ISSN: 2447-3359

REVISTA DE GEOCIÊNCIAS DO NORDESTE

Northeast Geosciences Journal

v. 10, nº 2 (2024)

https://doi.org/10.21680/2447-3359.2024v10n2ID36743

Contamination of water resources by pesticides used in commodities: assessment through simulation models

Contaminação dos recursos hídricos por agrotóxicos utilizados em commodities: avaliação por modelos de simulação

Joseph Simões Ribeiro[1]; Suellen Caroline Barbosa Neves[2]; Lizandra Ferreira Lameira[3]; Milene Karoline da Silva Galúcio[4]; Ygor Yuri Pereira da Silva[5]; Elcilene Mateus da Cruz [6] ;Ruy Bessa Lopes[7]

1 Universidade Federal do Oeste do Pará, Campus Tapajós/PPGSND, Santarém/PA, Brasil. Email: josephribeiro_@hotmail.com
ORCID: https://orcid.org/ https://orcid.org/0000-0001-9715-816X

2 Universidade Federal do Oeste do Pará, Campus Tapajós/PPG Biociências, Santarém/PA, Brasil. Email: scambiente@hotmail.com
ORCID: https://orcid.org/ https://orcid.org/0000-0002-0221-6855

3 Universidade Federal do Oeste do Pará, Campus Tapajós/ICTA, Santarém/PA, Brasil. Email: lizandraferreirlameir@hotmail.com
ORCID: https://orcid.org/ https://orcid.org/0000-0002-7442-5824

4 Universidade Federal do Oeste do Pará, Campus Tapajós/ICTA, Santarém/PA, Brasil. Email: milenekarol@gmail.com
ORCID: https://orcid.org/ https://orcid.org/0009-0007-5484-1795

5 Secretaria de Estado de Saúde Pública do Pará, 7°CRS/VISAMB, Belém/PA, Brasil. Email: yurisilvaa@hotmail.com
ORCID: https://orcid.org/0009-0003-1658-3079

6 Universidade Federal do Oeste do Pará, Campus Rondon, PROFMAT, Santarém/Pará, Brasil. Email: elcy.mta@gmail.com
ORCID: https://orcid.org/0009-0006-0308-5857

7 Universidade Federal do Oeste do Pará, Campus Tapajós/ICTA, Santarém/PA, Brasil. Email: ruybessa@yahoo.com.br
ORCID: https://orcid.org/0000-0002-4806-8835

Abstract: The aim of this study was to assess the impacts of the main pesticides used in monocultures in the Curuá-Una River Basin, using mathematical models, identifying the areas most susceptible to contamination. Five pesticides were selected: Glyphosate, Cypermethrin, Teflubenzuron, Chlorpyrifos and Methomyl. The models applied were the GUS Index, LEACH, SCI-GROW and the Curve Number Parameter, the latter aimed at assessing the risk in each area. The results indicated that Glyphosate and Methomyl have the greatest potential to contaminate surface and groundwater resources, while Cypermethrin, Teflubenzuron and Chlorpyrifos showed low mobility and lower risk to aquifers. Glyphosate and Chlorpyrifos showed residue concentrations of 117 and 0.109 µg/L in groundwater, respectively. The LEACH index indicated a high risk of surface water contamination for Glyphosate and Teflubenzuron. Based on the Curve Number Parameter, 97% of the basin area is susceptible to groundwater contamination by Glyphosate and Methomyl, while only 3% is at risk of surface water contamination. This data is fundamental for planning water resource monitoring programs and assessing environmental impacts, providing an efficient and cost-effective tool.

Keywords: Pesticides; Mathematical models; Water contamination.

Resumo: O objetivo deste estudo foi avaliar os impactos dos principais agrotóxicos utilizados em monocultivos na Bacia do Rio Curuá-Una, por meio de modelos matemáticos, identificando as áreas mais suscetíveis à contaminação. Foram selecionados cinco agrotóxicos: Glifosato, Cipermetrina, Teflubenzuron, Clorpirifos e Metomil. Os modelos aplicados foram o Índice de GUS, LEACH, SCI-GROW e o Parâmetro de Curve Number, este último visando avaliar o risco em cada área. Os resultados indicaram que Glifosato e Metomil apresentam maior potencial de contaminação de recursos hídricos superficiais e subterrâneos, enquanto Cipermetrina, Teflubenzuron e Clorpirifos mostraram baixa mobilidade e menor risco para os aquíferos. Glifosato e Clorpirifos apresentaram concentrações de resíduos de 117 e 0,109 µg/L em águas subterrâneas, respectivamente. O índice LEACH indicou alto risco de contaminação de águas superficiais para Glifosato e Teflubenzuron. Com base no Parâmetro de Curve Number, 97% da área da bacia é suscetível à contaminação do lençol freático por Glifosato e Metomil, enquanto apenas 3% apresenta risco de contaminação de águas superficiais. Esses dados são fundamentais para o planejamento de programas de monitoramento de recursos hídricos e avaliação de impactos ambientais, fornecendo uma ferramenta eficiente e econômica.

Palavras-chave: Pesticidas; Modelos matemáticos; Contaminação hídrica.

Recebido: 24/06/2024; Aceito: 26/08/2024; Publicado: 28/11/2024.

1. Introduction

Currently, agriculture is the leading sector of the Brazilian economy and relies heavily on inputs like pesticides to combat crop pests (IASCO-PEREIRA; LIBÂNIO, 2023). Since 2008, Brazil has held the position of the world's largest consumer of pesticides, with the main products used commercially on crops belonging to the classes of insecticides and herbicides (BOMBARDI, 2017; LONDRES, 2012).

In the State of Pará, specifically in the Western Region, agricultural activities have significantly expanded over the last 10 years, particularly in three cities: Santarém, Belterra, and Mojuí dos Campos. These cities produce 11% of the state’s soybeans, which has led to an increase in pesticide use on the crops (RIBEIRO, 2017). The intensive use of these compounds can lead to the contamination of water resources and potential harm to public health. It is estimated that only one-third of the applied pesticide reaches the target population, while the rest is dispersed into environmental compartments such as water and sediment, regardless of the application method (CHAIM et al., 1999; LOURENCETTI et al., 2005; RIBEIRO et al., 2007).

In the State of Pará, this issue currently affects the Western Region, particularly the municipalities of Santarém, Belterra, and Mojuí dos Campos, which have become prominent due to the expansion of the agricultural frontier in the late 1990s and early 2000s. (RIBEIRO, 2021). The intense occupation of land, driven by mechanized grain farming—primarily soybeans and corn—is the main activity responsible for this expansion (SOUMIS; ROULET; LUCOTTE, 2000).

The problem is further exacerbated by the fact that these municipalities are located in an area with abundant surface water resources and an extensive hydrographic network, divided into six basins: the Amazon River, the Tapajós River, the Arapiuns River, the Moju, Mojuí, and Curuá-Una Rivers, in addition to a large number of drainage basins throughout the surrounding area, highlighting the region's wealth in water resources.

Furthermore, the region is located above one of the largest aquifers in the world. According to Nascimento-Gaya (2022), the Alter do Chão Aquifer covers an area of 437,500 km². This aquifer is classified as a mixed type, with an unconfined upper part at a depth of 20 to 50 meters and a confined lower part at 430 meters (PENA, 2015). It consists of sedimentary rocks, such as siltstone and sandstone, which facilitate the movement of pesticides through the soil.

To preliminarily assess these potential contaminations, simplified predictive models such as the *Groundwater Ubiquity Score* (GUS) (WAUCHOPE et al., 1992), LEACH (BATCHELOR, 1990; PAPA et al., 2004), and Screening Concentration in GroundWater -SCI-GROW (USEPA, 2003) can be used.

