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Groundwater in Uruguay: Integrated Risk Assessment of Arsenic, Fluoride and Selenium Using Geostatistics and Quality Index

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Abstract

Groundwater is one of the main sources of drinking water in Uruguay and has traditionally been suitable for human consumption. However, increasing agricultural and industrial demand, coupled with a lack of updated hydrochemical data, has raised concerns about fluoride (F^-) and arsenic (As) contamination. In this study, hydrochemical data from 1,761 groundwater samples collected by the General Directorate of State Sanitary Services (OSE, personal communication, September 2025) and private sources across Uruguay (except Maldonado and Montevideo departments) were analysed. Arsenic concentrations ranged from 0.001 to 0.046 mg/L, with 5% of the samples exceeding the World Health Organization (WHO) recommended limit of 0.01 mg/L. Fluoride concentrations ranged from 0.04 to 2.5 mg/L, with 12% of samples exceeding the WHO limit of 1.5 mg/L. The highest fluoride concentrations were observed in the departments of Cerro Largo and Treinta y Tres, while arsenic anomalies were associated with sedimentary formations such as the Raigón and Mercedes formations. Selenium (Se) concentrations ranged from 0.1 mg/L to 0.5 mg/L. Multivariate statistical techniques, including Principal Component Analysis (PCA) and cluster analysis, revealed distinctive hydrochemical patterns. Furthermore, a Groundwater Quality Index (GrWQI) was developed, integrating pH, EC, F^-, As, and Se, with weighted contributions based on health risk. GrWQI values showed spatial heterogeneity, with several areas in the departments of Salto, Soriano, and Rocha presenting lower scores, indicating potential health risks. These findings highlight the urgent need for continued groundwater monitoring and management strategies.

Keywords: groundwater quality, fluoride, arsenic, selenium, Uruguay

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Agua subterránea en Uruguay: Evaluación integrada del riesgo por arsénico y fluoruro mediante geoestadística e índice de calidad del agua

Resumen

El agua subterránea es una de las principales fuentes de agua potable en Uruguay y tradicionalmente ha sido apta para el consumo humano. Sin embargo, la creciente demanda agrícola e industrial, sumada a la falta de datos hidroquímicos actualizados, ha suscitado inquietudes respecto a la contaminación por fluoruro (F^-) y arsénico (As). En este estudio se analizaron datos hidroquímicos de 1761 muestras de agua subterránea, recolectadas por la Dirección General de Servicios Sanitarios del Estado (OSE, comunicación personal, setiembre 2025) y fuentes privadas en todo Uruguay (excepto los departamentos de Maldonado y Montevideo). Las concentraciones de arsénico oscilaron entre 0,001 y 0,046 mg/L, y 5% de las muestras excedió la directriz de la Organización Mundial de la Salud (OMS) de 0,01 mg/L. Las concentraciones de fluoruro variaron entre 0,04 y 2,5 mg/L, y 12% de las muestras superó el umbral de la OMS de 1,5 mg/L. Las mayores concentraciones de fluoruro se observaron en los departamentos de Cerro Largo y Treinta y Tres, mientras que las anomalías de arsénico se asociaron con formaciones sedimentarias como Raigón y Formación Mercedes. Las concentraciones de selenio (Se) variaron entre 0,1 mg/L y 0,5 mg/L. Las técnicas estadísticas multivariadas, incluyendo el Análisis de Componentes Principales (ACP) y el análisis de conglomerados, revelaron patrones hidroquímicos distintivos. Además, se desarrolló un Índice de Calidad de Aguas Subterráneas (ICASP) que integra pH, CE, F^-, As y Se, con contribuciones ponderadas según el riesgo para la salud. Los valores del ICASP mostraron heterogeneidad espacial, con varias áreas en los departamentos de Salto, Soriano y Rocha con puntuaciones más bajas, lo que indica posibles riesgos para la salud. Estos hallazgos resaltan la urgente necesidad de implementar estrategias continuas de monitoreo y gestión de aguas subterráneas.

Palabras clave: calidad de agua subterránea, fluoruro, arsénico, selenio, Uruguay

Água Subterrânea no Uruguai: Avaliação Integrada de Risco por Arsênio e Fluoreto através de Geoestatística e um Índice de Qualidade da Água

Resumo

A água subterrânea é una das principales fontes de água potável no Uruguai e tradicionalmente é adequada para consumo humano. No entanto, as crescentes demandas agrícolas e industriais, combinadas com a falta de dados hidroquímicos atualizados, levantaram preocupações quanto à contaminação por flúor (F^-) e arsênio (As). Neste estudo, foram analisados dados hidroquímicos de 1,761 amostras de água subterrânea, coletadas pelo Departamento de Serviços Sanitários do Estado (OSE, comunicação pessoal, setembro de 2025) e fontes privadasemtodo o Uruguai (exceto os departamentos de Maldonado e Montevidéu). As concentrações de arsênio variaram de 0.001 a 0.046 mg/L, com 5% das amostras excedendo a diretriz da Organização Mundial da Saúde (OMS) de 0.01 mg/L. As concentrações de fluoreto (F^-) variaram entre 0.04 e 2.5 mg/L, com 12% das amostras ultrapassando o limite da OMS de 1.5 mg/L. As maiores concentrações de F^- foram observadas nos departamentos de Cerro Largo e Treinta y Tres, enquanto anomalias de arsênio foram associadas a formações sedimentares como RaigónandFormacion Mercedes. As concentrações de selênio (Se) variaram entre 0,1 mg/L e 0,5 mg/L.Técnicas estatísticas multivariadas, incluindo Análise de Componentes Principais (ACP) e análise de cluster, revelaram padrões hidroquímicos distintos. Além disso, foi desenvolvido um Índice de Qualidade da Água Subterrânea (IQQR), integrando pH, CE, F^-, As e Se, com contribuições ponderadas com base no risco à saúde. Os valores do IQQR mostraram heterogeneidade espacial, com diversas áreas nos departamentos de Salto, Soriano e Rocha apresentando pontuações mais baixas, indicativas de potenciais riscos à saúde. Esses achados ressaltam a necessidade urgente de estratégias contínuas de monitoramento e gestão das águas subterrâneas.

Palavras-chave: qualidade das águas subterrâneas, fluoreto, arsênico, selênio, Uruguai

1. Introduction

1.1 Groundwater Quality Challenges in Uruguay

Uruguay has long been recognised for its abundant and high-quality groundwater resources, which have historically served as a reliable source of drinking water for human consumption. However, in recent years, there has been a significant increase in well drilling activities to meet the growing demands of the productive and industrial sectors. This surge in groundwater extraction raises concerns about potential changes in water quality, particularly concerning naturally occurring contaminants such as fluoride and arsenic.

The Uruguayan national water company provides safe drinking water to approximately 94% of the population. However, in certain rural areas (Gamazo et al., 2018; Pamoukaghlián et al., 2024; Pizzorno et al., 2024), residents rely on private wells as their primary water source due to the lack of connection to the public water supply. These wells are often not subject to regular monitoring for contaminants such as arsenic and fluoride, posing potential health risks for those who consume this water (Gamazo et al., 2018).

Climate change-related issues, such as extended droughts (e.g., La Niña 2022–2023), further exacerbate these concerns by altering hydrological cycles (Rahmani & Fattahi, 2024) and potentially concentrating contaminants in aquifers (Kløve et al., 2014; Shukla et al., 2023). Hydrochemical changes in Uruguayan coastal aquifers due to drought periods were analyzed and reported (Pamoukaghlián et al., 2024), concluding that salinity variations in this area must be approached considering climate change and possible changes in the direction of ocean currents.

Cruz et al. (2014) analyzed the frequency, intensity, and duration of agronomic droughts in two key livestock-producing regions of Uruguay. Their findings did not reveal a clear increasing trend, highlighting the need for further investigation into the vulnerability of pastoral livestock systems to drought conditions. Advancing interdisciplinary research is essential to enhance the understanding of agronomic drought impacts within diverse economic, political, and social contexts in Uruguay.

Despite the fundamental role groundwater plays in Uruguay and the extensive analytical data produced by various public, private, and academic institutions, a comprehensive hydrochemical analysis of the country's aquifers remains lacking

This research analyses data on two potentially toxic elements found in Uruguay's groundwater: fluoride and arsenic, as a control methodology for applying in water management for irrigation and human consumption.

1.2 The Role of Chemical Parameters as Water Quality Indicators

Temperature plays a vital role in groundwater dynamics, as it influences chemical reactions, microbial activity, and the solubility of minerals (Stallard & Edmond, 1983). Variations in groundwater temperature can also reflect geothermal gradients or surface-water interactions, making it an important indicator of aquifer conditions. Similarly, pH is a fundamental parameter that governs the mobility of contaminants and the speciation of chemical species in groundwater (Appelo & Postma, 2004). Slight deviations in pH can significantly affect the solubility of metals such as arsenic and selenium, posing potential health risks if levels exceed regulatory limits.

Electrical conductivity (EC) serves as a proxy for total dissolved solids (TDS) and provides insights into the salinity of groundwater (Hem, 1985). Elevated EC values are often associated with agricultural runoff, seawater intrusion or mineral dissolution, all of which can affect water quality.

1.3 Potentially Toxic Elements Found in Uruguay's Groundwater: Fluoride, Arsenic, and Selenium

Arsenic contamination has been identified as a major global health concern, with millions of people exposed to unsafe levels through groundwater consumption (Smith et al., 2000). The presence of arsenic in groundwater is typically linked to geochemical processes such as the oxidation of sulphide minerals or reductive dissolution of iron oxides (Nordstrom, 2002).

Fluoride and selenium, while essential micronutrients at low concentrations, can become toxic when present in excess. Chronic exposure to high fluoride levels in drinking water has been associated with dental and skeletal fluorosis (Amini et al., 2008), while elevated selenium concentrations can lead to selenosis, a condition characterized by hair loss, nail brittleness, and neurological effects (Fordyce, 2007). These elements often originate from natural sources, such as volcanic rocks or sedimentary deposits, but their mobility is strongly influenced by pH, redox conditions, and the presence of competing ions (Smedley & Kinniburgh, 2002).

In nature, fluorine predominantly occurs as fluorides in minerals such as fluorspar (fluorite), cryolite, and fluorapatite. This element rank is the thirteenth most common in the Earth's crust, making up about 950 parts per million. Around 4 million tons of mineral fluorite are produced annually worldwide, with estimated reserves of about 120 million tons. Most soils contain approximately 330 ppm fluorine, usually between 150 to 400 ppm. However, some soils may have up to 1,000 ppm, and contaminated soils can reach 3,500 ppm (Hong et al., 2016).

Fluorine is ubiquitous in the environment, mostly originating from natural sources. These include standard erosion processes that release fluoride from rocks and minerals, volcanic activity, marine aerosol emissions, and partially natural biomass burning. There are various human-related sources of fluoride, which in some regions may impact the biosphere (Kar, 2022).

Fluorides are naturally present in the Earth's crust, found in rocks, coal, clay, and soil. They are released into the environment through natural processes such as the weathering of minerals, volcanic emissions, and marine aerosols (Agency for Toxic Substances and Disease Registry [ATSDR], 2003). Volcanic activity, including passive degassing and eruptions, contributes significantly to atmospheric hydrogen fluoride, with annual global emissions estimated between 0.6 and 6 million metric tons, approximately 10% of which may reach the stratosphere (Kern & Kelly, 2023).

In water, fluorides are associated with various ranges of compounds, with aluminium in freshwater, calcium and magnesium in seawater, and deposited into the sediment where they adhere strongly to sediment particles (Hong et al., 2016). At the same time, rock mineral dissolution can elevate the F^- concentration in groundwater; minerals such as fluorite or apatite can input F^- into the hydrogeological system (Mukherjee & Singh, 2018).

In soils, fluorides are strongly retained in the form of cryolite (Na_3AlF_6), fluorapatite ($Ca_5(PO_4)_3F$) and other phosphate rocks (Chatterjee et al., 2020). Leaching removes only a small amount of fluoride from soils (ATSDR, 2003).

Elevated fluoride concentrations in soils, often resulting from natural geochemical processes or anthropogenic activities, can pose significant risks to plant health and agricultural productivity. Fluoride accumulation in the rhizosphere may lead to phytotoxic effects (Gadi et al., 2021), including reduced nutrient uptake, impaired photosynthesis, and visible damage to foliage (Singh et al., 2023). These adverse effects are particularly concerning for sensitive crops and may vary depending on species, soil properties, and environmental conditions.

Geochemical studies reveal that fluoride exhibits its greatest stability when bonded with iron, aluminium, and calcium. Soil components containing these elements, such as clay minerals, calcium and magnesium compounds, and iron and aluminium compounds, retain labile fluoride effectively (Hong et al., 2016). Barrow and Ellis (1986) later suggested that at low pH, aluminium-fluoride complexes formed in the soil solution resulting in limited free F^- ions. Soils with higher calcium content showed increased effectiveness in fixing fluoride (Hong et al., 2016). The physicochemical properties of fluoride ions are the key to understanding their mobility and distribution in soils and their transport from porous media to groundwater. The electronegative fluoride ion replaces –OH/H2O groups attached to surface Al atoms as ligand exchange, loosening other Al–OH bonds (Moirana et al., 2024).

Hong et al. (2016) pointed out that the exposure of sensitive green plants to elevated fluoride concentrations for appropriate time intervals under controlled environmental conditions may produce one or more of the following effects: a slight paleness of the normal green pigment at leaf tips or margins that may extend to other parts of the leaf, a pale green area at the margins may turn to light beige and eventually reddish brown, sometimes called leaf scorch. However, there is a lack of information about the critical fluoride concentration affecting soil biota and plant growth.

