and, therefore,

**Table 4** - Retention factor ( $R_f$ ) and mobility potential of  $^{14}\text{C}$ -saflufenacil in nine Brazilian soils in soil TLC plates

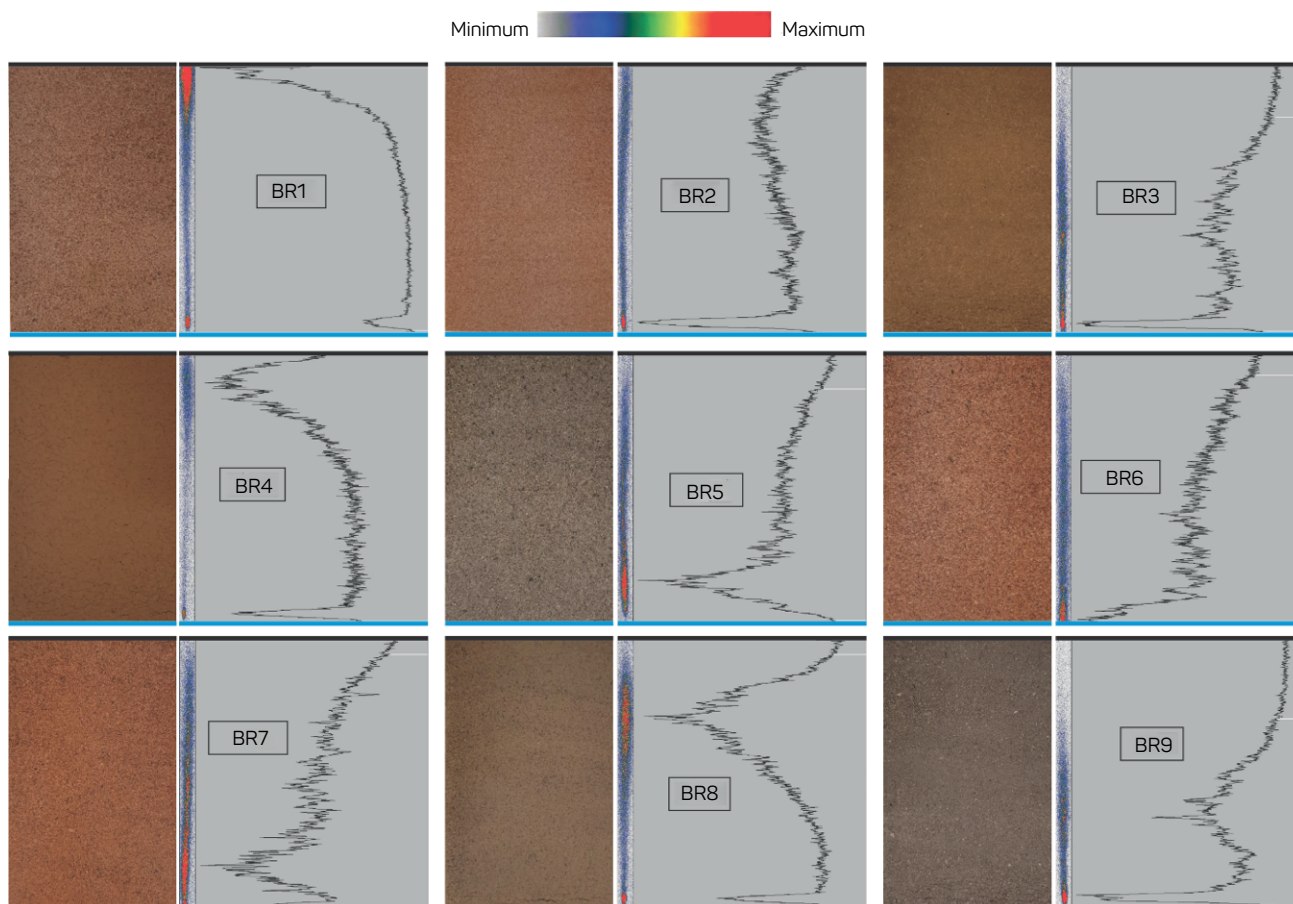
Soils	$R_f$	Mobility potential - Class <sup>b</sup>
BR1	$0.994 \pm 0.002^a$	Very mobile (5)
BR2	$0.992 \pm 0.003$	Very mobile (5)
BR3	$0.824 \pm 0.020$	Mobile (4)
BR4	$0.986 \pm 0.007$	Very mobile (5)
BR5	$0.842 \pm 0.028$	Mobile (4)
BR6	$0.895 \pm 0.030$	Mobile (4)
BR7	$0.951 \pm 0.016$	Very mobile (5)
BR8	$0.959 \pm 0.021$	Very mobile (5)
BR9	$0.703 \pm 0.005$	Mobile (4)

BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments. <sup>a</sup>Average  $\pm$  standard deviation of average ( $n = 2$ ). <sup>b</sup>According to classification by Helling and Turner (1968).

can be more easily moved from the sorption sites to the soil solution after their application, increasing their mobility potential in the soil profile (Monquero et al., 2012). These results have worrying implications regarding the risks of environmental contamination, especially from the surface and underground waters.

The mobility profile of  $^{14}\text{C}$ -saflufenacil on soil TLC plates (in one replicate) is shown in Figure 3. Colored areas on the chromatograms indicate the presence of  $^{14}\text{C}$ -saflufenacil. Blue color means lower levels of radiolabelled herbicide, while red suggests higher levels of herbicide.  $^{14}\text{C}$ -saflufenacil moved practically throughout the soil profile in most soils studied. However, in soil, BR1 has a more pronounced drag than other soils, which may reflect the higher percentage of desorption of the herbicide sorbed in the BR1 soil, resulting in a higher  $R_f$  value.

Studies carried out by Monquero et al. (2012) and Gannon et al. (2014) reported that saflufenacil has a decrease in leaching in soils with high OM contents.



BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments.

**Figure 3** - Mobility profile of  $^{14}\text{C}$ -saflufenacil in nine Brazilian soils on soil TLC plates. The image on the left shows the soil profile, and the one on the right shows the chromatogram on the left side and the  $^{14}\text{C}$ -saflufenacil mobility autoradiography on the right side after capillary elution with deionized water eluent. The blue line at the bottom of the soil TLC plates is the base of herbicide application, and the black line at the top represents the maximum vertical elution limit of the herbicide



In this present study, the results demonstrated a high mobility of saflufenacil even in soil with higher OC content, which can be explained by the weak sorption between saflufenacil and soils, which contributes to the desorption and herbicide mobility. As previously reported, the results found here suggest a high risk of contamination of surface and groundwater represented by saflufenacil even in soils with high sorption capacity. However, it is essential to highlight those factors other than soil OC, such as chemical composition (pH, CEC) and mineralogical (clay contents), play an essential role in the movement of saflufenacil (Gannon et al., 2014).

### 3.5 Main component analysis

Pearson's correlation analysis between the attributes of the nine soils studied was applied to discard the correlated properties and select those that contribute the greatest

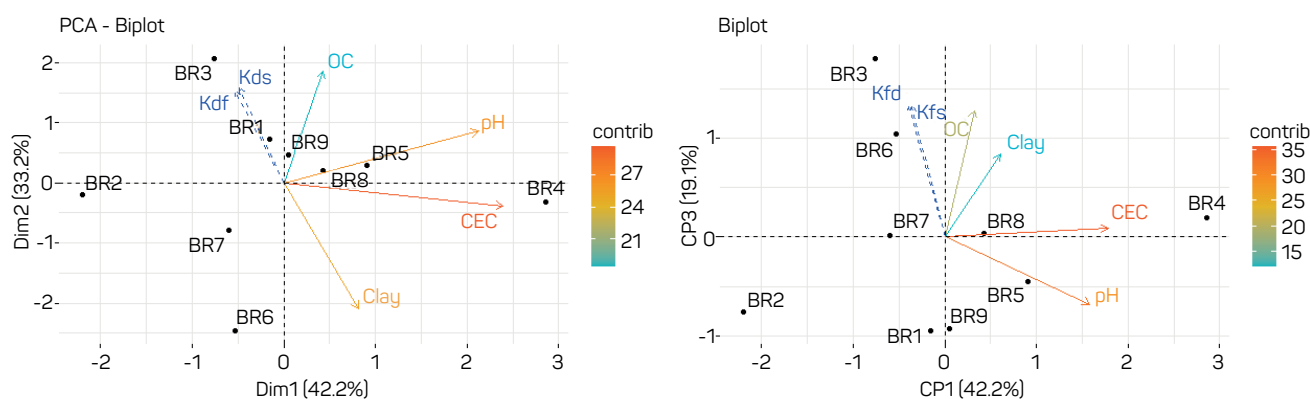
**Table 5** - Factor loadings for soil properties, Freundlich coefficient of sorption ( $K_{fs}$ ) and desorption ( $K_{fd}$ ) of <sup>14</sup>C-saflufenacil in nine soils, eigenvalues, total and accumulated variance