These mathematical models use the physicochemical properties of molecules to predict their mobility, contamination potential, and concentration in groundwater and surface water (JUNG et al., 2024). They serve as complementary tools in environmental assessment and are economically viable for the preliminary investigation of the contamination potential of water resources, especially since quantifying these compounds involves complex and costly analytical methods..

The main aim of this study was to carry out a preliminary investigation into the potential for contamination of water resources by the five pesticides most commonly used in soya cultivation in three municipalities in the west of Pará, in an attempt to pinpoint the potential risks for each area.

2. Methodology

2.1 Field site

This study was carried in the Western Region of the state of Pará and comprises three cities: Belterra, Mojuí dos Campos, and Santarém. Together, these cities cover an area of 27,285.043 km², bordering the municipalities of Medicilândia, Aveiro, Placas, Uruará, Jurutí, Prainha, Monte Alegre, Alenquer, Curuá, and Óbidos (Figure 1) (IBGE, 2023). The municipalities in the study area are bordered by the Curuá-Una River, which has a total drainage area of approximately 37,300 km². This river covers both municipalities, with its drainage areas surrounded by agricultural activities (JOÃO; TEIXEIRA; FONSECA, 2013; RIBEIRO, 2021).

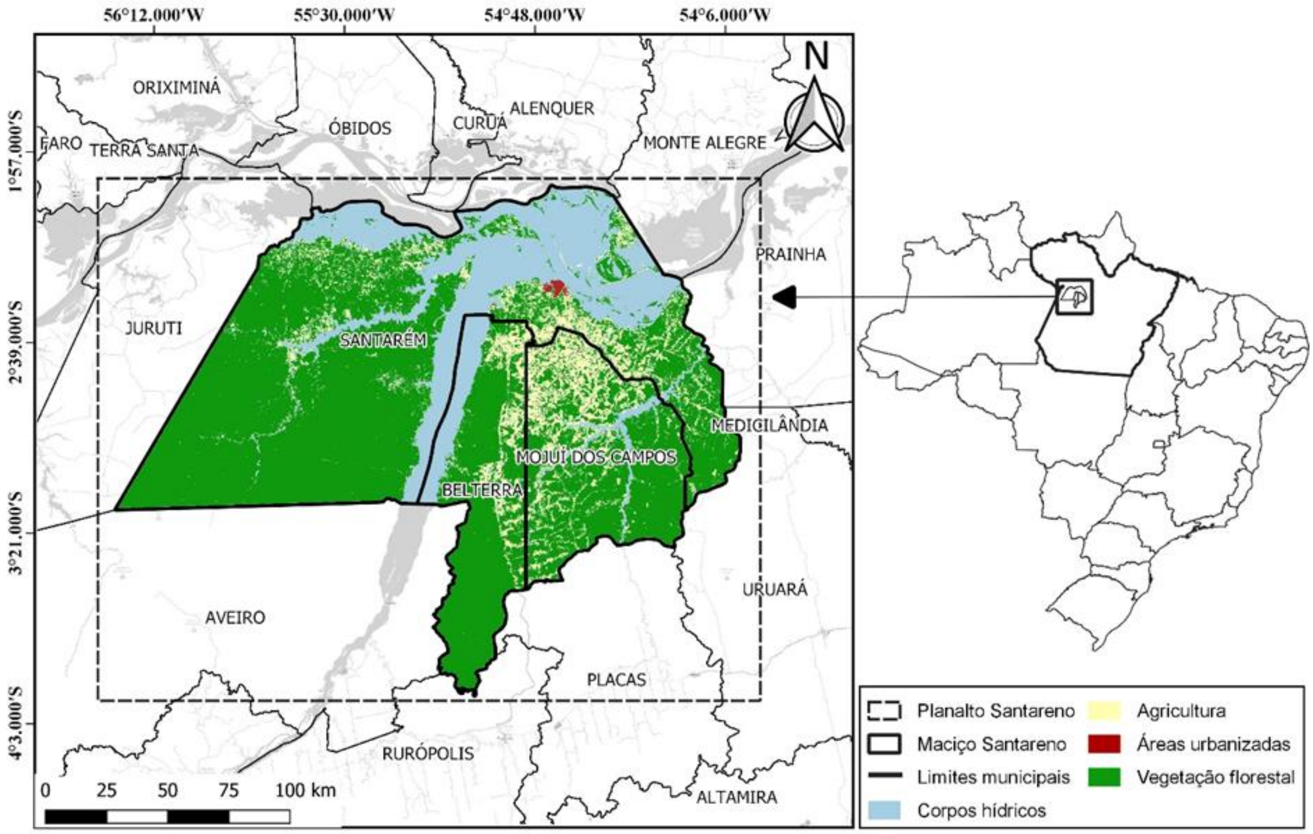

Figure 1 – Map showing the location of the studied municipalities.
Source: Elaborated by the authors (2024).

2.2 Hydrological contextualization

2.2.1 Groundwater

The region within the territorial boundaries encompasses the Alter do Chão Formation zone, which is primarily composed of siliciclastic deposits from the Alter do Chão Formation, associated with alluvial and lateritic deposits (SILVA; DESCOVI FILHO, 2023). The thickness of the exposed stratigraphic unit varies between 100 and 500 meters, and it is a porous aquifer with an exposed hydrolithological unit of the granular type 1. This formation covers the entire Amazon Sedimentary Basin (CUNHA; MELO; SILVA, 2007; JOÃO; TEIXEIRA; FONSECA, 2013).

According to the Brazilian Geological Survey, the hydrogeological system of the Alter do Chão Formation consists of two types of aquifers: a more superficial, unconfined aquifer with a thickness of around 50 meters, and a confined aquifer with an average thickness of 430 meters (JOÃO; TEIXEIRA; FONSECA, 2013). Less deep and unconfined areas are at a higher risk of contaminant infiltration compared to confined areas.

2.2.2 Surface water

For surface waters, the greatest risk comes from surface runoff into water bodies. The region has Dystrophic Yellow Latosols, which are deep soils (100 to 200 cm) with moderate infiltration rates, resistance, and tolerance to erosion. These soils are porous, with a textural gradient ranging from 1.20 to 1.50, and have a sandy or medium texture throughout the profile (SARTORI; LOMBARDI NETO; GENOVEZ, 2005).

According to Sartori, Lombardi Neto, and Genovez (2005), this type of soil has a moderate surface runoff rate. However, depending on land use and occupation, the soil can become impermeable, leading to the runoff of contaminants adsorbed onto organic matter, making it a more vulnerable area to chemical contamination (JATI; SILVA, 2017).

2.3 Survey of pesticides

To gather information on pesticide use, agronomic prescriptions issued between 2013 and 2017 by the Agricultural Defense Agency of the State of Pará (Agência de Defesa Agropecuária do Estado do Pará - ADEPARA) were analyzed. A second approach involved consulting agronomists working in the region, combined with presenting a preliminary list, compiled from information obtained from local retailers and ADEPARA, to identify the five most commonly used pesticides in soybean cultivation in the region.

The following products were identified: Roundup Original (Glyphosate), Cyptrin 250 CE (Cypermethrin), Dimilin (Teflubenzuron), Lorsban (Chlorpyrifos), and Lannate (Methomyl). The selection was also based on the volume sold, their relevance in the literature, and the physical and chemical properties of these compounds (LEWIS et al., 2016).