Additionally, the anthropogenic origin of fluoride is related to various human activities. Fluorosilicic acid, sodium hexafluorosilicate, and sodium fluoride are used in municipal water fluoridation processes (International Programme on Chemical Safety [IPCS], 1984), and their final disposal must be well-defined so that high levels of these pollutants do not reach natural waterways.

The potential essentiality of fluoride for animals and humans has been suggested, particularly concerning bone health (IPCS, 1984; *Some aromatic amines*, 1982). Research in several regions of New Zealand found that subclinical fluoride toxicosis may be linked to spontaneous humeral fractures in first-lactation dairy cows (Wehrle-Martinez et al., 2025).

Arsenic (As) is a naturally occurring element that poses significant environmental and health risks when present in elevated concentrations in groundwater used for drinking purposes. In Uruguay, this issue has become a focal point of recent research due to its environmental and public health implications, particularly in rural areas where groundwater serves as the primary source of potable water and agricultural irrigation. Groundwater arsenic concentrations in certain regions of Uruguay exceed both the World Health Organisation (WHO) guideline of 10 µg/L and the current national standard of 20 µg/L (Manganelli et al., 2007). This discrepancy underscores the need to align local regulations with international guidelines to better protect public health.

In Uruguay, the geographical distribution of arsenic in groundwater is not uniform. High arsenic levels have been found in areas like the Raigón aquifer in San José department (Machado et al., 2020; Manganelli et al., 2007; Wu et al., 2021). These concentrations are influenced by hydrogeological factors, including geochemical composition, redox conditions, and the presence of other inorganic parameters such as iron (Fe), manganese (Mn), and sulphate (SO_4^{2-}). Significant correlations between arsenic and these elements have been observed, suggesting that geochemical interactions play a key role in arsenic mobilization into groundwater (Machado et al., 2020). Moreover, Wu et al. (2021) employed combined machine learning techniques to estimate arsenic distribution, effectively showing the significant roles that depth and geological structures play in determining its occurrence. Furthermore, a correlation between the geochemical characteristics of drilling rocks and arsenic concentrations in groundwater has been explored, providing valuable insights for future mitigation strategies (Collazo et al., 2020; Pamoukaghlián et al., 2023).

Chronic exposure to As through contaminated drinking water has severe health implications. Inorganic arsenic species (Mañay et al., 2019), such as arsenite (As(III)) and arsenate (As(V)), are highly toxic and have been

associated with diseases such as skin cancer, cardiovascular disorders, and neurological impairments (Mañay et al., 2019; World Health Organization [WHO], 2022). In Uruguay, epidemiological studies have begun to assess the effects of low-dose arsenic exposure on rural populations, although knowledge gaps remain regarding the exact mechanisms of toxicity and individual susceptibility factors (Kordas et al., 2016).

To address this challenge, advanced analytical methodologies have been implemented to quantify and to speciate arsenic in water, soil, and food samples. Techniques such as hydride generation atomic absorption spectrometry (HG-AAS) and high-performance liquid chromatography coupled with inductively coupled plasma mass spectrometry (HPLC-ICP-MS) have provided precise data on the chemical forms of arsenic present in various matrices (Machado et al., 2020; Verger et al., 2018). These methods have been instrumental in understanding how As transforms and mobilises in the environment, particularly under flooded conditions such as those found in rice cultivation systems (Machado et al., 2020; Verger et al., 2018).

The relationship between arsenic in groundwater and its impact on agriculture, particularly rice cultivation, has also been studied. Rice is known to accumulate arsenic in its grains, raising additional concerns about food safety (Roel et al., 2022; Verger et al., 2018). As bioavailability in flooded soils and its transfer to rice grains emphasise, and the importance of controlling agricultural practices to minimise human exposure is a challenge in arsenic-contaminated environments. Improving access to cost-effective treatment technologies for rural communities and conducting deeper investigations into the long-term health effects of low-concentration arsenic exposure are needed.

Arsenic contamination in Uruguayan groundwater is due to natural causes (i.e., “geogenic” or “natural contamination”) and represents a complex challenge that requires an integrated approach combining environmental sciences, agronomy, and public health (Alvareda et al., 2025; Collazo et al., 2020; Mañay et al., 2019; Manganelli et al., 2007; Pamoukaghlián et al., 2023; Wu et al., 2021). Advances in analytical methodologies and growing awareness of associated risks have laid the groundwork for addressing this issue (Machado et al., 2020), but much remains to be done to ensure safe drinking water and protect the health of affected communities.

Selenium (Se) is an essential micronutrient for both humans and animals, playing a crucial role in antioxidant defence and thyroid hormone metabolism (Fordyce, 2007; Petrović, 2021). However, its geochemical behaviour makes it particularly complex, as the range between essential and toxic concentrations is narrow (Fordyce, 2007; Martens & Suarez, 1996; WHO, 2022). In groundwater systems, selenium occurs mainly as selenate (SeO_4^{2-}) and selenite (SeO_3^{2-}), whose mobility and bioavailability are strongly governed by pH, redox potential, and microbial activity (Petrović, 2021). Under oxidizing and alkaline conditions, such as those often found in semi-arid and coastal environments, selenium tends to be more mobile, increasing the risk of groundwater enrichment. Moderate Se concentrations in groundwater have been reported in sedimentary basins of South America, in oxidizing groundwaters from loess-type sediments in arid/semi-arid dry climates from the Chaco-Pampean plain (Argentina), frequently associated with marine sediments or volcanic ash deposits (Nicolli et al., 2010).

Although data on selenium occurrence in Uruguayan aquifers are still limited, its potential co-occurrence with fluoride and arsenic suggests that similar geogenic processes, such as mineral weathering and evaporative concentration during dry periods, may influence its distribution (Fernández-Martínez & Charlet, 2009). Chronic exposure to high selenium levels can lead to selenosis, with symptoms including gastrointestinal distress, nail and hair loss, and neurological disturbances (Fernández-Martínez & Charlet, 2009). Therefore, continued monitoring of selenium in groundwater is essential to distinguish natural background concentrations from anthropogenic inputs and to prevent long-term exposure in rural populations relying on groundwater for drinking and irrigation purposes.

In this study, hydrochemical data from 1,761 groundwater samples collected by the General Directorate of State Sanitary Services (OSE, personal communication, September 2025) and private sources across Uruguay (except Maldonado and Montevideo departments) were analysed.

1.4 Geological Framework

In Uruguay, there are some aquifers and aquifer systems that are particularly affected in terms of water quality regarding fluoride and arsenic.

The Guaraní Aquifer (conformed by Buena Vista, Cuchilla Ombú, Tacuarembó and Rivera Formations) is one of the most important aquifers in Uruguay, and fortunately, no elevated F or As values have been found in the phreatic aquifer, based primarily on information from the water intake wells of the Tacuarembó Formation. Data from the confined aquifer is not available for this study.

Carboniferous-Permian aquifers present quantity problems and, more generally, very poor water quality, and high F contents are not uncommon.

According to Bossi et al. (1998), the Carboniferous-Permian geologic formations that conform these aquifers and aquitards are: (a) San Gregorio Formation (Carboniferous-Permian), formed basically of psefites and pelites. (b) Tres Islas Fm. (Inferior Permian) predominantly composed of fine to coarse-grained psamites. The Melo Group includes Fraile Muerto, Mangrullo and Paso Aguiar Formations (De Santa Ana & Gutiérrez, 2000). Yaguarí Formation and Buena Vista Formation generally do not have quality problems. (c) Melo Group (Superior Permian), named in the literature as “gray shales” (“*politicos grises*”) and forming part of the aquifers and aquitards with the worst quality and quantity problems with conductivities up to 12762 uS/cm (Pamoukaghlián et al., 2019) (Tables S1 and S2 in Supplementary materials).

Looking at F anomalies, we can also find the high values associated to the Precambrian basement in the Illescas granite in the homonymous locality and Carapé Group (Bossi & Navarro, 1988) in Villa Serrana locality (Paleoproterozoic basement).

The Illescas granite is extended about 750 km^2 and is located in J. Batlle y Ordoñez and intrudes at the same time other granites, sienites and granophires. This is a rapakivi granite with a wiborgitic texture (Bossi & Gaucher, 2014). Its mineralogy is mainly composed of microcline, orthoclase, oligoclase, quartz, rutile, biotite, sphene, zircon and apatite. The apatite could be inputting F to the hydrogeological system. In a monographic unpublished work for the Hydrogeology course of the School of Sciences, Universidad de la República, by Eloisa Cocorel in 2019, there were reported F values of 1,7 and 1,4 for the Illescas granite-associated groundwater.

Regarding geology, the highest As levels are in the littoral part of the Rio Uruguay, in Cenozoic sediments of the Salto Formation and Cretaceous sediments, especially in the Mercedes Formation. In the Cenozoic sedimentary rocks of the Raigón Formation and the Salto Formation, there are also anomalous values.

In the Precambrian basement of the Piedra Alta Terrane, sometimes high Arsenic concentrations are found, curiously associated with high concentrations of the overlapping Raigón Aquifer System (Pamoukaghlián et al., 2023).

1.5 Uruguayan Groundwater Quality: Fluoride and Arsenic background

Concentrations ranging from 1.72 to 120.48 µg/L for total arsenic (tAs), 0.024 to 1.528 mg/L for fluoride (F^-), 0.62 to 211.38 µg/L for iron (Fe), and 0.11 to 8.705 µg/L for manganese (Mn) were reported by Machado et al. (2020) over Uruguay.

In 2019, a water quality study of the Permian aquifer system in the northeast region of Uruguay was performed, addressing quantity and quality water issues for human consumption. Melo Group, Yaguarí Formation and Tres Islas Formation's water quality analysis showed high levels of EC (48-12762 $uScm^{-1}$), Na^+ (2.5-2411 mg/L), Cl^- (0.5-2688 mg/L), F^- (0.6-3.0 mg/L), and the water quantity scarce due to shale lithology (Pamoukaghlián et al., 2019). These authors have also reported high values of F in the La Pedrera locality (Cerro Largo) up to 2.7 mg/L, corresponding to Fm. Tres Islas groundwater input. These authors also encountered high F levels in groundwater in Tacuarembó (Las Pajas locality), corresponding to a mixed input of the Tres Islas Formation and Melo Group.

High As concentrations were confirmed in water from private wells (P. Pizzorno, personal communication, 2024), whereas fluoride levels remained below the WHO guideline of 1.5 mg/L. In 2021, the first risk distribution models for arsenic in Uruguay's groundwater used a machine learning approach (Wu et al., 2021). This study utilised data from 504 arsenic wells across Uruguay, collected by the State Sanitary Services Department of Uruguay (OSE, Obras Sanitarias del Estado) (Wu et al., 2021). In 2023, a prior study on fluoride in groundwater revealed localised areas, primarily in the Southwest region of Uruguay, with elevated concentrations that exceed WHO guidelines (Alvareda et al., 2023).

1.6 Spatial Distribution of Fluoride and Arsenic in Groundwater Resources for Agricultural and Domestic Use in Uruguay

The findings underscore the urgent need for systematic monitoring of groundwater quality, as Uruguay's population could be exposed to elevated fluoride and arsenic levels, exceeding WHO guidelines (WHO, 2022). These results highlight the importance of implementing protective measures to safeguard public health.

The main objective of this work is to analyse available data and new results (N: 1761) about the distribution of Fluoride and Arsenic in groundwater concerning the hydrogeological framework of Uruguay. To develop this research, specific objectives are proposed:

1. Compile and organise a hydrochemical database integrating information from the State Sanitary Services Department (OSE) and private groundwater wells.

2. Identification of potential correlations of hydrochemical parameters in the groundwater dataset.

3. Elaborate maps of potential high-fluoride risk zones in untreated groundwater used for human and animal consumption to assess associated public and animal health risks.

4. Elaborate a groundwater quality index to evaluate possible risks for drinking water use.

2. Materials and Methods

2.1 Geology Mapping

Uruguayan geology was plotted in QGIS 3.2.2 with GRASS 7.4.1 accordingly to geological cartography available in the National Direction of Mining and Geology (DINAMIGE) (Olivet et al., 2024). Geological eras were color-coded using the RGB values adapted from CMYK (*Código de color RGB adaptado de CMYK*, 2023).

2.2 Hydrochemical Database

Data were obtained from previous monitoring efforts by OSE (OSE personal communication, September 2025), and additional new data from private wells were collected specifically to expand the dataset and assess fluoride

and arsenic distribution patterns. The total number of data points corresponds to 1,761 analysed groundwater samples from 659 wells, covering 278 localities and rural areas. No data from Montevideo and Maldonado departments were included.

Each groundwater sample presents data of an identification number (ID), UTM coordinates, Department, Locality, Date of collected sample, chemical parameters as Temperature (T), pH, electrical conductivity (EC), fluoride (F-), arsenic (As), selenium (Se), Hydraulic data as depth (meters), flow rate, piezometric level, static levels (SL), dynamic levels (DL), and the Aquifer.

The dataset spans the period from 2009 to 2022, with 92% of the samples concentrated between 2018 and 2019. Out of the 1,761 samples, arsenic concentrations were available for 1,361 samples, fluoride for 981 samples, and selenium for 66 samples.