Variables	CP1	CP2	CP3
Dependents (supplementary)			
$K_{fs}$	0.19	0.61	-0.69
$K_{fd}$	0.21	0.59	-0.69
Independent			
pH	-0.82*	0.33	0.35
OC	-0.16	0.72*	-0.67*
CEC	-0.93*	-0.15	-0.04
Clay	-0.31	-0.81*	-0.44
Eigenvalues	1.68	1.32	0.76
Total variance (%)	42.21	33.15	19.15
Accumulated variance (%)	42.21	75.37	94.52

\* Attributes with the greatest contribution in each component. CP: main component.

differences between the soils (Table S2). This process aims to minimize multicollinearity problems between independent variables in PCA (Chagas et al., 2019; Santos et al., 2019). Based on this, the properties (independent variables) used for PCA were pH, OC, CEC, and clay (Table 5). These variables were more effective in explaining the variability of the data in this study and have already been reported to play an essential role in the sorption of weak acid herbicides such as saflufenacil (Papiernik et al., 2012; Gannon et al., 2014; Barcellos Júnior et al., 2021). Therefore, PCA was applied to visualize the interrelationship between the independent variables pH, OC, CEC, and clay and their influence on the dependent variables  $K_{fs}$  and  $K_{fd}$  (supplementary). The supplementary variables were not included during the extraction of the components. However, they were mapped and projected in Figure 4 of the factor loadings to facilitate understanding the correlation with the soil variables.

PCA reduced the number of variables studied to three components (Table 5). These three components explained 94% of the variation in the original data. In addition to reducing the number of variables that explain the variation between soils, the PCA allowed us to visualize the influence of each variable in the formation of new variables (components). In the first component (CP1), responsible for 42% of the total variation, the CEC and pH variables greatest contributions to this variance were made. In the second component (CP2), which captured 33% of the total variation, clay and OC had a greater contribution in forming the component. For the third component (CP3), which explained 23.6% of the total variation, the OC variable had the greatest influence. The relative contribution of each of these variables in the sorbent processes depends on the weathering stage and the source material of the soil (Leal et al., 2013). The soils in this study were young (high CEC) and with pH almost neutral to very weathered (low CEC) and very acidic soils, and with variability in clay content, due to essential variations in paedogenetic processes (e.g., climate) in conditions tropical (Fontes,



BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments.

**Figure 4** - Factor loadings of the dependent ( $K_{fs}$  and  $K_{fd}$ ) and independent (pH, OC, CEC, and clay) variables of the <sup>14</sup>C-saflufenacil main component analysis in nine Brazilian soils, plotted in the CP1-CP2 (A) and CP1-CP3 (B) plane

Alleoni, 2006), which explains the greater contributions of pH, CEC, and clay in the total variability. On the other hand, the smaller contribution of OC to the total variance results from the lower heterogeneity of this characteristic in soils.