2.4 Mathematical models

2.4.1 GUS index

To assess the potential for groundwater contamination by pesticides, the simplified predictive model Groundwater Ubiquity Score (GUS) was used. This model predicts the mobility of a toxic compound infiltrating the soil and its likelihood of contaminating groundwater (WAUCHOPE et al., 1992).

$$GUS = log10\left(t_{1/2}\ solo\right)\ x\ [4 - log10(koc)] \quad \text{(Eq. 1)}$$

Where $t_{1/2}$ is the half-life of the compound in the soil (days) and Koc is the organic carbon partition coefficient ($mL.g^{-1}$). According to Dores and De-Lamonica-Freire et al. (2001), once this index is identified, pesticides are classified based on their tendency to leach into the subsurface domain, according to the following ranges (Table 1).

Table 1 – Groundwater Contamination Risk Classification According to the GUS Index.

GUS Index Classification Scale	
GUS < 1,8	Non-Leaching (NL)
1,8 < GUS ≤ 2,8	Transition Range (T)
GUS > 2,8	Leaching (L)

Source: Elaborated by the authors (2024).

2.4.2 LEACH Index

The LEACH index (Batchelor, 1990) describes the movement and pollution potential for surface waters.

$$LEACH = \left(SA\ x\ t_{1/2}\right) x\ (Pv\ x\ Koc) \quad \text{(Eq. 2)}$$

Where SA is the water solubility ($mg.L^{-1}$), Pv is the vapor pressure (MPa), and Koc is the organic matter adsorption coefficient ($mg.L^{-1}$). The interpretation of the results can be seen in Table 2.

Table 2 – Surface Water Contamination Risk Classification According to the LEACH Index.

LEACH Index Classification Scale	
LEACH <3	Low
3 LEACH ≤ 7	Medium
LEACH >7	High

Source: Elaborated by the authors (2024).

The lower the LEACH value, the lower the risk of contamination. These values are expressed on a logarithmic scale to allow for comparison with other indices.

2.4.3 Screening Concentration In Ground Water SCI-GROW

The SCI-GROW software - Screening Concentration In Ground Water (USEPA, 2003), estimates pesticide concentrations in groundwater, but only for regions where the water table is susceptible to pollution (LAUREANO et al., 2020). This susceptibility is mainly determined by the depth and whether the aquifer is confined or not (JOÃO; TEIXEIRA; FONSECA, 2013)..

These models use the physicochemical properties of molecules to predict contamination potential. For each active ingredient, the physical, chemical, and ecotoxicological characteristics were obtained from specialized databases like the PPDB: *Pesticide Properties Database* (UNIVERSITY OF HERTFORDSHIRE,2018), *Fate Pointers* (SRC,2018).

2.4.4 Curve Number Parameter

To assess the areas of highest risk, we used the Curve Number (CN) parameter method. The SCS-CN methodology classifies soils into four main groups based on their infiltration capacity and surface runoff generation, categorized as A, B, C, or D, with a progressive increase in runoff from A to D.

The soil hydrological groups were defined based on the reclassification of the soil map, following the guidelines established by Sartori, Lombardi Neto, and Genovez (2005), which are summarized in Table 2.

Table 3 – Hydrological classification of the soil for Brazilian conditions.

Group	Soil characteristics	Tipos de solo
A	Very deep soils (> 200 cm) with a high infiltration rate, resistance and tolerance to erosion, porous soils with a low textural gradient (< 1.20), medium texture, and well-drained or excessively drained soils.	Yellow Latosol, Red-Yellow Latosol, Red Latosol, all with clayey or very clayey textures and high macroporosity; Yellow Latosol and Red-Yellow Latosol, both with medium texture but without a sandy surface horizon.
B	Deep soils (100 to 200 cm) with a moderate infiltration rate, resistance and tolerance to erosion, porous soils with a textural gradient ranging from 1.20 to 1.50, and sandy or medium texture throughout the profile.	Yellow Latosol and Red-Yellow Latosol, both with medium texture but with a sandy surface horizon; Bruno Latosol; Red Nitisol; Quartzarenic Neosol; Red or Red-Yellow Argisol with sandy/medium, medium/clayey, clayey/clayey, or clayey/very clayey textures that do not exhibit abrupt textural changes.
C	Deep soils (100 to 200 cm) or shallow soils (50 to 100 cm) with low infiltration rates and low resistance to erosion. These soils have a textural gradient greater than 1.50 and are associated with low-activity clay.	Shallow Argissol without an abrupt textural change or Red Argissol, Red-Yellow Argissol, and Yellow Argissol, all deep with an abrupt textural change; Medium-textured Cambisol and Haplic or Humic Cambisol with physical characteristics similar to Latosols (latosolic); Ferrocárbic Spodosol; Fluvic Neosol.
D	Soils with very low infiltration rates offering minimal resistance to erosion, shallow soils (< 50 cm), shallow soils associated with abrupt textural changes, clayey soils associated with high-activity clay , and organic soils.	Litholic Neosol; Organosol; Gleysol; Chernozem; Planosol; Vertisol; Alisol; Luvisol; Plinthosol; mangrove soils; rock outcrops; Cambisols that do not fall into Group C; shallow Red-Yellow Argisol and Yellow Argisol, both associated with abrupt textural changes.

Source: Sartori, Lombardi Neto e Genovez (2005).

The SCS-CN model determines surface runoff using the following equations (USDA, 1986):

$$Q = \frac{(P - Ia)^2}{P - Ia + S} \quad \text{Eq. 3}$$

$$Ia = \frac{S}{5} \quad \text{Eq. 4}$$

$$Q = \frac{25400}{CN} - 254 \quad \text{Eq. 5}$$

Where:
Q = Surface Runoff (mm)
P = Precipitation (mm)
Ia = Initial Losses (mm)
S = Storage Parameter (mm)

The interpretation of the result is based on the variation of values, with CN values being dimensionless parameters that range from 0 to 100. High CN values, close to 100, represent a limiting condition of a completely impervious watershed, with a retention rate equal to zero (ANJINHO et al., 2018). A low CN, close to zero, indicates a high water infiltration rate, representing highly permeable watersheds, and high values where there is no surface runoff regardless of the accumulated rainfall.

Os valores de CN estabelecidos a partir da integração dos mapas de uso do solo de com o mapa de grupos hidrológicos, com base em valores estabelecidos pelo SCS (USDA, 1986) vistos na Tabela 4.

Table 4 – Classification of CN Classes.

CN Class	Classification
36 - 47 47- 57 57 – 68	Greater infiltration potential
68 – 79 79 - 89 89 - 100	Greater surface runoff potential

Fonte: Modified from USDA (1986).

2.5 Spatial Data Collection

The spatial data on land use and land cover in this study were obtained from the Mapbiomas platform, using data from the year 2022 (SOUZA et al., 2020). The information on soil types in the region was obtained from the EMBRAPA database, developed according to the new Brazilian Soil Classification System (EMBRAPA, 2014).

The Digital Terrain Model (DTM) used for watershed delineation was ANADEM, which corrected the vegetation bias in the Copernicus GLO-30 digital elevation model (DEM), with a spatial resolution of 30 meters (LAIPELT et al., 2024). For the assessment of land use and land cover accuracy and distance measurements from risk zones, Planet NICFI satellite images from August 2024 were used (PLANET LABS, 2024).

All cartographic information was analyzed in a Geographic Information System (GIS) using QGIS 3.38.11 software. In this study, the Universal Transverse Mercator (UTM) projection and the SIRGAS 2000/Brazil Polyconic reference system (EPSG: 5880) were adopted to facilitate metric calculations, as the study area is located between two UTM zones (21 and 22S).

3. Results and discussion

3.1 Mathematical models for predicting the risk of surface and groundwater contamination

For the use of SCI-GROW, the input parameters for the program were: active ingredient name, application rate (pounds per acre), number of applications per crop cycle, where label data were presented in liters and had to be converted to pounds, Koc, and soil half-life as shown in Table 5.

Table 5 – Input Parameters for the SCI-GROW Program..