Groundwater samples lacking aquifer information (N = 494) were classified as “Unknown Aquifer” and excluded from statistical analyses due to their uncertain hydrogeological origin. Their inclusion nevertheless underscores the need to strengthen geological and hydrogeochemical characterization in national groundwater databases.

2.3 Data Analysis

Data were analysed by descriptive statistics performed by R 4.4.2, RStudio®, to determine hydrochemical data ranges. Python® libraries such as Pandas and Matplotlib. Descriptive statistics were calculated, while spatial distribution maps were generated to identify high-risk areas. The geological context of elevated fluoride levels was explored. Private wells data was obtained from Alvareda et al. (2023) and from a master’s degree thesis (Texo, 2021). All data used in the study were identified by their name and hydrochemical composition, and observations were systematically recorded.

The methods employed ensured reproducibility and adherence to international standards for hydrochemical analysis. The database was expanded to include analyses between 2009 and 2022.

2.4 Data Preprocessing and Transformation for PCA and Clustering

Prior to multivariate analysis, specific transformations were applied to the dataset to meet the assumptions of normality and homoscedasticity. Electrical conductivity (EC) values were transformed using the square root function ($\sqrt{EC}$) to stabilize variance and reduce skewness. Arsenic concentrations were transformed using a base-10 logarithmic transformation, $\log10(As + 0.001)$, to manage the presence of zero and near-zero values and achieve a more symmetric distribution. Prior to conducting the Correlation matrix, Principal Component Analysis (PCA) and clustering, normality tests were performed on the transformations, deemed necessary to improve the reliability and interpretability.

First, a descriptive analysis of the data was carried out using computer tools using the Anaconda working environment with the Python 3 programming language and RStudio.

To assess the relationships between the transformed variables, the Pearson correlation coefficient was calculated. This method is appropriate for normally distributed data and measures the strength and direction of the linear relationship between two variables. Given that the data were normalized and transformed (logarithmic and square root transformations), the assumption of normality was met, allowing for the application of the Pearson correlation. The Pearson correlation coefficient ranges from -1 to +1, with values closer to +1 or -1 indicating a strong positive or negative linear relationship, respectively, and values closer to 0 indicating no linear relationship (Pearson, 1896).

2.4.1 Groundwater Quality Index (GrWQI) Calculation

To assess temporal variations in water quality, a Groundwater Quality Index (GrWQI) was calculated for each observation point across the departments of interest.

The GrWQI is computed as a modification from Ravikumar et al. (2013) to classify the quality of groundwater in various departments based on the concentration levels of five key water quality parameters: pH, EC, F^-, As, and Se. These parameters were chosen because of their significance in determining the safety and suitability of groundwater for drinking purposes.

GrWQI scores each parameter according to its concentration compared to health and safety limits, using a scale from 0 to 100, where higher scores indicate better water quality. Lower scores indicate poorer water quality. The specific classification for each parameter is as follows:

1. The pH score was determined based on the recommended range of 6.5–8.5 for drinking water. Values within this range were assigned a score of 100, while values outside this range were penalized accordingly.
2. The EC score was calculated considering typical ranges for groundwater. Higher EC values suggest greater levels of dissolved salts, with penalties applied for concentrations exceeding threshold limits.
3. The F^- score was based on the standard limits for drinking water, with values exceeding 1.5 mg/L resulting in a lower score, reflecting increasing health risks associated with fluoride contamination.
4. The As**:** Like fluoride, the arsenic score was based on recommended limits for safe drinking water (0.01 mg/L). Higher arsenic concentrations resulted in lower scores.
5. The selenium score was evaluated according to the guideline value for drinking water (40 µg/L). Concentrations below the limit were assigned higher scores, while concentrations exceeding 40 µg/L were penalized to reflect increasing health risks.

Each parameter was assigned a normalized score, which was then aggregated to compute the overall GrWQI. The WQI was calculated as the average of the individual scores for each parameter:

$$GrWQI = \frac{(pH\ score + EC\ score + F\ score + As\ score + Se\ score)}{n} \qquad \text{(Eq. 1)}$$

Where n is the number of parameters analyzed. If a well had less than five parameters measured, the GrWQI calculation was normalized to account for the missing data.

2.4.2 Weighted Scoring System

Finally, each parameter was assigned a specific weight, with higher negative weights given to the hazardous elements (**Arsenic, Fluoride**, and **Selenium)** to reflect their potential health risks. The weights were as follows:

- **As: -3** (highest negative weight due to its toxicity and associated health risks);
- **F^-: -2** (negative weight due to the risks of dental and skeletal fluorosis);
- **Se: -1** (negative weight due to the potential harmful effects of excessive selenium);
- **EC: -0.5** (a lower negative weight as high EC values indicate salinity or contamination, but generally have less severe health consequences);
- **pH: +0.5** (positive weight, as pH values within the acceptable range indicate better water quality).

To calculate the GrWQI, each parameter's score is multiplied by its respective weight. The weighted scores are then summed and averaged to compute the final GrWQI. In the case where a parameter is missing (i.e., `NA`), its score is excluded from the calculation, but the remaining available parameters still contribute to the final index.

2.4.3 Normalization of GrWQI

To ensure that the final GrWQI value is between 0 and 100, the index is normalized by adjusting the weighted scores of all parameters. This is done by applying the following equation (Eq. 2):

$$Normalized\ GrWQI = \frac{(GrWQI - GrWQImin)}{(GrWQImax - GrWQImin)}\ x\ 100 \qquad \text{(Eq. 2)}$$

Where GrWQI min and GrWQI max are the minimum and maximum values.

This normalization ensures that the final GrWQI values fall within the 0-100 scale, where 100 represents the best water quality and 0 the worst.

2.4.4 Classification of Groundwater Quality Based on GrWQI

The resulting GrWQI is used to classify the groundwater quality into three categories:

- Water of Excellent Quality: GrWQI values close to 100 (typically above 90) indicate high water quality, safe for drinking without health risks.
- Water of Acceptable Quality: GrWQI values between 80 and 90 represent acceptable water quality, where some parameters may be approaching or slightly exceeding safe limits. These waters may require monitoring or treatment.
- Water of Poor Quality: GrWQI values below 80 indicate poor water quality with potential health risks. This category typically includes areas with elevated concentrations of contaminants such as arsenic, fluoride, or selenium, or where other parameters exceed safe limits.

The GrWQI provides an integrated measure of water quality, combining the effects of multiple parameters and their relative health risks to classify groundwater quality comprehensively.

2.4.5 Temporal Analysis of GrWQI

The GrWQI was calculated for each well across all available temporal measurements, focusing on departments with the highest risk of fluoride and arsenic contamination. For these departments, the temporal evolution of the GrWQI was analyzed to assess trends in water quality over time. The analysis focused on identifying fluctuations in water quality and potential periods of worsening or improvement, allowing for a detailed temporal perspective on the water quality dynamics in the most affected regions.

3. Results

After the hydrochemical and hydraulic database (N: 659) was cleaned, null values and blank entries were removed to enable statistical analysis (including information from Tables S1 and S2 in Supplementary materials). Outliers were retained. The distribution of the 504 wells (cleaned data) considered for the study is shown in Figure 1.

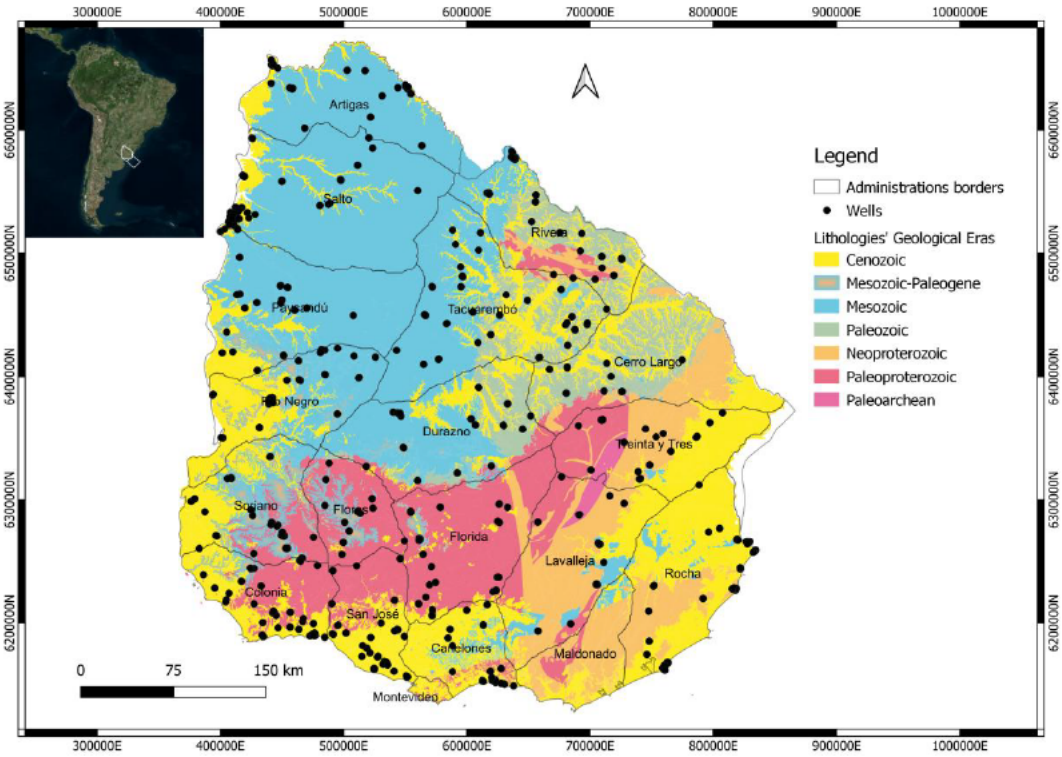

Figure 1. Location of Uruguay showing geological features and the distribution of 504 groundwater wells with complete hydrochemical data

3.1 Data analysis

3.1.1 Descriptive Statistics of Groundwater Monitoring Variables

A total of 504 wells were analyzed to assess the variability and central tendencies of key groundwater monitoring variables, including temperature (T), pH, electrical conductivity (EC), arsenic (As), fluoride (F^-), and selenium (Se). The descriptive statistics for these variables are summarized in Table 1, providing insights into their distribution and potential implications for groundwater quality.

Table 1. Summary Statistics. Descriptive statistics for groundwater monitoring variables

Variable	Min	Max	Median	Mode	Mean	SD	CV	Q1	Q3
T (°C)	2	28	18	19	16.4	6.4	39.3	16.0	21.0
pH	5.60	8.40	7.20	7.20	7.19	0.33	4.54	7.10	7.40
EC (µS/cm)	1	2996	598	644	638	490.2	76.8	223.5	842.5
As (mg/L)	0.001	0.046	0.004	0.002	0.007	0.006	92.9	0.002	0.011
F (mg/L)	0.231	2.50	0.350	0.350	0.515	0.256	49.7	0.350	0.630
Se (mg/L)	0.100	0.500	0.200	0.200	0.214	0.094	44.0	0.200	0.200

3.1.2 Temperature (T)

The temperature of groundwater ranged from 2 °C to 28 °C, with a median value of 18 °C and a mean of 16.4 °C. The mode, representing the most frequently observed temperature, was 19 °C, indicating that this value is common across the dataset. The standard deviation (SD) of 6.4 °C reflects moderate variability in groundwater temperatures, while the coefficient of variation (CV) of 39.3% suggests relatively high relative dispersion. The interquartile range (IQR), spanning from 16.0 °C to 21.0 °C, highlights that most wells exhibit temperatures within this range. These results suggest that groundwater temperatures are influenced by both seasonal variations and local geothermal gradients.

3.1.3 pH

The pH values of the groundwater samples ranged from 5.60 to 8.40, with a median and mode of 7.20, indicating slightly alkaline conditions. The mean pH was 7.19, aligning closely with the median, which suggests a symmetric distribution around the central tendency. The low standard deviation (0.33) and coefficient of variation (4.54%) indicate minimal variability in pH levels across the wells. The IQR, ranging from 7.10 to 7.40, further confirms that most wells have pH values within a narrow range. These findings suggest that groundwater pH is relatively stable, likely due to buffering mechanisms in the aquifer system.

3.1.4 Electrical Conductivity (EC)

Electrical conductivity (EC), a proxy for dissolved solids in groundwater, exhibited a wide range of values, from 1 µS/cm to 2996 µS/cm, reflecting significant spatial variability. The median EC was 598 µS/cm, while the mean was slightly higher at 638 µS/cm, suggesting a right-skewed distribution influenced by a few high-conductivity outliers. The mode of 644 µS/cm indicates the most frequently observed EC value. The standard deviation (490.2 µS/cm) and coefficient of variation (76.8%) highlight substantial variability in EC levels, likely driven by differences in geological composition and anthropogenic influences. The IQR, spanning from 223.5 µS/cm to 842.5 µS/cm, encompasses most of EC values, emphasizing the heterogeneity of groundwater salinity.

3.1.5 Arsenic (As)

Arsenic concentrations ranged from 0.001 mg/L to 0.046 mg/L, with a median of 0.004 mg/L and a mean of 0.007 mg/L. The mode of 0.002 mg/L indicates that low arsenic concentrations are most common. However, the high coefficient of variation (92.9%) and standard deviation (0.006 mg/L) suggest significant variability, potentially linked to localized contamination sources or geochemical processes. The IQR (Q3-Q1), spanning from 0.002 mg/L to 0.011 mg/L, captures the bulk of the data but also highlights the presence of elevated arsenic levels in some wells. Arsenic shows a distribution pattern comparable to fluoride, largely governed by the geochemical composition of aquifer materials and water-rock interactions that mobilize arsenic through specific hydrochemical mechanisms. These findings underscore the importance of monitoring arsenic concentrations to ensure compliance with health-based guidelines.