The three main components were represented in the factorial plane PC1–PC2 and PC1–PC3 (Figure 4A and 4B, respectively) to identify which variables were more correlated with  $K_{fs}$  and  $K_{fd}$ . In the Figure 4A (PC1–PC2), has a high positive correlation of  $K_{fs}$  and  $K_{fd}$  with OC. On the other hand, pH, clay, and CEC were negatively correlated with  $K_{fs}$  and  $K_{fd}$ . In the PC1 – PC3 space (Figure 4B), OC and clay were positively correlated with  $K_{fs}$  and  $K_{fd}$ , while pH and CEC were negatively correlated with  $K_{fs}$  and  $K_{fd}$ . Despite the lower contribution of OC to data variability, OC was the parameter with the highest correlation with sorption (high  $K_{fs}$  values)

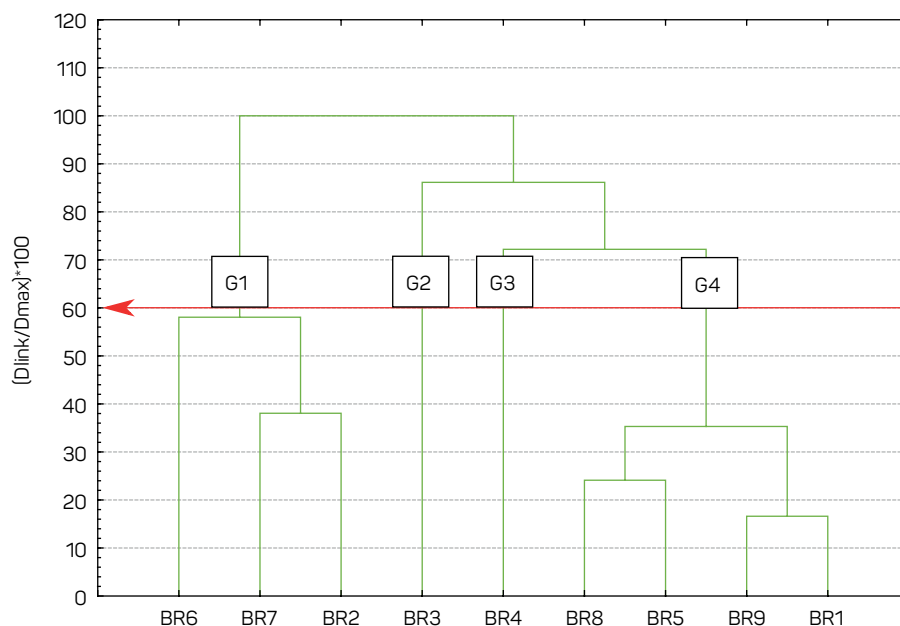
The PCA allowed discriminating the nine soils into four groups, considering the similarity of pH, CEC, clay content, and OC (Figure 5). The union of BR6, BR7, and BR2 soils in the same group is due to the lower pH values. BR3 remained isolated in one group due to its higher OC content, while the group with BR4 soil was characterized by higher pH and CEC values. In the other group, BR5, BR9, and BR2 stood out for their low clay contents.

By analysing the soil clusters with the respective  $K_{fs}$  and  $K_{fd}$  data, proximity was noted in the sorption between soil samples within the same group. Despite these results, this study focused on only nine Brazilian soils, limiting the generalizability of the findings to a broader range of soil types. It is essential to use a more significant number of soil samples to increase the correlation between groupings

and saflufenacil behaviour, generating broader and more accurate results to estimate the herbicide behavior in different types of soils (Chagas et al., 2019). The study mainly focused on saflufenacil sorption-desorption dynamics without considering other factors like microbial activity, which could influence herbicide behavior in soils.

The results of this study reveal important implications for the behavior and environmental fate of saflufenacil in soil. The findings suggest that saflufenacil application in Brazilian soils may yield diverse sorption and mobility outcomes due to the significant physicochemical variability across soils. We study highlights the potential risk of saflufenacil as a mobile pollutant in soil profiles, emphasizing the importance of considering soil properties for accurate risk assessment and decision-making in weed control strategies. This study highlights the potential risk of saflufenacil as a mobile pollutant in soil profiles, emphasizing the importance of considering soil properties for accurate risk assessment and decision-making in weed control strategies. The application of PCA, considering a more significant number of soil samples and using the variables pH, CEC, clay content, and OC, allows considering different saflufenacil dose recommendations for each soil group, as well as estimating the impact of the application of saflufenacil in soils from other regions. Undoubtedly, this would reduce the amount of physicochemical analysis of soils. It would be necessary to analyze few properties and only a tiny number of soils in each group, providing simpler, faster, and broader information for safe decision-making on the application of saflufenacil for weed control.