Composto	**Litres(hectare)**	**Pounds (hectare)**	**N°. of Applications**	***Koc*(mg.L^{-1})**	***t ½ soil* (days)**
Roundup original (Glyphosate)	4	8,82	2	1424	96
Cyptrin (Cypermethrin)	0,10	0,22	2	307558	85
Dimilin (Teflubenzuron)	0,14	0,31	2	26062	92
Lorsban (Chlorpyrifos)	1	2,2	2	5509	175
Lannate (Methomyl)	6	13,23	2	72	46

Koc *- soil organic matter adsorption coefficient.* $t_{1/2}$ *- time required for chemical or physical degradation to remove half of the substance from the environment.*
Source: Created by the authors (2024).

The calculated results for the GUS, LEACH, and SCI-GROW indices can be observed in Table 6, which also includes risk data for surface and groundwater.

Table 6 presents a detailed analysis of the risk of water resource contamination by five commonly used agricultural compounds, utilizing three different prediction models: GUS, LEACH, and SCI-GROW. Additionally, the table indicates the Potential Risk for Surface Water (PRSW) and Potential Risk for Groundwater (PRGW) associated with each compound.

Roundup Original (Glyphosate)

- GUS: Glyphosate exhibited a GUS value of 0.32, indicating that it does not undergo significant leaching, as reflected by its "NL" (Non-Leaching) classification.
- LEACH: In the LEACH model, glyphosate showed a high risk of surface water contamination, with a value of 9.172.
- SCI-GROW: Its estimated concentration in groundwater was high, reaching 117 µg/L, which represents a significant risk to this type of resource.
- PRSW/PRGW: The combination of these factors results in a high risk of contamination for surface waters (H) and a medium risk for groundwater (M)

Cyptrin 250 CE (Cypermethrin)

- GUS: Cypermethrin had a GUS value of -2.3, indicating that it does not undergo leaching (NL).
- LEACH: In the LEACH model, the risk of surface water contamination was classified as low, with a value of 2.851.
- SCI-GROW: No concentrations of cypermethrin were detected in groundwater (ND), suggesting a low risk of contamination.
- PRSW/PRGW: These results indicate a moderate risk for surface waters (M) and a low risk for groundwater (L).

Dimilin (Teflubenzuron)

- GUS: Teflubenzuron was also classified as non-leaching, with a GUS value of -1.15.
- LEACH: It presented a moderate risk in the LEACH model, with a value of 7.861, indicating a significant potential for surface water contamination.
- SCI-GROW: No concentrations of this compound were detected in groundwater (ND).
- PRSW/PRGW: The risk was classified as moderate for surface waters (M) and low for groundwater (L).

Lorsban (Chlorpyrifos)

- GUS: Chlorpyrifos had a very low GUS value (0.01), indicating that it does not undergo leaching (NL).
- LEACH: It presented a low risk in the LEACH model, with a value of 2.989.
- SCI-GROW: The estimated concentration in groundwater was very low (0.109 µg/L), indicating a low risk.
- PRSW/PRGW: The risk was classified as low for both surface waters (L) and groundwater (L).

Lannate (Methomyl)

- GUS: Methomyl was classified as highly leaching, with a GUS value of 3.56.
- LEACH: In the LEACH model, it presented a high risk for surface waters, with a value of 8.836.
- SCI-GROW: The concentration in groundwater was estimated at 17.2 µg/L, indicating a high risk.
- PRSW/PRGW: Due to these factors, methomyl was classified as high risk for both surface waters (H) and groundwater (H).

The data presented in Table 6 indicate that among the compounds analyzed, methomyl poses the highest risk of contamination for both surface and groundwater, being classified as highly mobile and leaching. This compound warrants special attention due to its significant potential for environmental impact.

Glyphosate, conversely, also shows a considerable risk to surface waters, although its impact on groundwater is more limited. Despite being classified as "non-leaching" by the GUS index, the high estimated concentration in groundwater, according to the SCI-GROW model, suggests the need for rigorous monitoring.

Conversely, cypermethrin, teflubenzuron, and chlorpyrifos showed low risks of groundwater contamination according to the GUS and SCI-GROW models. However, it is important to note that both teflubenzuron and chlorpyrifos may pose a moderate to high risk for surface water contamination, according to the LEACH model. This indicates that these substances can still be a concern for water quality, especially in areas where their use is intensive.

Table 6 – Risk of water resource contamination according to each prediction model.

Composto	**GUS**	**LEACH**	**SCI-GROW (ug.L^{-1})**	**PRSW**	**PRGW**
Roundup original (Glyphosate)	0,32/ NL	9,172	117	H	M
Cyptrin 250 CE (Cypermethrin)	-2,3/ NL	2,851	ND	M	L
Dimilin (Teflubenzuron)	-1,15/ NL	7,861	ND	M	L
Lorsban (Chlorpyrifos)	0,01/ NL	2,989	0,109	L	L
Lannate (Methomyl)	3,56/ LE	8,836	17,2	H	H

NL *- Non-Leaching;* ***LE****- Leaching.* ***PRSW*** *- risco para águas superficiais* ***PRGW****- risco para águas subterrâneas.* ***ND*** *– Not detected.* ***A*** *- High;* ***M*** *– Moderate;* ***B*** *– Low.*
Fonte: Created by the authors (2024).

3.2 *Curve Number* parameters for predicting risk areas

To assess the risks to the Curuá-Uma basin, it is essential to consider land use, soil type, and terrain slope. Analyzing land use and occupation is paramount in this context. As illustrated in Figure 2, about 26% of the basin area is dedicated to agriculture, with livestock farming and the monoculture of soybeans and corn being the main activities utilizing pesticides. The native forest occupies 66% of the basin, predominantly in more remote areas less impacted by human activity. These areas are crucial for maintaining biodiversity, regulating the hydrological cycle, and protecting soils from erosion, as well as preserving water bodies, as discussed by Aguiar, Peleja, and Sousa (2014).

Within the anthropized area of the basin, pasture occupies the largest portion, covering 20% of the total area. This occupation reflects a significant transformation of the natural landscape for agricultural activities. The conversion of forests and other native vegetation into pastures can result in soil degradation, increased erosion, and river sedimentation due to surface runoff, as well as a significant loss of biodiversity (PAULA; ESCADA; ORTIZ, 2022).

Regarding the most impactful activity in chemical use, soybean and corn cultivation occupies 4% of the basin area. The expansion of soy reflects the advancement of mechanized agriculture in the region, a significant factor in land use change. This monoculture exerts considerable pressure on the environment, including soil quality degradation, pesticide contamination, and deforestation (MASCARENHAS; ARAÚJO; SILVA, 2021).

In addition to these, other temporary crops occupy 4% of the basin. These crops may include rice, melon, watermelon, among others. Although they occupy a smaller portion of the basin, the frequent crop rotation and intensive land use for agriculture can significantly impact soil quality and local hydrology, contributing to changes in ecological and hydrological processes.