3.1.6 Fluoride (F^-)

Fluoride concentrations varied from 0.231 mg/L to 2.50 mg/L, with a median and mode of 0.350 mg/L, indicating that this value is both central and frequent. The mean fluoride concentration was slightly higher at 0.515 mg/L, reflecting the influence of a few high-fluoride wells. The standard deviation (0.256 mg/L) and coefficient of variation (49.7%) suggest moderate variability, possibly due to differences in geological formations or water-rock interactions. The IQR, spanning from 0.350 mg/L to 0.630 mg/L, encompasses most fluoride values, but the upper range approaches levels that could pose health risks if consumed over prolonged periods.

3.1.7 Selenium (Se)

Selenium concentrations ranged from 0.1 mg/L to 0.5 mg/L, with a median and mode of 0.2 mg/L, indicating that this value is both central and frequent. The mean selenium concentration was slightly higher at 0.214 mg/L, reflecting a relatively symmetric distribution. The standard deviation (0.094 mg/L) and coefficient of variation (44.0%) suggest moderate variability, likely influenced by differences in soil composition and redox conditions. The IQR, spanning from 0.2 mg/L to 0.2 mg/L, indicates minimal spread in the central portion of the data, suggesting that selenium levels are relatively consistent across most wells. The coincidence values of Q1, median, and Q3 for Se reflect the low dispersion of the dataset. This pattern is attributed to the limited variability in measured concentrations and the rounding of analytical results, which were mostly reported as 0.2 mg/L.

3.2 Correlation Analysis

The skewness and kurtosis values for each transformation were assessed to ensure improved normality (Hatem et al., 2022). The results indicated that the log-transformed and square root-transformed arsenic values exhibited better distribution characteristics compared to the original data. Following these transformations, the data were scaled to ensure that each variable contributed equally to the PCA and clustering results.

The original data for As showed a skewness of 1.65 and kurtosis of 3.62, indicating positively skewed, leptokurtic distribution; and for EC showed a skewness of 1.38 and kurtosis of 3.35, indicating positively skewed, slightly leptokurtic distribution.

The As data was transformed as log (As + 0.001) and EC as squared root. After transformation, the log-transformed data of As exhibited a skewness of 0.372 and kurtosis of -1.091, and for the square root of EC (skewness: 0.046 and kurtosis: -0.12), indicating a more symmetric distribution and reduced heavy tails compared to the original data, a near-normal distribution with minimal skew and a slightly platykurtic shape, providing the most favourable results in terms of normality.

Following these transformations, the data were scaled to ensure that each variable contributed equally to the Correlation matrix, PCA, and clustering results.

The Correlation matrix (Pearson) of the transformed variables reveals several important relationships between the parameters analyzed in Table 2. A moderate negative correlation was observed between As log (Arsenic concentration transformed) and pH (−0.603), suggesting that higher levels of arsenic are generally associated with lower pH values. This finding aligns with previous studies indicating that acidic conditions may enhance the solubility and mobility of arsenic in groundwater systems.

Table 2. Pearson correlation matrix of hydrochemical variables (pH, EC_sqrt: square root of EC, F: fluoride, As_log: arsenic log10, and Se: selenium)

Variable	pH	EC_sqrt	F	As_log	Se
pH	1.000	0.190	-0.218	-0.603	0.057
EC_sqrt	0.190	1.000	-0.211	0.392	-0.013
F	-0.218	-0.211	1.000	-0.038	-0.771
As_log	-0.603	0.392	-0.038	1.000	-0.278
Se	0.057	-0.013	-0.771	-0.278	1.000
T	0.409	0.254	0.583	-0.282	-0.534

Fluoride (F) and temperature (T) show a high positive correlation (0.583), which may suggest increased fluoride release at higher temperatures, possibly linked to deep sources or desorption processes.

EC_sqrt and As_logis positively correlated (0.392), which may be related to higher ionic strength in areas with elevated arsenic concentrations.

Additionally, the Se (selenium) variable exhibits a significant negative correlation with F^- (fluoride) (−0.771), indicating an inverse relationship between these two elements. This could suggest that higher concentrations of fluoride are generally associated with lower selenium concentrations, potentially due to geochemical processes that influence their co-occurrence in groundwater.

The correlation between EC_sqrt (square root transformation of EC) and F^- was also noteworthy (0.392), reflecting a moderate positive relationship. This suggests that fluoride concentrations tend to increase with higher

conductivity, which may be indicative of more mineralized groundwater, where fluoride and other ions are more readily available.

The relationships observed in the matrix are valuable for understanding the geochemical interactions in the study area, which could inform future monitoring and remediation strategies. Notably, while correlations were generally weak to moderate, they provide insights into the potential geochemical processes affecting groundwater quality. It is worth noting, however, that Pearson correlation analysis is only an initial exploratory tool, and further approaches such as ionic ratios, saturation indices, or hydrogeochemical modeling would be required to confirm specific geochemical processes. These findings will be important for designing efficient groundwater monitoring networks and informing decision-making for water quality management in the region.

3.3 Distribution of As, F^-, and Se over Uruguayan Departments

To analyse the variability and distribution of fluoride and arsenic concentrations across different departments, boxplot was generated (Figure 2), as well as for Se (Figure S1, Supplementary materials), as an initial general analysis of the situation in the Uruguayan country. Data from Montevideo and Maldonado departments were not considered, as these areas were not included in the groundwater dataset provided by OSE (the national water company) (OSE, personal communication, September 2025). However, an expanded national database that includes these departments is currently being developed to support future studies on groundwater quality across the entire country.

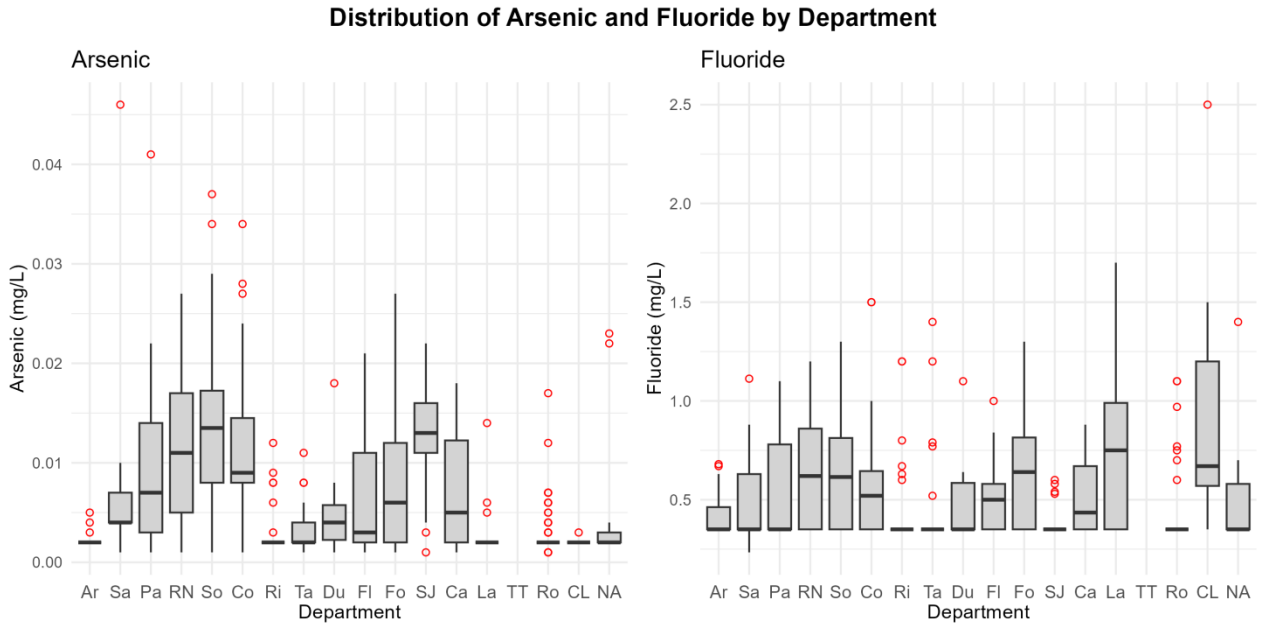

Figure 2. Boxplot for fluoride (right) and arsenic (left) by 17 Uruguayan departments

Department abbreviations: Artigas: Ar, Salto: Sa, Paysandú: Pa, Río Negro: RN, Soriano: So, Colonia: Co, Rivera: Ri, Tacuarembó: Ta, Durazno: Du, Florida: Fl, Flores: Fo, San José: SJ, Canelones: C, Lavalleja: La, Treinta y Tres: TT, Rocha: Ro, Cerro Largo: CL. NA: No available data.

Fluoride concentrations in groundwater ranged from 0.231 to 2.5 mg/L. The higher median values and broader ranges are observed in departments such as Cerro Largo, Flores, Lavalleja, Río Negro, and Soriano, suggesting localized areas with elevated fluoride levels. Outliers, particularly above 1.5 mg/L, are noted in several departments. The highest value (2.5 mg/L) was detected in the Cerro Largo department, exceeding the WHO guideline maximum of 1.5 mg/L. This anomaly is likely associated with the geological characteristics of the Tres Islas Formation, which may contribute to elevated fluoride levels through natural leaching processes.

Regarding As, departments such as Colonia, Río Negro, San José, and Soriano exhibit higher median concentrations compared to others. Although overall As levels remain relatively low, several outliers exceed 0.02 mg/L, mainly in Colonia, Paysandú, Salto, Soriano, and Treinta y Tres.

Selenium concentrations were generally low across Uruguay, ranging from 0.10 to 0.50 mg/L (mean = 0.21 mg/L, median = 0.20 mg/L). Detectable Se levels were found in a few departments, mainly Canelones, Salto, Rivera, Flores, and Cerro Largo. The highest median value was observed in Canelones (0.45 mg/L), while Salto and Rivera presented moderate levels (around 0.20 mg/L). All detected concentrations exceeded the WHO guideline value of 0.01 mg/L, indicating that selenium enrichment, although spatially limited, can occur in specific hydrogeochemical environments (Fernández-Martínez & Charlet, 2009; Nicolli et al., 2010; WHO, 2022). This pattern suggests that Se distribution may be linked to the geochemical composition of local aquifer materials or to reducing conditions that favour selenium mobilization.

These results highlight a spatial heterogeneity in groundwater quality, with certain departments showing a greater tendency toward elevated fluoride and arsenic concentrations, which may influence groundwater use for drinking and irrigation purposes.

3.4 Principal Component Analysis (PCA) and Clusters Analysis

3.4.1 Principal Component Analysis (PCA)

The principal component analysis (PCA) revealed that the first two principal components (PC1 and PC2) together explain approximately 65.34% of the total variance in the dataset, with PC1 alone accounting for 41.67% and PC2 for 23.68%. PC3 and PC4 account for an additional 17.93% and 16.72%, respectively, leading to a cumulative variance explanation of 100% when all four components are considered. Results from PCA can be found in Table S3 of the Supplementary material.

According to the PCA Loadings, PC1 is mainly associated with negative loadings of pH (-0.568), arsenic (-0.545), fluoride (-0.517), and EC_sqrt (-0.337). This suggests that PC1 captures a general gradient where higher pH, arsenic, and fluoride concentrations, as well as electrical conductivity, tend to co-vary. PC2 is predominantly influenced by EC_sqrt (0.883) with a strong positive loading and to a lesser extent by fluoride (-0.462). This indicates that PC2 reflects variability mainly related to electrical conductivity, somewhat opposing fluoride concentrations. PC3 shows a strong positive association with arsenic (0.834), suggesting that this component captures variability specifically linked to arsenic concentrations independent of the other variables. PC4 is characterized by a high positive loading of pH (0.707) and a strong negative loading of fluoride (-0.637), indicating a secondary axis of variability related to the interplay between pH and fluoride levels.

Principal Component Analysis (PCA) combined with K-means clustering identified four distinct hydrochemical groups among the groundwater samples. The first two principal components (PC1 and PC2), which together explained approximately 65.34% of the total variance, were sufficient to differentiate these clusters. PC1 was primarily associated with higher fluoride (F), arsenic (As), and pH values, while PC2 was mainly driven by the variability in electrical conductivity (EC). This indicates that groundwater geochemistry is largely influenced by both salinity-related processes and the enrichment of fluoride and arsenic, likely controlled by water-rock interaction and mineral dissolution mechanisms.

3.4.2 Clusters Analysis

Clusters of each department are presented in Table S4 in Supplementary material, and Figure 3 illustrates the projection of groundwater wells onto the first two principal components (PC1 and PC2), coloured by the four clusters identified through K-means clustering.