In general, the studied soils showed weak sorption by saflufenacil, which can be attributed to the anionic



BR1: Ultisol Typic Hapludult; BR2: Quartzipsamments; BR3: Alfisol Aqualf; BR4: Inceptisol Ochrept; BR5: Ferrohumiluvic Spodosol; BR6: Ultisol Rhodic Paleudult; BR7: Oxisol Typic Hapludox; BR8: Typic Plinthustalfs; BR9: Quartzipsamments.

**Figure 5** - Dendrogram of similarity of the nine soils in four groups, obtained from the Ward method and the Euclidean distance, as a function of the variables pH, CEC, clay content, and OC.

character of the herbicide. As a result, saflufenacil had a high potential for mobility in soils. The PCA shows that, through the variables pH, CEC, clay content, and OC, it is possible to group soil samples with similar patterns of saflufenacil sorption and generalize them to new soils. However, further investigation is needed to understand better the effects of soil properties on the behaviour and environmental fate of saflufenacil in tropical soils. For example, future investigations could focus on integrating modeling approaches that incorporate soil variability to predict saflufenacil behavior accurately in diverse soil types, aiding in decision-making for sustainable herbicide use.

#### 4. Conclusions

Saflufenacil is weakly sorbed in different types of tropical soils, and the sorption process is reversible. Its mobility varies from mobile ( $R_f = 0.703$ ) to very mobile ( $R_f = 0.994$ ), indicating that this herbicide has leaching potential in soils studied.

The sorption-desorption capacity and mobility of saflufenacil depend on the soil's physical and chemical attributes, mainly pH, CEC, clay, and OC content, and, therefore, it is vital to analyze them to predict the impacts of herbicide application on the environment. The PCA is an essential tool that helps to clarify how the effects of soil properties influence herbicide behaviour.

The OC content in Brazilian soils has a direct role in saflufenacil sorption and desorption. BR3 soil (soil with

highest organic carbon; OC = 2,1%) exhibits greater sorption ( $K_d = 1,85 \text{ L kg}^{-1}$ ), value 5.5 times greater than the BR1 (soil with lower sorption; with OC = 0,6%). Therefore, the application of saflufenacil to tropical soils, especially those with low levels of CO (< 1%), may result in a greater potential risk of contamination of surface and groundwater in neighbouring agricultural and non-agricultural areas, particularly those with intensive use and ineffectiveness of saflufenacil.

#### Author's contributions

FSO: methodology, writing original draft. VT: resources. KFM: conceptualization. VLT: supervision. TMST: methodology. BCCF and HAL: writing, review and editing. DVS: supervision and funding acquisition.

#### Acknowledgements

The authors thank the Higher Education Personnel Improvement Coordination (*Coordenação de Aperfeiçoamento de Pessoal do Ensino Superior, Brasil – Capes*).

#### Funding

This study was financed in part by the *Coordenação de Aperfeiçoamento de Pessoal do Ensino Superior, Brasil (Capes) - Finance Code 001*.