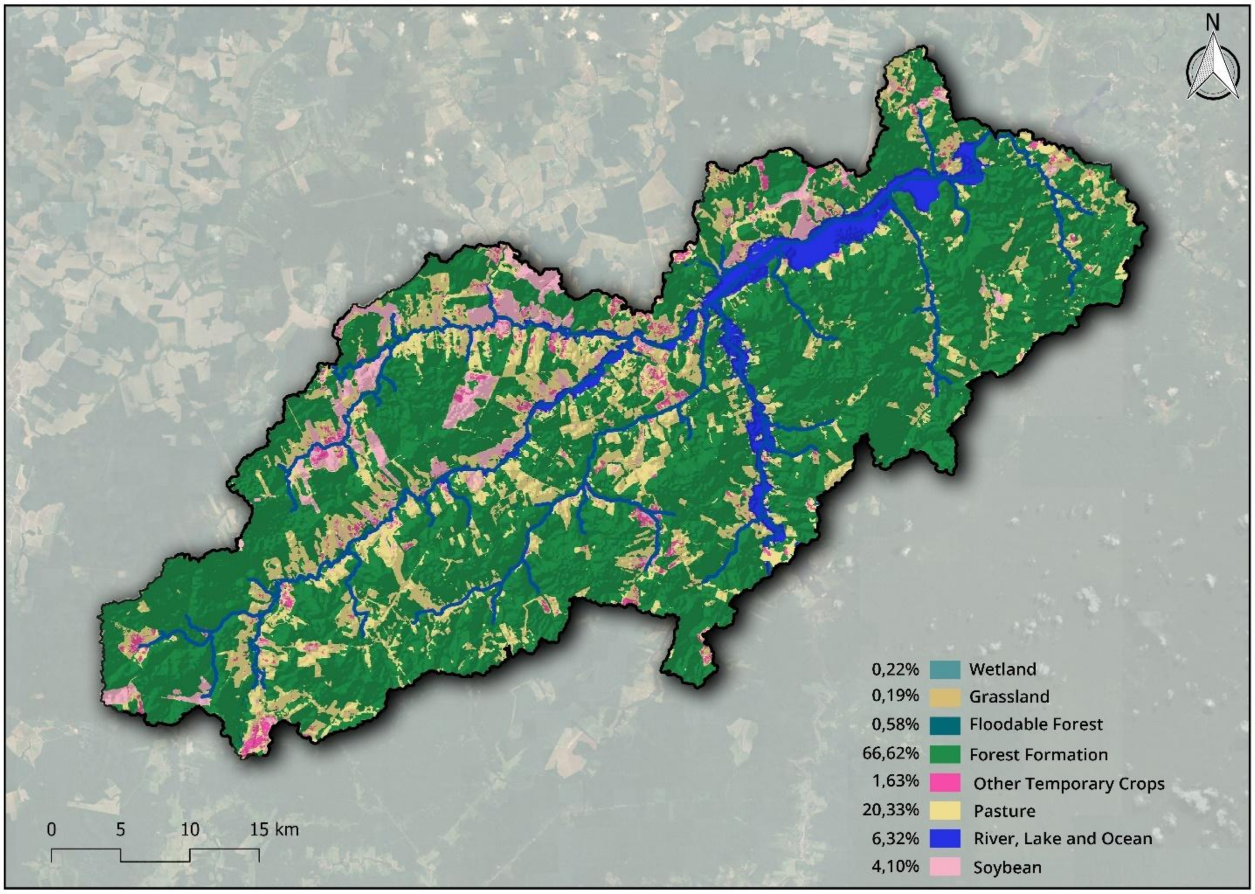

Figure 2 – Land use and occupation map of the Curuá-Una basin.
Source: Created by the authors (2024).

Figure 3 shows the hydrogeological map of the Curuá-Una River basin, which is part of the Amazon Sedimentary Basin. Within this basin, the Alter do Chão Formation stands out for its hydrogeological system, where, in the Curuá-Una River region, the aquifer is unconfined and has an approximate depth of 50 meters (João, Teixeira, & Fonseca, 2013). This characteristic demonstrates a high susceptibility to groundwater contamination by compounds with lower affinity for organic matter.

Among the molecules with the greatest potential for contamination, methomyl and glyphosate are notable, as both can contaminate both groundwater and surface water. According to Lewis (2016), methomyl has a low organic carbon sorption coefficient (Koc) of 72 m³/kg, indicating that it has a low tendency to adsorb onto soils and sediments, thereby facilitating its mobility in water. Its octanol-water partition coefficient (Kow) of 0.6 is also low, meaning that it is highly soluble in water and thus has a greater potential to contaminate aquifers.

Additionally, according to Lewis (2016), glyphosate also has a low Koc (1,424 m³/kg), which contributes to its mobility in aquatic environments. However, its Kow is extremely low (-3.4 m³/kg), reflecting its high solubility in water and lower tendency to adsorb to organic matter. This combination of physicochemical properties for both compounds indicates that in areas like the Curuá-Una River basin, there is a considerable risk of groundwater contamination.

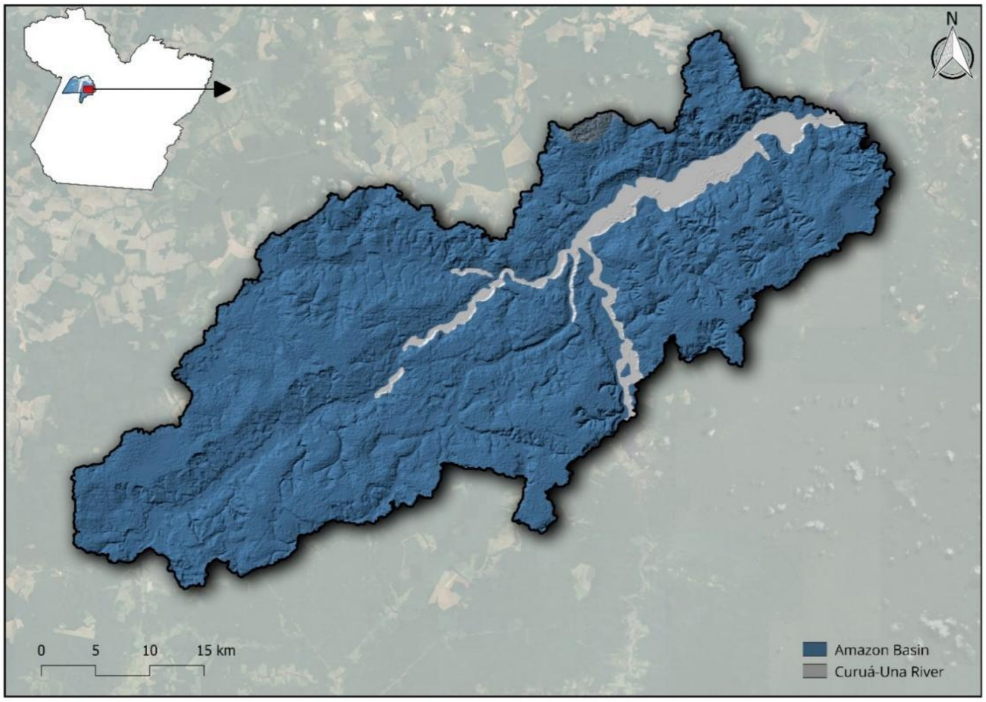

Figure 3 – Hydrogeological Map of the Curuá-Una Basin..
Source: Created by the authors (2024).

To discuss the susceptibility to infiltration and percolation of pesticides in the Curuá-Una River basin based on the products used, it is essential to consider the risks associated with the behavior of each chemical substance in relation to the characteristics of the basin, as presented in Table 6. Thus, in Figure 4, we can observe the risk areas for both surface and groundwater.

The Curve Number (CN) method assigns values to different soil types and vegetation cover, reflecting their capacity to absorb or repel water. It can be observed that about 59% of the area is more vulnerable to groundwater contamination, while less than 3% presents a risk of surface water contamination. Thus, 59% of the basin has a high infiltration rate, 25% has a moderate rate, and 13% is classified as having low infiltration, resulting in approximately 97% of the area being vulnerable to groundwater contamination.

Lower CN values, as indicated in the lighter yellow areas on the map (36-47), suggest a greater infiltration potential. This means that the soil in these regions is more porous and permeable, allowing water, and consequently contaminants such as pesticides, to penetrate more easily into the soil. These areas are more susceptible to contamination by substances with low affinity for organic matter and higher hydrophilicity, such as glyphosate, since these substances can reach deeper soil layers and eventually the groundwater (GROS et al., 2017).