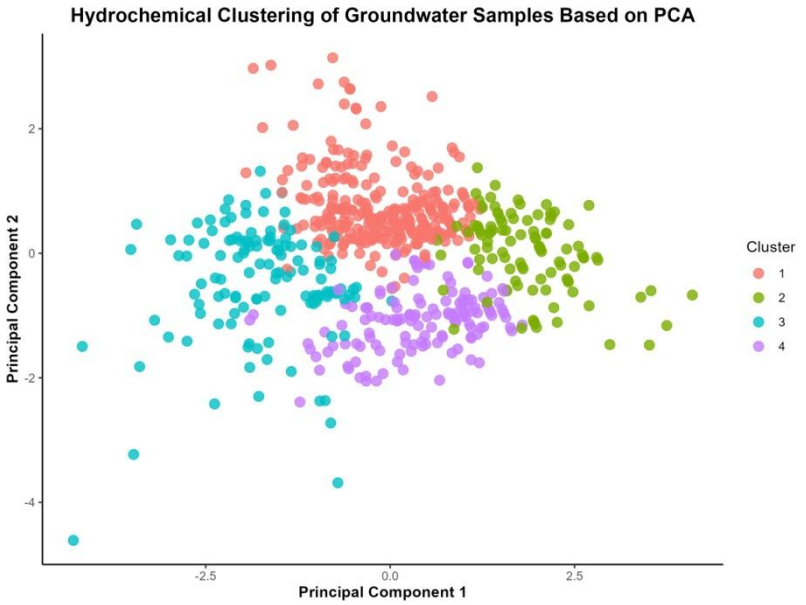

Figure 3. Hydrochemical clustering of the groundwater samples, discriminated by PCA

The biplot clearly demonstrates the spatial separation among hydrochemical groups in the reduced PCA space, where PC1 reflects the joint influence of pH, fluoride, and arsenic concentrations, and PC2 is mainly driven by electrical conductivity. Cluster 1 occupies the upper-central region, suggesting moderate to high levels of chemical constituents. Cluster 2 is distinctly shifted toward the right along PC1, indicating lower fluoride and arsenic content. Cluster 3 is in the lower-left quadrant, associated with higher fluoride and arsenic and lower salinity. Cluster 4 is positioned closer to the lower-central region, representing wells with low mineralization and moderate geochemical signatures. This multivariate structure reinforces the notion that different geochemical processes, such as silicate weathering, redox-driven arsenic mobilization, and variations in mineral dissolution, govern groundwater composition across the country.

Cluster 1 (n = 291) is composed mainly of wells distributed across Artigas, Canelones, Colonia, Durazno, Flores, Florida, Lavalleja, Paysandú, Río Negro, Rivera, Rocha, Salto, San José, Soriano, Tacuarembó, and Treinta y Tres. This group is characterized by groundwater with moderate to elevated fluoride and arsenic concentrations, and slightly alkaline pH values. These characteristics suggest a dominant influence of silicate weathering and potential leaching from volcanic or sedimentary aquifer materials. However, a more detailed hydrogeochemical analysis would be required to confirm these processes. The mean EC was 910 µS/cm (median = 755 µS/cm), suggesting relatively high ionic content in the groundwater of this cluster. This could indicate the presence of dissolved salts or other dissolved ions, such as sulphates or chlorides, which may be sourced from the local geology or land use practices. The average fluoride concentration was 0.423 mg/L (median = 0.35 mg/L), which is above the WHO guideline value (WHO, 2022) of 1.5 mg/L for F^- in drinking water, indicating potential geogenic fluoride contamination. The As was relatively low, with a mean of 0.00614 mg/L (median = 0.004 mg/L), which may suggest limited mobilization of arsenic under the current geochemical conditions. The pH value, averaging 7.27 (median = 7.26), indicates neutral to slightly alkaline water, which is common in many groundwater systems where carbonate minerals are present, buffering the water to neutral pH.

Cluster 2 (n = 103) includes wells predominantly located in Río Negro and Florida. The mean EC in Cluster 2 was lower at 400 µS/cm (median = 384 µS/cm), suggesting that the groundwater in this cluster is less mineralized compared to Cluster 1. The fluoride concentration was 0.363 mg/L on average (median = 0.35 mg/L), indicating a moderate level of fluoride that may also be geogenic, as fluoride often occurs naturally in certain volcanic or sedimentary rocks. The As concentration was much lower at 0.0024 mg/L, on average (median = 0.002 mg/L),

which may indicate a more favourable redox environment for the immobilization of arsenic, or a lower availability of iron and organic matter needed for As mobilization. The pH of 6.65 (median = 6.7) suggests slightly acidic conditions, which could promote the dissolution of certain minerals like aluminium and iron oxides, potentially influencing the fate of As.

Cluster 3 (n = 128) includes wells predominantly located in Colonia, Paysandú, Río Negro, Salto, and Soriano. This cluster represents groundwater with comparatively lower fluoride and arsenic levels and moderate electrical conductivity, reflecting less mineralized water possibly associated with younger recharge zones or different lithological settings. Cluster 3 exhibited the highest EC of 778 µS/cm (median = 708 µS/cm), pointing to a higher concentration of dissolved solids, possibly from mineral dissolution or anthropogenic contamination (e.g., agricultural runoff). The F^- concentration was notably high, with an average of 0.911 mg/L (median = 0.84 mg/L), indicating significant fluoride enrichment, which could be attributed to the leaching of fluoride-rich minerals such as fluorspar or phosphate rocks. The As concentration in this cluster was the highest, averaging 0.0139 mg/L (median = 0.014 mg/L), which suggests that the groundwater may be influenced by reducing conditions that facilitate the release of arsenic from iron oxyhydroxides. A high F^- and As co-occurrence could also indicate a shared geochemical process such as the dissolution of arsenic-bearing minerals (e.g., arsenopyrite) under low redox potential. The pH of 7.38 (median = 7.4) indicates mildly alkaline conditions, which are typically associated with the dissolution of carbonates and the precipitation of hydroxides, both of which can impact the solubility of trace metals like arsenic.

Cluster 4 (n = 137) had the lowest EC at 109 µS/cm (median = 83 µS/cm), which suggests relatively low mineralization, likely representing a region with fresh groundwater or limited interaction with mineralized rocks. The average fluoride concentration was 0.460 mg/L (median = 0.35 mg/L), indicating moderate levels of fluoride, which might be linked to local rock types that contain soluble fluoride-bearing minerals. The arsenic concentration was 0.00667 mg/L on average (median = 0.005 mg/L), suggesting moderate arsenic levels, which could be related to the dissolution of arsenic-bearing minerals under specific redox conditions. The pH of 7.30 (median = 7.3) suggests near-neutral conditions, like Cluster 1, which could reflect a balance between processes such as carbonate dissolution and the buffering effect of dissolved bicarbonates. The departments with values closest to the mean for EC, As, and pH in Cluster 4 primarily include those with higher pH values, such as Lavalleja, Treinta y Tres, and Canelones. However, Cluster 4 appears to encompass several departments with significantly lower values in terms of EC, such as Cerro Largo, Soriano, and Artigas. This suggests that Cluster 4 represents a range of behaviours in relation to these parameters.

Overall, the cluster separation highlights the hydrogeochemical heterogeneity of Uruguay's groundwater resources, emphasizing the necessity for targeted monitoring strategies adapted to different water quality typologies.

3.5 Spatial Distribution Maps

Spatial distribution maps revealed localized hotspots of fluoride contamination, particularly in areas with specific lithological features (Figure 4). These findings suggest that the exposure risks are not uniformly distributed, with certain populations being disproportionately affected.

The maps depict the mean concentration of fluoride and arsenic in groundwater. Fluoride concentrations are represented by a color gradient from light pink (lowest concentrations) to dark red (highest concentrations). Similarly, the arsenic map follows the same color gradient, highlighting regions with elevated arsenic concentrations. Both maps show that some departments have higher concentrations, with distinct geographic patterns influenced by lithological factors. These findings emphasize the spatial variability in contamination levels, indicating that certain regions may be at higher risk for fluoride and arsenic exposure.

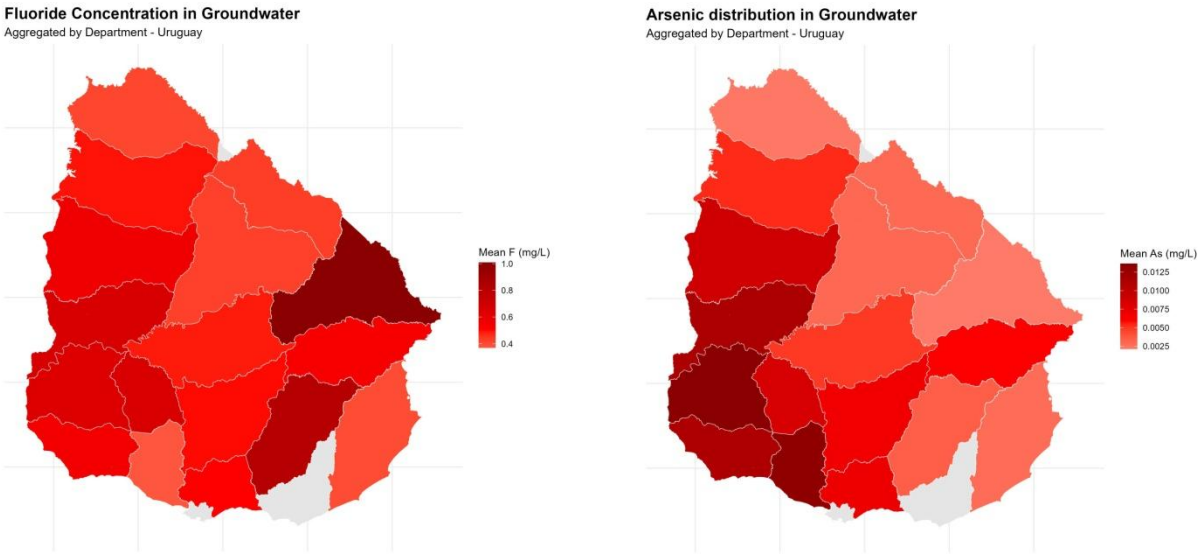

Figure 4. Spatial distribution of fluoride (left) and arsenic (right) concentrations in groundwater by department in Uruguay

3.6 Relationship Between Aquifer Type and Arsenic and Fluoride Concentrations

The relationship between aquifer type and the mean concentrations of As and F^- in the groundwater samples was evaluated (N = 1006). The data were grouped by hydrogeological system (identified in the Aquifer column), and the mean concentrations were calculated for each group of Wells (Table 3). Even with missing data, such Aquifer and for some samples, the analysis showed clear patterns.

Table 3 presents Aquifer data categorized by OSE and private users, both relating to groundwater sources.

To facilitate the identification of general trends and minimize the influence of extreme values, mean concentrations of arsenic and fluoride were calculated for each aquifer group.

Table 3 includes both fractured aquifers (crystalline basement and Arapey aquifer) and sedimentary aquifers. Last mentioned comprise Carboniferous-Permian aquifers (Melo Group, Tres Islas Fm, and Yaguarí Fm related aquifers aquitards); Kretacic aquifers (Mercedes Fm and Guichon Fm related aquifers), and Cenozoic age aquifers (Raigon Fm, Villa Soriano Fm, Paso del Puerto Fm, and Chuy Fm related aquifers).

Exploratory analysis revealed substantial differences in arsenic (As) and fluoride (F^-) concentrations among the studied aquifer systems. Sedimentary aquifers, particularly the Raigón Formation, exhibited the highest mean arsenic concentration (0.014 mg/L) among the aquifers with a substantial number of samples (N = 50). Similarly, the Mercedes Formation (0.013 mg/L, N = 17), the combined Guichón/Mercedes aquifer (0.011 mg/L, N = 28), and the Guichón Formation alone (0.009 mg/L, N = 11) also showed elevated arsenic concentrations. These results point to the Cretaceous sedimentary units, particularly Guichón and Mercedes, and the Cenozoic Raigón aquifer as important sources of arsenic in groundwater. The Paso del Puerto Formation displayed the highest mean As concentration overall (0.023 mg/L) but given the limited number of samples (N = 7), this result should be interpreted with caution. Similarly, the Villa Soriano Formation also showed a high mean As concentration (0.014 mg/L, N = 4).

In contrast, fractured aquifers, such as the crystalline basement (Fractured Aquifer) and the Arapey basalt aquifer, showed lower mean arsenic concentrations (0.004–0.007 mg/L). These low values are consistent with the limited presence of arsenic-bearing minerals and reduced water-rock interaction in hard rock aquifers compared to sedimentary environments.

Table 3. Mean concentrations of arsenic (As) and fluoride (F^-) by aquifer

Aquifer	As (mg/L)	F^-(mg/L)	N
Arapey	0.004	0.450	135
Arapey / Yaguarí	0.002	0.350	2
Basalt	0.004	0.538	6
Chuy	0.002	0.381	37
Chuy / Grupo Rocha	0.002	0.350	3
Fractured Aquifer	0.007	0.593	151
Fray Bentos	0.005	0.379	2
Fray Bentos/ Arapey	0.008	0.381	2
Fray Bentos/ Guichón	0.007	0.264	1
Grupo Rocha	0.002	0.350	1
Guichón	0.009	0.425	11
Guichón / Arapey	ND	0.350	1
Guichón / Mercedes	0.011	0.751	28
Melo	0.002	0.615	2
Mercedes	0.013	0.692	17
Paso del Puerto	0.023	0.350	7
Piedras de Afilar	0.002	0.825	2
Puerto Gómez	0.002	0.350	2
Raigón	0.014	0.383	50
Salto	0.007	0.580	2
Salto / Arapey	0.004	0.317	1
Salto / Fray Bentos	0.006	0.372	2
Tacuarembó	0.002	0.350	23
Tres Islas	0.002	1.400	4
Unknown	0.007	0.506	494
Villa Soriano	0.014	0.350	4
Yaguarí	0.004	0.350	12
Yaguarí / Fractured Aquifer	ND	0.350	2

ND indicates no data available. N: number of samples considered.