#### References

- Azcarate MP, Montoya JC, Koskinen WC. Sorption, desorption, and leaching potential of sulfonylurea herbicides in Argentinean soils. *J Environ Sci Health B*. 2015;50(4):229-37. Available from: <https://doi.org/10.1080/03601234.2015.999583>
- Badische Anilin and Soda Fabrik – BASF. Agricultural products: KIXORTM herbicide: worldwide technical brochure (GL-69288). Durham: BASF Agricultural Products Group; 2008.
- Bakhtyari S, Shirvani M, Shariatmadari H. Adsorption-desorption behavior of 2,4-D on NCP-modified bentonite and zeolite: implications for slow-release herbicide formulations. *Chemosphere*. 2013;90:699-705. Available from: <https://doi.org/10.1016/j.chemosphere.2012.09.052>
- Barbieri GF, Pigatto CS, Leães GP, Kruse ND, Agostinetto D, Ulguim AR. Physicochemical properties of soil and rates of saflufenacil in emergence and growth of soybean. *J Plant Protect Res*. 2021;61:176-82. Available from: <https://doi.org/10.24425/JPPR.2021.137026>
- Barcellos Júnior LH, Pereira GAM, Matos CC, Souza PSR, Agazzi LR, Silva EMG et al. Influence of organic matter in sorption of the saflufenacil in Ferralsols. *Bull Environ Contam Toxicol*. 2021;107:263-8. Available from: <https://doi.org/10.1007/s00128-020-02800-5>
- Budd CM, Soltani N, Robinson DE, Hooker DC, Miller RT, Sikkema PH. Control of glyphosate resistant Canada fleabane with saflufenacil plus tankmix partners in soybean. *Can J Plant Science*. 2016;96(6):989-94. Available from: <https://doi.org/10.1139/CJPS-2015-0332>
- Chagas PSF, Souza MF, Dombroski JLD, Oliveira Junior RS, Nunes GHS, Pereira GAM et al. Multivariate analysis reveals significant diuron-related changes in the soil composition of different Brazilian regions. *Sci Rep*. 2019;9(1):1-12. Available from: <https://doi.org/10.1038/s41598-019-44405-x>
- Environmental Protection Agency – EPA. Fate transport and transformation test guidelines: OPPTS 835.1210 soil thin layer chromatography. Washington: Environmental Protection Agency; 1998.
- Flessner ML, Wehtje GR, McElroy JS, Howe JA. Methiozolin sorption and mobility in sand-based root zones. *Pest Manag Sci*. 2015;71(8):1133-40. Available from: <https://doi.org/10.1002/ps.3896>
- Fontes MPF, Alleoni LRF. Electrochemical attributes and availability of nutrients, toxic elements, and heavy metals in tropical soils. *Sci Agric*. 2009;63(6):589-608. Available from: <https://doi.org/10.1590/S0103-90162006000600014>
- Gámiz B, Velarde P, Spokas KA, Celis R, Cox L. Changes in sorption and bioavailability of herbicides in soil amended with fresh and aged biochar. *Geoderma*. 2019;337:341-9. Available from: <https://doi.org/10.1016/j.geoderma.2018.09.033>