In the darker regions of the color scale, corresponding to higher CN values (above 68), the soil has a lower infiltration capacity and a greater tendency for surface runoff. The soil is more compact or has a ground cover that does not favor water infiltration (PESSOA-DE-SOUZA et al., 2017).

In these areas, rainwater or irrigation water is more likely to run off the surface rather than infiltrate, which may reduce the risk of groundwater contamination by pesticides but increase the likelihood of chemical runoff into surface water bodies such as rivers and lakes.

The image reveals that the areas most susceptible to infiltration, indicated by lower CN values (light yellow) and an average CN of 47, are mainly distributed in the southern and southwestern regions of the map. Conversely, the darker blue areas, which indicate higher soil compaction and greater surface runoff, are concentrated in the northern and northeastern portions. Table 4 provides a more detailed breakdown of the percentage of each area within the Curuá-Una basin.

Areas with low infiltration potential, indicated by higher CN values, are more associated with risks of surface pollution, directly affecting the water quality in rivers and other bodies of water. In these areas, rainwater or irrigation water is more likely to run off the surface rather than infiltrate, which may reduce the risk of groundwater contamination by pesticides but increase the likelihood of chemical runoff into surface water bodies such as rivers and lakes.The Curve Number (CN) method assigns values to different soil types and vegetation cover, reflecting their capacity to absorb or repel water. It can be observed that about 59% of the area is more vulnerable to groundwater contamination, while less than 3% presents a risk of surface water contamination. Thus, 59% of the basin has a high infiltration rate, 25% has a moderate rate, and 13% is classified as having low infiltration, resulting in approximately 97% of the area being vulnerable to groundwater contamination.

Lower CN values, as indicated in the lighter yellow areas on the map (36-47), suggest a greater infiltration potential. This means that the soil in these regions is more porous and permeable, allowing water, and consequently contaminants such as pesticides, to penetrate more easily into the soil. These areas are more susceptible to contamination by substances with low affinity for organic matter and higher hydrophilicity, such as glyphosate, since these substances can reach deeper soil layers and eventually the groundwater (GROS et al., 2017).

In the darker regions of the color scale, corresponding to higher CN values (above 68), the soil has a lower infiltration capacity and a greater tendency for surface runoff. The soil is more compact or has a ground cover that does not favor water infiltration (PESSOA-DE-SOUZA et al., 2017).

In these areas, rainwater or irrigation water is more likely to run off the surface rather than infiltrate, which may reduce the risk of groundwater contamination by pesticides but increase the likelihood of chemical runoff into surface water bodies such as rivers and lakes.

The image reveals that the areas most susceptible to infiltration, indicated by lower CN values (light yellow) and an average CN of 47, are mainly distributed in the southern and southwestern regions of the map. Conversely, the darker blue areas, which indicate higher soil compaction and greater surface runoff, are concentrated in the northern and northeastern portions. Table 4 provides a more detailed breakdown of the percentage of each area within the Curuá-Una basin.

Areas with low infiltration potential, indicated by higher CN values, are more associated with risks of surface pollution, directly affecting the water quality in rivers and other bodies of water. In these areas, rainwater or irrigation water is more likely to run off the surface rather than infiltrate, which may reduce the risk of groundwater contamination by pesticides but increase the likelihood of chemical runoff into surface water bodies such as rivers and lakes.

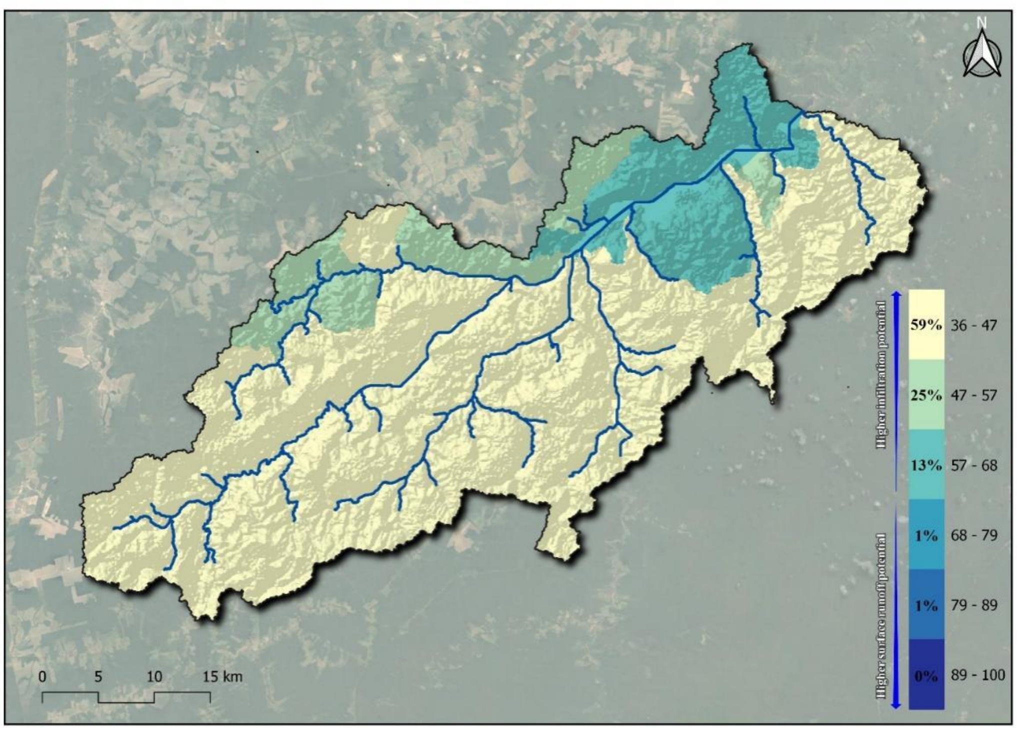

Figure 4 – Risk Map of Water Resource Contamination in the Curuá-Una Basin.
Source: Created by the authors (2024).

Tabela 4 – Percentual em área do parâmetro CN.

CN Class	Percentage of area	Classification
36 - 47	59%	
47- 57	25%	Higher infiltration potential
57 – 68	13%	
68 – 79	1%	
79 - 89	1%	Higher surface runoff potential
89 - 100	>0,5 %	

Source: Created by the authors (2024).

When assessing the vulnerability to contaminant infiltration and relating the physicochemical properties of the molecules, we can infer the areas where each substance has the greatest potential for contamination (Figure 5). In the case of glyphosate, the substance presents a high risk of surface water contamination, especially in areas identified with lower infiltration potential (59%, as shown in Figure 4), where surface water can easily transport the herbicide to water bodies. The risk to groundwater, however, is considered moderate, likely due to infiltration into less permeable soil zones, which act as barriers to deep penetration.

The behavior of cypermethrin, according to the basin's susceptibility, indicates a moderate risk for surface waters and a low risk for groundwater. The moderate risk for surface waters can be explained by the presence of areas with varying potentials for infiltration and percolation, with a greater tendency for retention on the surface due to the substance's low water solubility and high affinity for organic matter.

Teflubenzuron also presents a moderate risk for surface waters and a low risk for groundwater. The moderation of surface risk may be associated with areas of the basin with more compacted soils or lower infiltration rates, where the substance may remain longer before being degraded or transported superficially.

Chlorpyrifos was classified as low risk for both surface and groundwater. This could be related to the fact that this substance tends to adhere to soil and organic matter, reducing its mobility on the surface and at depth. The characteristics of the basin, which include areas of lower infiltration and percolation potential, reinforce this low-risk classification.