Significant average levels of fluoride were detected in both Guichón/Mercedes aquifer (0.751 mg/L F^-) and the Mercedes Formation (0.692 mg/L F^-), indicating that Cretaceous sedimentary formations also play a key role as sources of fluoride. The Tres Islas Formation had a high average fluoride concentration (1,4 mg/L F^-, N = 4), but these results should be interpreted cautiously because there were only a few samples.

A substantial portion of the samples (N = 494) could not be associated with a specific aquifer formation and were therefore classified under “Unknown Aquifer.” These samples were excluded from the statistical analysis, as they may correspond to different hydrogeological systems. Nonetheless, their presence highlights the need to improve geological and hydrogeochemical characterization in groundwater monitoring programs across the country.

3.7 Groundwater Quality Based on the GrWQI

Normalized GrWQI mean values results for each well (N = 1006) by department, aquifer, and year are presented in Table S5 in Supplementary materials.

The GrWQI values provide a comprehensive overview of groundwater quality across various departments in Uruguay. By integrating five key parameters (pH, EC, F^-, As, and Se) and applying a weighted, normalized scoring system, the GrWQI reflects both the chemical safety and the suitability of groundwater for human consumption. The index emphasizes contaminants with higher health risks (arsenic, fluoride, and selenium) through higher negative weights, while rewarding parameters within acceptable standards (e.g., pH).

1. Overall Trends and Quality Distribution:

The normalized GrWQI values obtained exhibit a broad variability across the study area, ranging from values near 0 to approximately 100. This distribution highlights significant spatial differences in groundwater quality, with some departments demonstrating excellent conditions, while others are severely impacted by contamination. In general, most wells displayed low GrWQI scores, indicating widespread groundwater quality concerns.

2. Departments with Poor Groundwater Quality:

Several departments, including Rocha, Soriano, and Salto, show a substantial number of wells with GrWQI values below 20. These low scores point to high concentrations of hazardous elements, particularly arsenic and fluoride, exceeding safe drinking water limits. Given the weighted importance of these parameters, the results suggest a critical need for focused mitigation and management in these regions.

3. Spatial Variability and Potential Localized Contamination:

The significant variation in GrWQI values within departments suggests not only regional differences but also localized contamination sources. In departments such as Flores, Treinta y Tres, and Soriano, minimum GrWQI values indicate that while the average groundwater quality may be moderate, specific observation points exhibit severely degraded water quality. This heterogeneity underscores the importance of site-specific assessments alongside broader regional evaluations.

4. Spatial Variability of GrWQI by Department:

The spatial variability of the Groundwater Quality Index (GrWQI) across the Uruguayan departments between 2009 and 2019 is shown in Figure 5. The mean GrWQI values (Table S6, Supplementary material) indicate generally moderate groundwater quality in most departments, although some regions exhibit wider interquartile ranges, reflecting some local variability and potential influence of hydrogeological or anthropogenic factors.

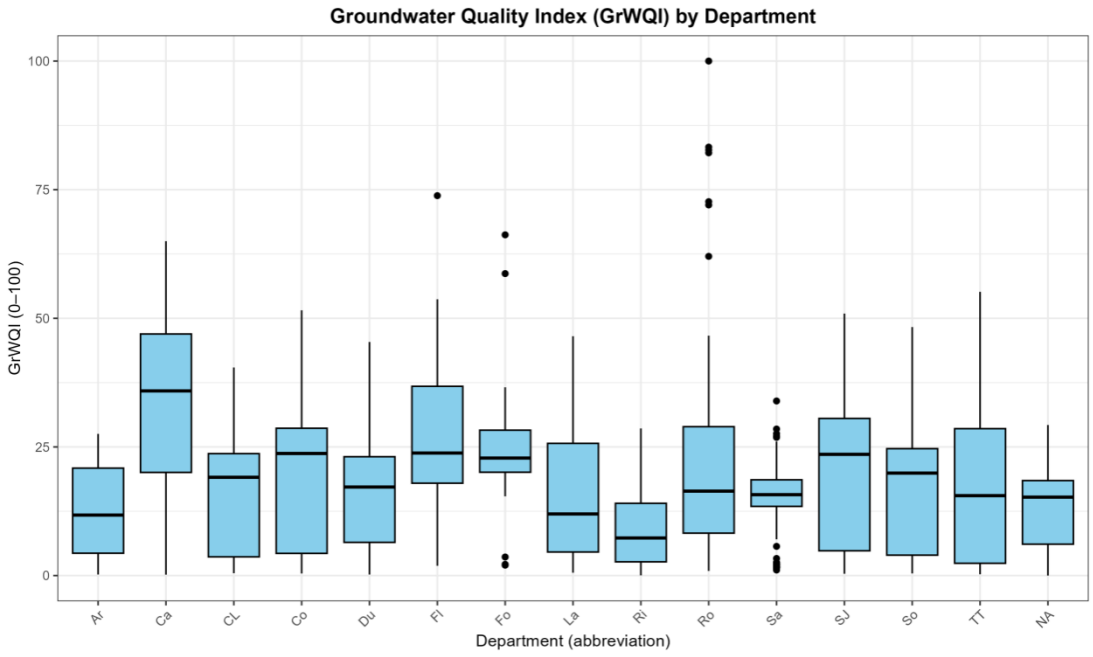

Figure 5. Spatial distribution of the Groundwater Quality Index (GrWQI) across Uruguayan departments during 2009-2019

Boxplots represent the variability and central tendency of groundwater quality, evidencing spatial heterogeneity among departments. NA: not available data.

The distribution of normalized Groundwater Quality Index (GrWQI, 0-100) values across departments highlights substantial spatial variability in groundwater quality. Departments such as **Canelones (mean GrWQI = 33.1)** and **Florida (25.3)** exhibit higher median values and relatively moderate variability, indicating better overall groundwater quality. In contrast, **Rivera (9.1)** and **Tacuarembó (10.4)** show the lowest mean GrWQI values, reflecting consistently lower water quality and higher risk of contaminants exceeding safe limits.

This spatial heterogeneity highlights the importance of regional-scale monitoring and the need to consider both natural and land-use related drivers of groundwater quality.

4. Discussion

4.1 Groundwater Hydrochemistry

Groundwater is a critical resource for drinking water supply, agriculture, and industrial activities worldwide. However, its quality is increasingly threatened by natural processes and anthropogenic activities, which can introduce contaminants or alter hydrochemical properties (Mukherjee & Singh, 2018). Understanding the variability of key groundwater parameters such as T, pH, EC and concentrations of As, F^-, and Se is essential for assessing its suitability for irrigation, human consumption, and other uses.

The variability observed in these parameters underscores the importance of systematic monitoring and statistical analysis to identify trends, assess risks, and inform management strategies. The following discussion interprets the descriptive statistics presented in Table 1 within the broader context of groundwater quality assessment, highlighting both the implications for human health and the need for targeted interventions.

The observed differences in EC, F^-, As, and pH values across the clusters analysis are indicative of various geochemical processes occurring in the groundwater.

- Fluoride and Arsenic Behaviour: In general, fluoride and arsenic concentrations are influenced by the dissolution of minerals from the surrounding geology. Fluoride is often mobilized from fluoride-rich minerals under neutral to alkaline conditions (Li et al., 2020; Pazand & Aghavali, 2022), which is consistent with the relatively high concentrations found in Clusters 1, 3, and 4 (Figure 3). Arsenic, on the other hand, is commonly released in reducing environments, particularly when iron oxyhydroxides, which can absorb arsenic, are reduced to iron (Fe^{2+}), resulting in the release of arsenic into solution (Yadav et al., 2015). Cluster 3 may be experiencing this process, as higher arsenic concentrations were observed in this group, particularly under slightly alkaline conditions that may favour the dissolution of arsenic-bearing minerals.
- Redox Conditions: Redox conditions in these aquifers vary according to the pH, with Cluster 2 being more acidic and Cluster 1 and Cluster 3 more alkaline, based on their pH values. The acidic conditions in Cluster 2 might be enhancing the solubility of certain metals, such as iron and aluminum, which could influence the fate of arsenic by causing its adsorption onto iron oxides (Foster & Chilton, 2003; Solaiman et al., 2009; Xu et al., 2025; Yadav et al., 2015). The slightly alkaline conditions in Clusters 1 and 3 promote carbonate mineral dissolution, likely leading to higher EC values in these areas.
- Ion Exchange and Mineral Dissolution: The relatively high EC values in Clusters 1, 3, and 4 could also be attributed to ion exchange processes, where calcium, sodium, and magnesium ions from the groundwater interact with minerals in the aquifer matrix. This can lead to the release of dissolved ions, further increasing the EC. This hypothesis requires further hydrogeochemical analysis for confirmation. Additionally, the dissolution of salts such as sulfates or chlorides can also contribute to the elevated EC levels.

4.2 Hydrogeology and Hydrochemical Process

The variation in water chemistry across the clusters suggests a complex interplay of geological, chemical, and environmental factors that influence groundwater composition. These findings highlight the importance of understanding local hydrogeochemical processes in managing water quality and assessing potential health risks, especially concerning fluoride and arsenic concentrations (Li et al., 2024).

Aquifer lithology and geological origin play a pivotal role in determining groundwater quality. In sedimentary aquifers, paleoenvironmental and paleogeographic conditions, together with source rock composition, influence the resulting lithology and, consequently, the mineralogy directly related to groundwater quality. Uruguayan sedimentary aquifers, particularly those of Cretaceous and Cenozoic age (especially Raigón Aquifer and Litoral Kretacis System Aquifer), tend to pose a greater risk for natural arsenic and fluoride contamination, whereas fractured volcanic and crystalline basement aquifers in general exhibit lower concentrations of these elements. This pattern is consistent with global observations (Mukherjee et al., 2024), where sedimentary environments are often associated with elevated geogenic arsenic and fluoride levels. Moving forward, research efforts should prioritize the refinement of aquifer classification schemes, the expansion of spatial and temporal sampling networks, and the detailed investigation of the geochemical processes driving contaminant mobilization. Such initiatives are essential for improving groundwater resource management and developing effective strategies to mitigate public health risks.

Future research should focus on refining aquifer classification, expanding sample coverage, and investigating the geochemical mechanisms responsible for contaminant mobilization, to support better groundwater management and risk mitigation.

4.3 Importance of the Weighted GrWQI Approach

The weighted GrWQI approach successfully captured the differential health impacts of various contaminants (Li et al., 2021; Poonia et al., 2021), offering a more realistic and risk-sensitive evaluation of groundwater quality compared to simple averaging. This methodology allows prioritization of high-risk areas based on health hazards rather than purely chemical thresholds, enhancing the relevance of the results for public health planning (Gaagai et al., 2023).

The detailed analysis of GrWQI by department highlights the spatial heterogeneity of groundwater quality across Uruguay. Departments such as Canelones and Florida consistently show higher mean GrWQI values, indicating better overall water quality, whereas Rivera and Tacuarembó exhibit the lowest scores, reflecting potential localized contamination and increased health risks. This department-level assessment reinforces the utility of the weighted GrWQI approach, enabling authorities to identify priority areas for monitoring and intervention. By integrating both the mean values and variability (standard deviation and range), stakeholders can develop more targeted management strategies (Rawat & Singh, 2018), ensuring resources are allocated efficiently and high-risk zones are closely monitored over time.

The GrWQI values offer a comprehensive overview of groundwater quality across various departments in Uruguay. These results underscore the value of the weighted GrWQI approach for prioritizing monitoring and management efforts, allowing resources to focus on areas with higher health risks.

GrWQI is a useful indicator for temporal monitoring. Temporal fluctuations in groundwater quality should be regularly assessed to identify trends of deterioration or improvement. Departments with consistently low or variable GrWQI values may benefit from enhanced surveillance programs, ensuring that emerging risks are promptly detected and addressed. Mapping the GrWQI index by department can help municipalities manage resources more effectively.

4.4 Public Health Implications

The widespread occurrence of low GrWQI scores, mainly because of increased concentrations of arsenic, fluoride, and selenium, is frequently observed and may have implications for public health (Gaagai et al., 2023; Li et al., 2021; Mañay et al., 2019). Long-term exposure to these elements can lead to serious conditions, such as carcinogenic effects, skeletal fluorosis, and other chronic health issues (Jha et al., 2020; Machado et al., 2020; Rawat & Singh, 2018). Wells with extremely low GrWQI values require urgent intervention, either through water treatment, provision of alternative safe water supplies, or public health advisories.

Implementing measures to mitigate these risks requires an integrated public health approach that combines scientific knowledge with policy, social, and technological actions (Jha et al., 2020). In Uruguay, as in many regions affected by geogenic contamination (Alvareda et al., 2025; Machado et al., 2020; Mañay et al., 2019; Pamoukaghlián et al., 2023; Wu et al., 2021), coordinated programs for monitoring, early detection, and management of arsenic and fluoride in groundwater are essential. Uruguay should promote both technological and nature-based solutions to reduce exposure, while strengthening community awareness and including geogenic contamination in health and environmental policy discussions. The effectiveness of these strategies should be periodically evaluated and updated according to new scientific evidence and environmental conditions (Jha et al., 2020).

4.5 Classification and Practical Applications

The GrWQI provides a simple yet powerful tool for classifying groundwater from excellent to poor quality based on combined chemical and health criteria (Jha et al., 2020). Its application supports decision-making in groundwater management (García Chávez et al., 2025; Jha et al., 2020), highlighting areas that require urgent remediation, continued monitoring, or protection efforts.