- Gannon TW, Hixson AC, Keller KE, Weber JB, Knezevic SZ, Yelverton FH. Soil properties influence saflufenacil phytotoxicity. *Weed Sci.* 2014;62(4):657-63. Available from: <https://doi.org/10.1614/WS-D-13-001711>
- Grossmann K, Hutzler J, Caspar G, Kwiatkowski J, Brommer CL. Saflufenacil (Kixor™): biokinetic properties and mechanism of selectivity of a new protoporphyrinogen IX oxidase inhibiting herbicide. *Weed Sci.* 2011;59(3):290-98. Available from: <https://doi.org/10.1614/WS-D-10-00179.1>
- Halimah M, Ismail BS, Nashriyah M, Maznah Z. Mobility studies of <sup>14</sup>C-chlorpyrifos in Malaysian oil palm soils. *Bull Environ Contam Toxicol.* 2016;96(1):120-4. Available from: <https://doi.org/10.1007/s00128-015-1685-3>
- Helling CS, Turner BC. Pesticide mobility: determination by soil thin-layer chromatography. *Science.* 1968;162(3853):562-3. Available from: <https://doi.org/10.1126/ciencia.162.3853.562>
- Hiller E, Tatarková V, Šimonovičová A, Bartal' M. Sorption, desorption, and degradation of [4-chloro-2-methylphenoxy] acetic acid in representative soils of the Danubian Lowland, Slovakia. *Chemosphere.* 2012;87(5):437-44. Available from: <https://doi.org/10.1016/j.chemosphere.2011.12.021>
- International Union of Pure and Applied Chemistry – IUPAC. Pesticide properties database. Zurich: International Union of Pure and Applied Chemistry; 2021[access Feb 15, 2021]. Available from: <https://sitem.herts.ac.uk/aeru/ppdb/en/Reports/1244.htm>
- Kah M, Brown CD. Adsorption of ionisable pesticides in soils. In: Kah M, Brown CD organizers. *Reviews of environmental contamination and toxicology.* Berlin: Springer; 2006. p.149-217. Available from: [https://doi.org/10.1007/978-0-387-32964-2\\_5](https://doi.org/10.1007/978-0-387-32964-2_5)
- Kah M, Sigmund G, Xiao F, Hofmann T. Sorption of ionizable and ionic organic compounds to biochar, activated carbon and other carbonaceous materials. *Water Res.* 2017;124:673-92. Available from: <https://doi.org/10.1016/j.watres.2017.07.070>
- Kumar N, Mukherjee I, Varghese E. Adsorption-desorption of tricyclazole: effect of soil types and organic matter. *Environ Monit Assess.* 2015;187(3):1-10. Available from: <https://doi.org/10.1007/s10661-015-4280-5>
- Leal RM, Alleoni LR, Tornisielo VL, Regitano JB. Sorption of fluoroquinolones and sulfonamides in 13 Brazilian soils. *Chemosphere.* 2013;92(8):979-85. Available from: <https://doi.org/10.1016/j.chemosphere.2013.03.018>
- Li W, Zhang Y, Jia H, Zhou W, Li B, Huang H. Adsorption-desorption and leaching behaviors of tetraniliprole in three typical soils of China. *Bull Environ Contam Toxicol.* 2019a;103(4):623-9. Available from: <https://doi.org/10.1007/s00128-019-02688-w>
- Li X, Grey T, Price K, Vencill, W, Webster T. Adsorption, desorption, and persistence of fomesafen in soil. *Pest Manag Sci.* 2019b;75(1):270-8. Available from: <https://doi.org/10.1002/ps.5112>
- Limousin G, Gaudet JP, Charlet L, Szenknect S, Barthès V, Krimissa M. Sorption isotherms: a review on physical bases, modeling, and measurement. *App Geochem.* 2007;22:249-75. Available from: <https://doi.org/10.1016/j.apgeochem.2006.09.010>
- Liu X, Wu H, Hu T, Chen X, Ding X. Adsorption and leaching of novel fungicide pyraoxystrobin on soils by <sup>14</sup>C tracing method. *Environ Monit Assess.* 2018;190(2):1-10. Available from: <https://doi.org/10.1007/s10661-017-6458-5>
- Marín-Benito JM, Sánchez-Martín MJ, Ordax JM, Draoui K, Azejjel H, Rodríguez-Cruz MS. Organic sorbents as barriers to decrease the mobility of herbicides in soils. Modelling of the leaching process. *Geoderma.* 2018;313:205-16. Available from: <https://doi.org/10.1016/j.geoderma.2017.10.033>
- Martins EC, Melo VF, Bohone JB, Abate G. Sorption and desorption of atrazine on soils: the effect of different soil fractions. *Geoderma.* 2018;322:131-39. Available from: <https://doi.org/https://doi.org/10.1016/j.geoderma.2018.02.028>
- Marinho ACCS, Portela JC, Silva EF, Dias NS, Sousa Júnior FS, Silva AC, Silva JF. Organic matter, and physicochemical attributes of a cambisol under different agricultural uses in a semi-arid region of Brazil. *Austr J Crop Sci.* 2016;10(1):32-41.
- Matallo MB, Franco DAS, Almeida SDB, Cerdeira AL. Sorption and desorption of saflufenacil in two soils in the state of São Paulo with different physical and chemical attributes. *Planta Daninha.* 2014;32(2):393-9. Available from: <https://doi.org/10.1590/S0100-83582014000200017>
- Mehdizadeh M, Mushtaq W, Siddiqui SA, Ayadi S, Kaur P, Yeboah S et al. Herbicide residues in agroecosystems: fate, detection, and effect on non-target plants. *Rev Agric Sci.* 2021;9:157-67. Available from: [https://doi.org/10.7831/ras.9.0\\_157](https://doi.org/10.7831/ras.9.0_157)
- Mendes KF, Olivatto GP, Sousa RN, Junqueira LV, Tornisielo VL. Natural biochar effect on sorption-desorption and mobility of diclosulam and pendimethalin in soil. *Geoderma.* 2019b;347:118-25. Available from: <https://doi.org/10.1016/j.geoderma.2019.03.038>
- Mendes KF, Sousa RN, Takeshita V, Alonso FG, Régio APJ, Tornisielo VL. Cow bone char as a sorbent to increase sorption and decrease mobility of hexazinone, metribuzin, and quinclorac in soil. *Geoderma.* 2019a;343:40-9. Available from: <https://doi.org/10.1016/j.geoderma.2019.02.009>
- Monqueiro PA, Sabbag R, Orzari I, Hijano N, Galvani Filho M, Dallacosta V et al. [Saflufenacil and residual leaching after drought periods]. *Planta Daninha.* 2012;30(2):415-23. Portuguese. Available from: <https://doi.org/10.1590/S0100-83582012000200022>
- OECD - Organization for Economic Co-operation and Development. OECD Guidelines for the Testing of Chemicals: Test Number 106, Adsorption – Desorption Using a Batch Equilibrium Method, OECD: Paris, p. 44; 2000. Available from: [chromeextension://efaidnbmnnnibpca-pjpcgclefndmkaj/https://archive.epa.gov/scipoly/sap/meetings/web/pdf/106\\_adsorption\\_desorption\\_using.pdf](chromeextension://efaidnbmnnnibpca-pjpcgclefndmkaj/https://archive.epa.gov/scipoly/sap/meetings/web/pdf/106_adsorption_desorption_using.pdf)
- Papiernik SK, Koskinen WC, Barber BL. Low sorption, and fast dissipation of the herbicide saflufenacil in surface soils and subsoils of an eroded prairie landscape. *J Agric Food Chem.* 2012;60(44):10936-41. Available from: <https://doi.org/10.1021/jf303271p>