Conversely, methomyl was classified as high risk for both surface and groundwater. This classification may be attributed to its high mobility potential, combined with the characteristics of the basin, which include areas with high susceptibility to percolation and infiltration. The regions of the basin that favor greater infiltration (indicated in darker blue in the figure) may facilitate the transport of this substance to groundwater, while areas with lower infiltration favor surface runoff into rivers and lakes.

The analysis of contamination risks in the Curuá-Una River basin reveals a significant variation in the mobility and persistence of pesticides, depending on the chemical properties of the products. It can be observed that certain pesticides cause damage to both surface and groundwater, altering the basin's physical and hydrological characteristics. It is crucial that this information be used to guide the management and application of these products in the region, minimizing environmental impact and preserving the quality of both surface and groundwater.

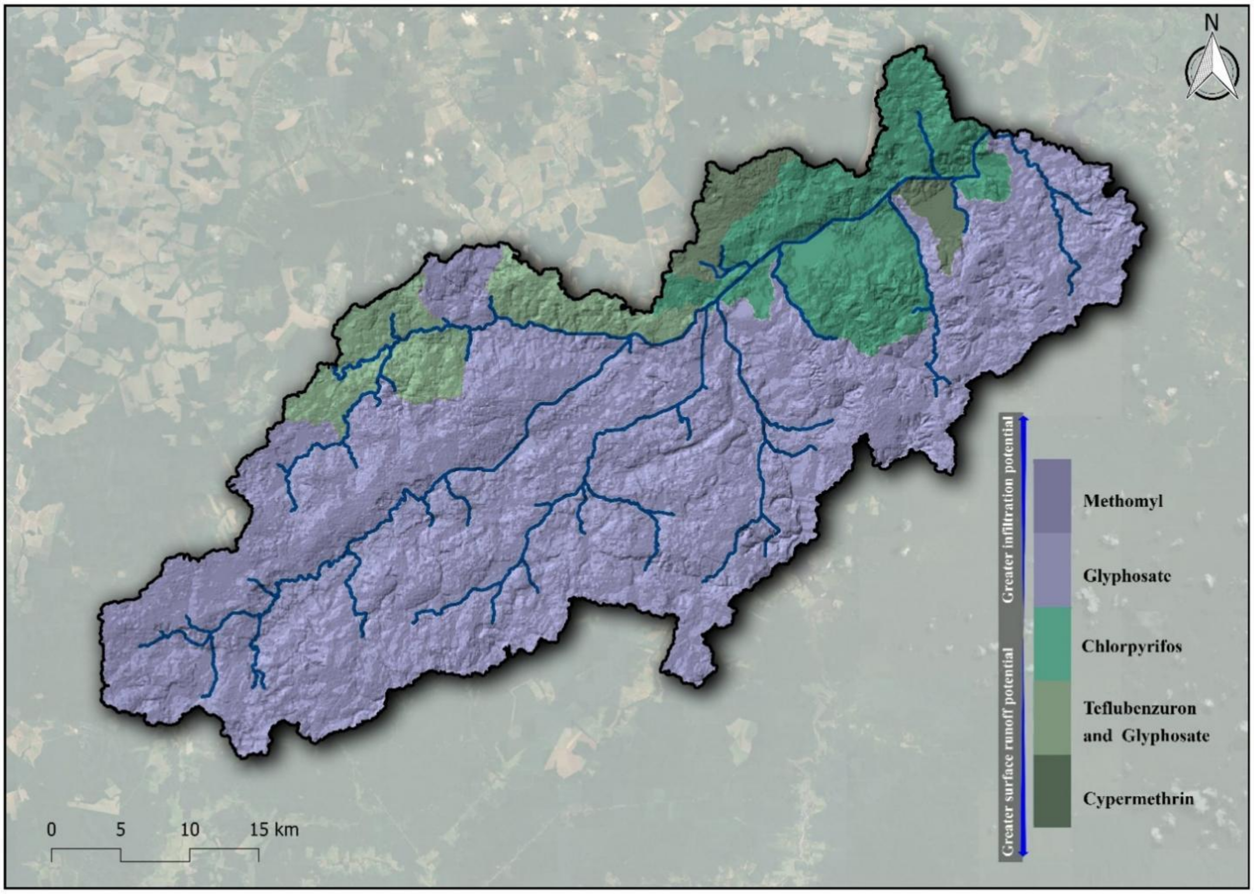

Figure 5 – Risk Map of Water Resource Contamination in the Curuá-Una Basin.
Source: Created by the authors (2024).

4. Final considerations

Based on the analyses conducted, this study clearly demonstrated the potential for pesticide contamination of water resources in the Curuá-Una River basin, utilizing predictive models and hydrological parameters such as the Curve Number. The combination of factors such as soil structure, permeability, and surface runoff capacity allowed for the identification of areas more vulnerable to the infiltration and runoff of chemical substances, which is essential for planning management and conservation practices.

The results indicate that approximately 59% of the study area is at high risk of groundwater contamination due to the high infiltration rate, while less than 3% is subject to surface water contamination. Substances like glyphosate and methomyl stood out for their potential environmental impact on both groundwater and surface water. Conversely, pesticides such as cypermethrin and chlorpyrifos presented lower risks, though they still require monitoring.

Therefore, this study not only provides a robust foundation for understanding the dynamics of pesticide contamination in the region but also offers an effective tool for environmental managers and agencies. The application of mathematical models, such as GUS and LEACH, combined with the Curve Number methodology, has proven to be a valuable technique for environmental and agricultural management. It aids in decision-making regarding where and how to implement soil and water management practices to mitigate the environmental risks associated with the use of chemical products in agriculture. These tools have demonstrated to be fast, efficient, and cost-effective in assessing the risk of water resource contamination.

Acknowledgements

We extend our gratitude to all collaborators from the Pará State Agricultural Defense Agency for their assistance in organizing and tabulating the agronomic records, as well as to everyone involved in the preparation of this manuscript.

References

AGUIAR, C. P. O. de; PELEJA, J. R. P.; SOUSA, K. N. S. Qualidade da água em microbacias hidrográficas com agricultura nos municípios de Santarém e Belterra, Pará. *Revista Árvore*, v. 38, n. 6, p. 983–992, 2014.

ANJINHO, P. da S. et al. Espacialização do parâmetro Curve Number (CN) na bacia hidrográfica do Ribeirão do Lobo para o período de 1985 E 2017. In: SIMPÓSIO DO PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIAS, 33., 2018, São Carlos, SP. *Anais* [...]. São Carlos, SP: Escola de Engenharia de São Carlos, 2018.

BATCHELOR, B. Leach models: Theory and application. *Journal of Hazardous Materials*, v. 24, n. 2–3, p. 255–266, 1990.

BOMBARDI, L. M. (org.). *Geografia do Uso de Agrotóxicos no Brasil e Conexões com a União Europeia*. São Paulo, SP: FFLCH - USP, 2017.

CHAIN, A. Impacto ambiental de agroquímicos e biopesticidas. *Rev. Bras. Toxicol.*, v. 8, n. 1, p. 9-10, 1995.

CUNHA, P. R. da C.; MELO, J. H. G.; SILVA, O. B. da. Bacia do Amazonas. *Boletim de Geociências - Petrobras*, v. 15, n. 2, p. 227–251, 2007.

DORES; DE-LAMONICA-FREIRE, E. M. Contaminação do ambiente aquático por pesticidas. Estudo de caso: águas usadas para consumo humano em Primavera do Leste, Mato Grosso – Análise preliminar. *Quimica Nova*, Vol. 24, No. 1, 27-36, 2001.

EMBRAPA - EMPRESA BRASILEIRA DE PESQUISA AGROPECUÁRIA. *Mapa de Solos*. Brasília, DF, 2014. Disponível em: http://www.dpi.inpe.br/amb_data/Shapefiles/soloEmbrapa.zip. Acesso em: 22 fev. 2024.