In Uruguay, the implementation of Water Safety Plans (WSPs) has become a cornerstone of national water policy, aligning with WHO's recommendations for risk-based management from source to consumer (Iriburo et al., 2019). Since 2012, the national water utility (OSE) has progressively developed and applied WSPs across its supply systems, supported by the National Water Plan in 2017 and the regulatory framework established by URSEA in 2018 (Rodríguez et al., 2019). This transition transformed the WSPs from a voluntary recommendation into a legal requirement, setting clear targets for full implementation in all water supply systems by 2030.

By 2019, OSE had already implemented WSPs in major cities such as Salto, Dolores, Mercedes, and Colonia del Sacramento, with additional systems under development in Paysandú and the Metropolitan Area (Rodríguez et al., 2019; Virginia et al., 2019). These advances demonstrate Uruguay's commitment to proactive risk management, integrating continuous monitoring, operational control, and staff training to ensure the safety and sustainability of drinking water supply. Such progress provides a valuable framework for managing contamination risks related to arsenic and fluoride, reinforcing the need for adaptive, region-specific monitoring strategies.

These findings underscore the importance of implementing regional water quality management strategies, especially in departments with identified risks. Efforts to reduce contamination, improve water treatment practices, and enhance public awareness about safe water usage are crucial steps in ensuring that all departments in Uruguay maintain safe drinking water standards in the future.

Further research should expand the dataset and improve models to better assess risk.

5. Conclusions

This study represents the first in-depth assessment of the spatial distribution of arsenic and fluoride in Uruguay's groundwater systems. Research conducted by integrating geostatistical approaches, multivariate statistical analysis, and applying a weighted Groundwater Quality Index (GrWQI) establishes clear links between water quality, geological origin, and the characteristics of different aquifer types.

Descriptive and multivariate analyses demonstrated considerable variation in groundwater chemistry among departments, with arsenic and fluoride concentrations frequently surpassing WHO guidelines in certain locations. Principal Component Analysis and cluster classification identified distinct groundwater typologies characterized by unique geochemical profiles, underscoring the significance of geological and hydrogeological influences on contaminant mobilization. Notably, several regions exhibited parameters –most prominently arsenic and fluoride– that consistently exceeded recommended drinking water standards, indicating national-scale heterogeneity in groundwater composition. Cluster 3 was specifically correlated with the highest concentrations of arsenic and fluoride and comprised wells from Colonia, Paysandú, Río Negro, Salto, and Soriano.

The GrWQI combined complex chemical data into a single index sensitive to risk, and provides a practical and health-focused tool for guiding groundwater management and prioritizing monitoring efforts across departments. Areas with the lowest GrWQI scores reflect reduced water quality and elevated potential health risks. Such zones may be suitable candidates for further remediation measures, expanded monitoring, and public health initiatives.

This work provides a baseline for evaluating national groundwater quality. Future efforts may involve enhancing aquifer characterization, creating predictive risk models, and combining health surveillance data. These measures support the management of groundwater resources and the safety of drinking water supplies in Uruguay.

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Transparency of Data

Data not available: The data set that supports the results of this study is not publicly available.

Author Contribution Statement

	E Alvareda	K Pamoukaghlián	M Cáceres	L Bessone	J Ramos	S Da Rocha	R Panzl	P Gamazo
Conceptualization	■	■						
Data curation	■		■					
Formal analysis	■	■	■					
Funding acquisition	■							
Investigation	■	■	■	■	■	■	■	■
Methodology	■	■	■			■	■	
Project administration	■							
Resources				■	■			■
Software	■			■				
Supervision	■							
Validation	■							
Visualization	■				■			
Writing – original draft	■							
Writing – review and editing	■	■						

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Supplementary Material

Table S1. Well data table showing water quality of the Permian aquifers

UTM Zone	UTM-X	UTM-Y	Z(m)	Department	Locality	Q (m^3/h)	Depth (m)	SL (m)	Hydrogeo Unit	EC (uS/cm)	Cl^- (mg/L)	Na^+ (mg/L)	F^- (mg/L)	Hardness (mg/L)	Alk (mg/L)
21 J	771900	6460508	136	Cerro Largo	Isidoro Noblia	7	205	1.14	GM/TI	301	18	46		44	101
21 J	771994	6461083	129	Cerro Largo	Isidoro Noblia	36.6	163	0	GM/TI	224	6.9	17		43	63
21J	782262	6461293	155	Cerro Largo	La Mina - E60	0.48	33	15.22	Y						
21H	775046	6436324	150	Cerro Largo	Pueblo Nando - E34	0.66	62	18.4	Y	567	7.7	30		294	293
21 H	774622	6413476	96	Cerro Largo	La Pedrera	1.7	130	0	TI	355	10	15	2.7	153	157
21H	725863	6388232	227	Cerro Largo	Cerro de las Cuentas	1.32	37.8	11.6	SG/TI	228	21	13	0.69	98	87
21 H	722333	6418485	151	Cerro Largo	Ramón Trigo - Esc. 83	0.4	60	9.5	GM/Y	546	48	75		98	160
21 H	722297	6418412	149	Cerro Largo	Ramón Trigo - Esc. 83	1.2	32	5	GM/Y	418		39		133	163
21 H	732833	6400267	150	Cerro Largo	Fraile Muerto	12	198	20	TI						
21 H	733113	6400596	150	Cerro Largo	Fraile Muerto	12	176	22.67	GM	638	57	66	0.67	159	190
21 H	715125	6394351	137	Cerro Largo	Tres Islas	2.5	60	7.35	TI	104	3.7	2.5		53	60
21 H	753733	6391184	209	Cerro Largo	Guazunambí	6.1	93	21.2	Y	105	8.2	8.2		24	29
21 H	740815	6385255	222	Cerro Largo	Ganem - Esc. 33	0	70		GM/Y						
21 H	741124	6384834	225	Cerro Largo	Ganem - Esc. 33	0	80		GM/Y						
21 H	740551	6385549	216	Cerro Largo	Ganem - Esc. 33	0	130		GM/Y	312					
21 J	641523	6397541	137	Durazno	Cuchilla de Ramirez - E57	1.2	102	4.61	GM	455		17		192	211
21 H	517284	6334221	87	Durazno	Los Tapes - E23	2.5	64	7.1	SG/B	661	15	67	0.65	212	314
21J	716366	6519604		Rivera	Cerrillada	0.25	21		Y		5			54	56
21J	716407	6519737		Rivera	Cerrillada	0.2	18		Y						
21J	652561	6525438	58	Rivera	La Calera - E13	1.8	18.7	6.6	Y	551		43		221	274
21J	667067	6523202	157	Rivera	Tres Puentes - E104	7.2	96	7.01	Y	619		30		256	301
21 J	709331	6497335	163	Rivera	Arroyo Blanco	7.2	55	4.81	Y	359	15	41		152	102
21 J	725524	6495854	139	Rivera	Hospital	1.2	33	2.5	TI	1147	107	197		153	359
21J	725493	6495900	130	Rivera	Hospital	0.8	62	3.4	TI	831	50	139		144	350
21J	712583	6477782		Rivera	Alborada (Plano 27348)	1	26	3.9	Y						
21 H	704054	6478896	159	Rivera	Chircas de Caraguatá	1.8	30	3.15	Y	553		12		287	263
21 H	675411	6516573	191	Rivera	Cerro Pelado	5.2	40	8.08	Y	550		38		314	229
21 H	713413	6454646	137	Rivera	Sarandí del Río Negro	1.2	56		GM	799	13	122	0.65	192	364
21 J	693271	6516166		Rivera	La Puente	6.6	62	5.02	Y	739	29			219	305
21 J	636923	6475459	238	Tacuarembó	Picada Quirino - E41	0	60		GM	10061	2688	313		169	75
21 J	635837	6475043	276	Tacuarembó	Poblado Heriberto	0	60		GM						
21 J	635849	6474405	135	Tacuarembó	Poblado Heriberto	0	25		GM						
21 H	700470	6454698	142	Tacuarembó	Paso Mariano	0	100		Y						
21 H	700469	6454668	146	Tacuarembó	Paso Mariano	0	44		Y	770					
21 H	684631	6462465	179	Tacuarembó	Puntas de Cinco Sauces	5	30	5.12	Y	48		7.5		14	
21 H	698012	6443869	149	Tacuarembó	Caraguata al Norte	1.2	70	8.3	Y	608	14	32		295	314
21 H	687372	6437669		Tacuarembó	Toscas de Caraguatá	4.2	51	7.12	Y						
21 H	687569	6438134	112	Tacuarembó	Toscas de Caraguatá	12	22		Y	559	0.5	52		201	258
21 H	685326	6449425		Tacuarembó	Paso Linvido	0	56		Y						
21 H	685273	6448631	110	Tacuarembó	Paso Linvido - E100	6	30	3.73	Y	366		53		467	78
21 H	697879	6443530	141	Tacuarembó	Caraguatá al Norte - E38	3	60	3.8	GM/Y	700	26	47		192	295
21 J	644710	6472253		Tacuarembó	Ansina	0.5	55.5	6.5	Y/SG						
21H	631920	6466302	106	Tacuarembó	Pueblo Semper	0	90		GM						
21J	631950	6466075	104	Tacuarembó	Pueblo Semper - E135	1	11	3.7	GM	360		34		138	169
21H	650269	6462280	128	Tacuarembó	Pueblo del Barro - (PL)	1.2	38		GM	526		88	0.59	86	270
21 J	671297	6461198	320	Tacuarembó	Los Rosas	3	90	1	GM/Y	2561	136	474	0.71	176	256
21H	650229	6462336	123	Tacuarembó	Pueblo del Barro	0	43		GM/Y						
21 J	672204	6461192	143	Tacuarembó	Los Rosas	0	70		GM/Y						
21H	671607	6448811	135	Tacuarembó	Puntas de Carretera	0.25	60	0	GM	3960		701		228	252
21H	670240	6448916	132	Tacuarembó	Puntas de Carretera	0.25	70	8.1	GM	1317	47	276	0.65	32	422
21 H	674573	6448005	111	Tacuarembó	Puntas de Carretera	0.6	100		GM	6760					
21 H	681320	6443793	151	Tacuarembó	Las Arenas	2.9	44	3	Y	197		26		47	95
21 H	677114	6446439	139	Tacuarembó	Las Arenas	0	50		GM/Y						
21 H	677807	6446012	138	Tacuarembó	Las Arenas	0.4	44	1.7	Y	216		16		79	89
21 H	610749	6446275	167	Tacuarembó	Cerros de Clara	0.55	30	12.5	Y	361	30	19		93	75
21H	682099	6416995	110	Tacuarembó	Las Chircas - E29	0.2	69	22.8	GM	12670		2411		1581	107
21 H	681831	6425579	125	Tacuarembó	Cerro Pereira	1.2	27	2.13	GM	944	60	145	1	419	178
21 H	684783	6410673		Tacuarembó	Las Pajas	0.8	80	23.15	GM/TI	3160	564	588	3		
21 H	684268	6410620	129	Tacuarembó	Las Pajas - PPLER	2.4	80	23.8	GM/TI	2762	555	49	2.9	142	339
21 H	681491	6407095		Tacuarembó	Las Pajas - PPLER	1.3	60	0.38	GM/TI	594	76	588	3	195	212
21 H	681544	6406144	106	Tacuarembó	Las Pajas	2.5	30	14.5	GM/TI	714	19	61	3	287	288
21H	681407	6407952	116	Tacuarembó	Las Pajas	5	22		TI	444		19	0.79	203	206
21 H	659187	6415483	104	Tacuarembó	Los Feos - E128	1	75	8	GM	1426	143	66	1	242	292
21 H	679015	6422134	117	Tacuarembó	Las Chircas	0	55		GM						
21 H	679108	6424041	143	Tacuarembó	Las Chircas	0	40		GM						
21 H	577087	6413871	175	Tacuarembó	Achar	1.8	25	9.2	Y	622	15	35		306	268
21 H	626714	6462234	103	Tacuarembó	Paso de los Novillos	4	40	0	GM/B	3210	687	629	0.81	21	129
21 H	625444	6462221	103	Tacuarembó	Paso de los Novillos	0.45	50	3	B	3530	760	763	0.67	28	131
21 H	626230	6462105	104	Tacuarembó	Paso de los Novillos	0	50		GM/B						
21 H	624612	6463147	126	Tacuarembó	Paso de los Novillos	0	8.5		A/B						
21 H	625064	6462677	102	Tacuarembó	Paso de los Novillos	0	53		GM/B						

Source. Extracted and modified from Pamoukaghlián et al. (2019).