Paszko T, Muszyński P, Materska M, Bojanowska M, Kostecka M, Jackowska I. Adsorption and degradation of phenoxyalkanoic acid herbicides in soils: a review. *Environ Toxicol Chem*. 2016;35(2):271-86. Available from: <https://doi.org/10.1002/etc.3212>

Raimi MO, Vivien OT, Alima O, Akpojubaro EH, Williams EA. Articulating the effect of pesticides use and sustainable development goals (SDGs): the science of improving lives through decision impacts. *Res World Agric Econ*. 2021;2(1):1-8. Available from: <https://doi.org/10.36956/RWAE.V2I1.347>

Santos LOG, Souza MF, Chagas PSF, Teófilo TMS, Formiga MAP, Me-deiros RCA et al. Multivariate analysis, and multiple linear regression as a tool to estimate the behavior of hexazinone in Brazilian soils. *Environ Monit Assess*. 2019;191:1-11. Available from: <https://doi.org/10.1007/s10661-019-7893-2>

Singh N, Singh SB. Sorption-desorption behavior of metsulfuron-methyl and sulfosulfuron in soils. *J Environ Sci Health B*. 2012;47(3):168-74. Available from: <https://doi.org/10.1080/03601234.2012.632262>

Yavari S, Sapari NB, Malakahmad A, Razali MAB, Gervais TS, Yavari S. Adsorption-desorption behavior of polar imidazolinone herbicides in tropical paddy fields soils. *Bull Environ Contam Toxicol*. 2020;104:121-7. Available from: <https://doi.org/10.1007/s00128-019-02759-y>

Yue L, Ge C, Feng D, Yu H, Deng H, Fu B. Adsorption-desorption behavior of atrazine on agricultural soils in China. *J Environ Sci*. 2017;57:180-9. Available from: <https://doi.org/10.1016/j.jjes.2016.11.002>

Zhang Y, Li W, Zhou W, Jia H, Li B. Adsorption-desorption characteristics of pyraclonil in eight agricultural soils. *J Soils Sediments*. 2020;20(3):1404-12. Available from: <https://doi.org/10.1007/s11368-019-02471-8>