GROS, P. et al. Glyphosate binding in soil as revealed by sorption experiments and quantum-chemical modeling. *Science of The Total Environment*, v. 586, p. 527–535, 2017.

IASCO-PEREIRA, H. C.; LIBÂNIO, G. Investimentos externos diretos da china no brasil: a presença de empresas chinesas na economia brasileira nos séculos XX E XXI. *Revista de Economia Contemporânea*, v. 27, 2023.

IBGE - INSTITUTO BRASILEIRO DE GEOGRAFIA E ESTATÍSTICA. *Panorama populacional do estado do Pará.* Brasília, DF, 2023. Disponível em: https://cidades.ibge.gov.br/brasil/pa/panorama. Acesso em: 20 jul. 2023.

JATI, D. A.; SILVA, J. T. da. Estudos geo-hidrológicos da bacia do rio Curuá-Una, Santarém, Pará: Aplicação do modelo hidrológico de grandes bacias (MGB-IPH). *Revista Brasileira de Geografia Física*, v. 10, n. 4, p. 1296–1311, 2017.

JOÃO, X. da S. J.; TEIXEIRA, S. G.; FONSECA, D. D. F. *Mapa Geodiversidade do Estado do Pará*. Brasília, DF: CPRM - Serviço Geológico do Brasil, 2013. Disponível em: https://rigeo.sgb.gov.br/handle/doc/14705.

JUNG, G. et al. Evaluation of soil pesticide leaching to groundwater using undisturbed lysimeter: development of the pesticide groundwater leaching scoring system (PLS). *Environmental Science and Pollution Research*, , v. 31, n. 14, p. 21973–21985, 2024.

LAIPELT, L. et al. ANADEM: A Digital Terrain Model for South America. *Remote Sensing,* v. 16, n. 13, p. 2321, 2024.

LAUREANO, J. de J. et al. Análise da qualidade da água subterrânea. *Águas Subterrâneas*, v. 35, n. 1, 2020.

LEWIS, K. A. et al. An international database for pesticide risk assessments and management. *Human and Ecological Risk Assessment: An International Journal,* v. 22, n. 4, p. 1050–1064, 2016.

LONDRES, F. *Agrotóxicos no Brasil: um guia para ação em defesa da vida*. Rio de Janeiro, RJ: AS-PTA – Assessoria e Serviços a Projetos em Agricultura Alternativa, 2012.

LOURENCETTI, C.; SPADOTTO, C. A.; SANTIAGO-SILVA, M.; RIBEIRO, M. L. Avaliação do potencial de contaminação de águas subterrâneas por pesticidas: comparação entre métodos de previsão de lixiviação. *Pesticidas: Revista Ecotoxicologia e Meio Ambiente*, v. 15, p. 1-14, 2005.

MASCARENHAS, G. M. de A.; ARAÚJO, L. M. de; SILVA, J. A. T. e. Agrotóxicos, dominação e fronteiras: significação, relação e perspectivas sobre o pacote tecnológico agrícola e a Amazônia brasileira. *Revista Brasileira de Políticas Públicas*, v. 10, n. 3, 2021.

NASCIMENTO-GAYA, M. R. et al. Modelamento hídrico: um estudo de caso da refinaria REMAN. *Revista Fuentes el Reventón Energético*, v. 20, n. 2, 2022.

PAPA, E. et al. Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan). *Water Research*, v. 38, n. 16, p. 3485–3494, 2004.

PAULA, D. S. de; ESCADA, M. I. S.; ORTIZ, J. de O. Análise multitemporal do uso e cobertura da terra na Amazônia: A expansão da Agricultura de Larga Escala na Bacia do Rio Curuá-Una. *Revista Brasileira de Cartografia*, v. 74, n. 2, p. 379–398, 2022.

PENA, Rodolfo F. Alves. *Aquífero Alter do Chão*; Brasil Escola. Disponível em: https://brasilescola.uol.com.br/brasil/aquifero-alter-chao.htm. Acesso em 07 de junho de 2024.

PESSOA-DE-SOUZA, M. A. et al. Pesticides off site by runoff – Principles And Practices. *Caderno de Ciências Agrárias*, v. 9, n. 3, p. 119–125, 2017.

PLANET LABS. *Norway's International Climate and Forests Initiative Satellite Data Program*. 2024. Disponível em: https://www.planet.com/nicfi/. Acesso em: 22 fev. 2024.

RIBEIRO, J. S. *Cenário de uso, consumo e classificação de risco dos agrotóxicos na nova fronteira agrícola do Oeste do Pará*. 2021. 140 f. - Dissertação (Mestrado em Sociedade, Ambiente e Qualidade de Vida) - Programa de Pós-Graduação em Sociedade, Ambiente e Qualidade de Vida, Universidade Federal do Oeste do Pará, Santarém, PA, 2021.

RIBEIRO, J. S. *Simulação da contaminação dos recursos hídricos por pesticidas na lavoura temporária no entorno da BR-163*, Santarém, Pará. 2017. 64 f. TCC (Graduação) - Curso de Bacharelado em Ciências Biológicas, Instituto de Ciência e Tecnologia das Águas - Icta, Universidade Federal do Oeste do Pará, Santarém, 2017.

RIBEIRO, M. L. et al. Contaminação de águas subterrâneas por pesticidas: avaliação preliminar. *Química Nova*, v. 30, n. 3, p. 688-694, 2007.

SARTORI, A.; LOMBARDI NETO, F.; GENOVEZ, A. M. Classificação Hidrológica de Solos Brasileiros para a Estimativa da Chuva Excedente com o Método do Serviço de Conservação do Solo dos Estados Unidos Parte 1: Classificação. *Revista Brasileira de Recursos Hídricos*, v. 10, n. 4, p. 5–18, 2005.

SILVA, Y. A.; DESCOVI FILHO, L. L. V. Análise da vulnerabilidade intrínseca do Aquífero Alter do Chão no município de Santarém - Pará - Brasil. In: DAVID, M. E. V. et al. (org.). *Contribuições à Geologia da Amazônia*. Belém, PA: Sociedade Brasileira de Geologia - Núcleo Norte, 2023. v. 12, p. 212–225.

SOUMIS, N.; ROULET, M.; LUCOTTE, M. Characterization of pesticide consumption in the county of Santarém, Pará, Brazil. *Acta Amazônica*, v. 30, n. 4, p. 615–615, 2000.

SOUZA, C. M. et al. Reconstructing Three Decades of Land Use and Land Cover Changes in Brazilian Biomes with Landsat Archive and Earth Engine. *Remote Sensing*, v. 12, n. 17, p. 2735, 2020.

SRC. *Fate Pointers*, 2018 Disponível em:<http://esc.syrres.com/fatepointer/search.asp>. Acessado em 09/02/2024.

UNIVERSITY OF HERTFORDSHIRE. *PPDB: Pesticide Properties Database*, 2018. Disponível em: < https://sitem.herts.ac.uk/aeru/ppdb/en/atoz.htm >. Acessado em 09/02/2018.

USDA - UNITED STATES DEPARTMENT OF AGRICULTURE. N*atural Resources Conservation Service. Urban hydrology for small watersheds*. Technical release, v. 55, p. 2–6, 1986.

USEPA - UNITED STATES ENVIRONMENTAL PROTECTION AGENCY. *SCI-GROW Description*. Washington, DC, USA, USA, 2003. Disponível em: https://archive.epa.gov/oppefed1/web/html/scigrow_description.html. Acesso em: 16 fev. 2024.

WAUCHOPE, R. D. et al. The SCS/ARS/CES Pesticide Properties Database for Environmental Decision-Making. *Rev Environ Contam Toxicol*, v. 123, n. 1, p. 1–155, 1992.