Table S2. Well data table showing water quality (As, Fe, Mn, Zn, Pb, Cd, Cr, Cu, Se) of the Permian aquifers

UTM Zone	UTM-X	UTM-Y	Z(m) (m)	Department	Locality	As (mg/L)	Fe (mg/L)	Mn (mg/L)	Zn (mg/L)	Pb (mg/L)	Cd (mg/L)	Cr (mg/L)	Cu (mg/L)	Se (mg/L)
21 J	771900	6460508	136	Cerro Largo	Isidoro Noblia		5.4	0.03	5.4	0.002	< 0,004	0.004		< 0,004
21 J	771994	6461083	129	Cerro Largo	Isidoro Noblia		0.07	0.03	0.13	0.002	< 0,004	< 0,002	<0,06	< 0,004
21J	782262	6461293	155	Cerro Largo	La Mina - E60		1.9					< 0,002	<0,06	
21H	775046	6436324	150	Cerro Largo	Pueblo Nando - E34		0.31	0.25	0.004	0.002	< 0,004	< 0,002	<0,06	<0,002
21 H	774622	6413476	96	Cerro Largo	La Pedrera		1.2	0.14	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21H	725863	6388232	227	Cerro Largo	Cerro de las Cuentas		0.006		0.004	0.002	0.002	< 0,002	<0,06	< 0,004
21 H	722333	6418485	151	Cerro Largo	Ramón Trigo - Esc. 83		0.44	0.07	0.2	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	722297	6418412	149	Cerro Largo	Ramón Trigo - Esc. 83		0.26	0.03	0.19	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	732833	6400267	150	Cerro Largo	Fraile Muerto									
21 H	733113	6400596	150	Cerro Largo	Fraile Muerto		0.5	0.06	0.11	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	715125	6394351	137	Cerro Largo	Tres Islas		0.34	0.03	0.004	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	753733	6391184	209	Cerro Largo	Guazunambí				0.71	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	740815	6385255	222	Cerro Largo	Ganem - Esc. 33									
21 H	741124	6384834	225	Cerro Largo	Ganem - Esc. 33									
21 H	740551	6385549	216	Cerro Largo	Ganem - Esc. 33									
21 J	641523	6397541	137	Durazno	Cuchilla de Ramirez - E57		0.19		0.76	0.002	0.002	< 0,002	<0,06	<0,002
21 H	517284	6334221	87	Durazno	Los Tapes - E23		0.06	0.03	0.04	0.002	0.002	< 0,002	<0,06	< 0,004
21J	716366	6519604		Rivera	Cerrillada		0.7							
21J	716407	6519737		Rivera	Cerrillada									
21J	652561	6525438	58	Rivera	La Calera - E13		0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21J	667067	6523202	157	Rivera	Tres Puentes - E104		0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,04	< 0,004
21 J	709331	6497335	163	Rivera	Arroyo Blanco				0.04	<0,002	<0,0004	<0,002	<0,06	
21 J	725524	6495854	139	Rivera	Hospital	0.013	0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21J	725493	6495900	130	Rivera	Hospital	0.008	0.07	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21J	712583	6477782		Rivera	Alborada (Plano 27348)									
21 H	704054	6478896	159	Rivera	Chircas de Caraguatá		0.06			<0,002	<0,0004	<0,002	<0,06	
21 H	675411	6516573	191	Rivera	Cerro Pelado					<0,002	<0,0004	<0,002	<0,06	
21 H	713413	6454646	137	Rivera	Sarandí del Río Negro		0.21	0.17	0.07	0.004	< 0,004	< 0,002	<0,06	<0,002
21 J	693271	6516166		Rivera	La Puente					<0,002	<0,0004	<0,002	<0,06	
21 J	636923	6475459	238	Tacuarembó	Picada Quirino - E41		0.66	0.46	1.8	0.002	< 0,004	< 0,002	<0,06	<0,003
21 J	635837	6475043	276	Tacuarembó	Poblado Heriberto									
21 J	635849	6474405	135	Tacuarembó	Poblado Heriberto									
21 H	700470	6454698	142	Tacuarembó	Paso Mariano									
21 H	700469	6454668	146	Tacuarembó	Paso Mariano									
21 H	684631	6462465	179	Tacuarembó	Puntas de Cinco Sauces				0.39	< 0,002	< 0,000	< 0,002	< 0,06	< 0,002
21 H	698012	6443869	149	Tacuarembó	Caraguata al Norte		7.3	0.03	0.14	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	687372	6437669		Tacuarembó	Toscas de Caraguatá									
21 H	687569	6438134	112	Tacuarembó	Toscas de Caraguatá		0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	685326	6449425		Tacuarembó	Paso Linvido									
21 H	685273	6448631	110	Tacuarembó	Paso Linvido - E100	0.009	0.1	0.03	0.13	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	697879	6443530	141	Tacuarembó	Caraguatá al Norte - E38		0.09	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 J	644710	6472253		Tacuarembó	Ansina									
21H	631920	6466302	106	Tacuarembó	Pueblo Semper		0.5			0.002	< 0,004	< 0,002	<0,06	
21J	631950	6466075	104	Tacuarembó	Pueblo Semper - E135	0.006	0.7	0.15	0.15	0.002	< 0,004		<0,06	
21H	650269	6462280	128	Tacuarembó	Pueblo del Barro - (PL)		0.06	0.03	0.09	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 J	671297	6461198	320	Tacuarembó	Los Rosas		0.78	0.06	0.06	0.003	< 0,004	0.003	<0,06	< 0,004
21H	650229	6462336	123	Tacuarembó	Pueblo del Barro									
21 J	672204	6461192	143	Tacuarembó	Los Rosas									
21H	671607	6448811	135	Tacuarembó	Puntas de Carretera		0.1	0.03	0.82	0.002	< 0,004	< 0,002	<0,06	< 0,004
21H	670240	6448916	132	Tacuarembó	Puntas de Carretera		0.06	0.03	0.09	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	674573	6448005	111	Tacuarembó	Puntas de Carretera									
21 H	681320	6443793	151	Tacuarembó	Las Arenas		0.06	0.03	0.29	0.002	< 0,004	< 0,002	<0,06	<0,002
21 H	677114	6446439	139	Tacuarembó	Las Arenas									
21 H	677807	6446012	138	Tacuarembó	Las Arenas		0.3	0.05	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21 H	610749	6446275	167	Tacuarembó	Cerros de Clara		0.29		0.23	<0,002	<0,0004	<0,002	<0,06	<0,002
21H	682099	6416995	110	Tacuarembó	Las Chircas - E29	0.01	0.92	0.06	0.39	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	681831	6425579	125	Tacuarembó	Cerro Pereira					<0,002	<0,0004	<0,002	<0,06	
21 H	684783	6410673		Tacuarembó	Las Pajas						< 0,004			
21 H	684268	6410620	129	Tacuarembó	Las Pajas - PPLER					<0,002	<0,0004	<0,002	<0,06	
21 H	681491	6407095		Tacuarembó	Las Pajas - PPLER		0.24	0.03	0.04	0.002	< 0,004	0.003	<0,06	<0,002
21 H	681544	6406144	106	Tacuarembó	Las Pajas		0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21H	681407	6407952	116	Tacuarembó	Las Pajas		0.06	0.03	0.04	0.002	< 0,004	< 0,002	<0,06	<0,002
21 H	659187	6415483	104	Tacuarembó	Los Feos - E128		0.06	0.03	0.14	0.002	< 0,004	< 0,002	<0,06	< 0,004
21 H	679015	6422134	117	Tacuarembó	Las Chircas									
21 H	679108	6424041	143	Tacuarembó	Las Chircas									
21 H	577087	6413871	175	Tacuarembó	Achar				0.04	<0,002	<0,0004	0.008	<0,06	
21 H	626714	6462234	103	Tacuarembó	Paso de los Novillos					<0,002	<0,0004	< 0,002	< 0,06	< 0,002
21 H	625444	6462221	103	Tacuarembó	Paso de los Novillos					<0,002	<0,0004	< 0,002	< 0,06	< 0,002
21 H	626230	6462105	104	Tacuarembó	Paso de los Novillos									
21 H	624612	6463147	126	Tacuarembó	Paso de los Novillos									
21 H	625064	6462677	102	Tacuarembó	Paso de los Novillos									

Source. Extracted and modified from Pamoukaghlián et al. (2019).

Table S3. Results of the importance of components in the PCA and the loadings

Importance	**PC1**	**PC2**	**PC3**	**PC4**
Standard deviation	1.2910	0.9732	0.8469	0.8179
Proportion of variance	0.4167	0.2368	0.1793	0.1672
Cumulative proportion	0.4167	0.6534	0.8328	1.0000
Loadings				
EC_sqrt	-0.3370	0.8831	-0.1202	-0.3033
As_log	-0.5445	-0.0759	0.8335	0.0536
pH	-0.5683	-0.0312	-0.4196	0.7070
F^-	-0.5165	-0.4619	-0.3385	-0.6365

Table S4. Results of departments by cluster

Cluster	**Department**
1	Salto
1	Canelones
1	Rocha
1	Río Negro
1	Treinta y Tres
1	Soriano
1	Florida
1	Paysandú
1	Colonia
1	San Jose
1	Durazno
1	Tacuarembó
1	Lavalleja
1	Artigas
1	Flores
1	Rivera
2	Salto
2	Río Negro
2	Cerro Largo
2	Canelones
2	Rocha
2	Paysandú
2	Rivera
2	Tacuarembó
2	Durazno
2	San Jose
2	Flores
2	Treinta y Tres
2	Florida
2	Artigas
2	Soriano
2	Lavalleja
3	Salto
3	Soriano
3	Florida
3	Flores

Cluster	Department
3	Lavalleja
3	Rivera
3	Paysandú
3	Río Negro
3	Treinta Y Tres
3	Cerro Largo
3	Rocha
3	Colonia
3	Tacuarembó
3	San Jose
3	Canelones
3	Durazno
4	Salto
4	Rocha
4	Cerro Largo
4	Florida
4	Durazno
4	Paysandú
4	Soriano
4	Canelones
4	Treinta y Tres
4	Tacuarembó
4	San Jose
4	Río Negro
4	Rivera
4	Colonia
4	Lavalleja
4	Artigas
4	Flores

Table S5. Mean Groundwater Quality Index (GrWQI) values by aquifer system in Uruguay

Aquifer System	Number of Samples (n)	Mean GrWQI
Arapey Aquifer	117	15.3
Fractured Aquifer (Precambrian Basement)	151	18.6
Raigón Aquifer	51	16.4
Paso del Puerto Aquifer	6	14.4
Yaguarí Aquifer	12	11.0
Chuy Aquifer	37	13.7
Cretaceous Aquifers (Mercedes/Guichón)	55	19.8
Tres Islas Formation	4	16.2
Salto Aquifer	4	8.0
Villa Soriano Formation	4	15.7

Table S6. Mean normalized Groundwater Quality Index (GrWQI) by department (2009-2019)

Department	Mean GrWQI	SD	Min_GrWQI	Max_GrWQI	N
Canelones	33.1	19.6	0.2	65.0	49
Florida	25.3	15.7	1.9	73.8	54
Flores	23.7	14.6	2.0	66.2	29
Rocha	21.8	20.3	0.9	100.0	95
Colonia	21.1	12.9	0.4	51.6	78
San Jose	20.7	13.8	0.4	50.9	68
Soriano	18.6	13.9	0.4	48.3	74
Treinta y Tres	17.7	16.0	0.3	55.1	26
Río Negro	17.1	7.5	1.9	29.3	45
Durazno	16.5	11.2	0.2	45.4	35
Lavalleja	16.4	12.7	0.6	46.5	23
Cerro Largo	16.2	12.1	0.5	40.4	25
Salto	15.0	7.0	1.1	33.9	146
Paysandú	14.6	6.9	0.2	26.4	63
Artigas	13.1	8.6	0.2	27.5	51
Tacuarembó	10.4	7.5	0.0	28.8	79
Rivera	9.1	7.3	0.0	28.6	66

Note. Mean of GrWQI (0-100), SD: Standard Deviation, Minimum: Min_GrWQI, Maximum: Max_GrWQI, and N: Number of Samples.

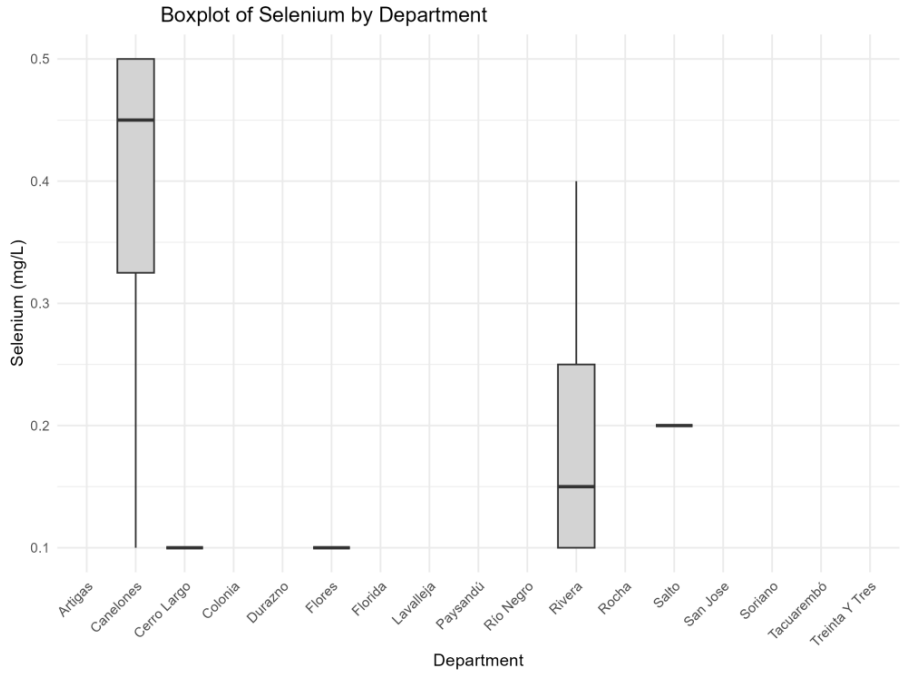

Figure S1. Boxplot for selenium (Se) by 17 Uruguayan departments

Departments: Artigas, Canelones, Cerro Largo, Colonia, Durazno, Flores, Florida, Lavalleja, Paysandú, Río Negro, Rivera, Rocha, Salto, San José, Soriano, Tacuarembó, and Treinta y Tres.