Produced Water Chemistry for Environmental & Agricultural Utilization

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Key Terms

Produced Water

Water that is produced as a byproduct during oil and gas extraction.

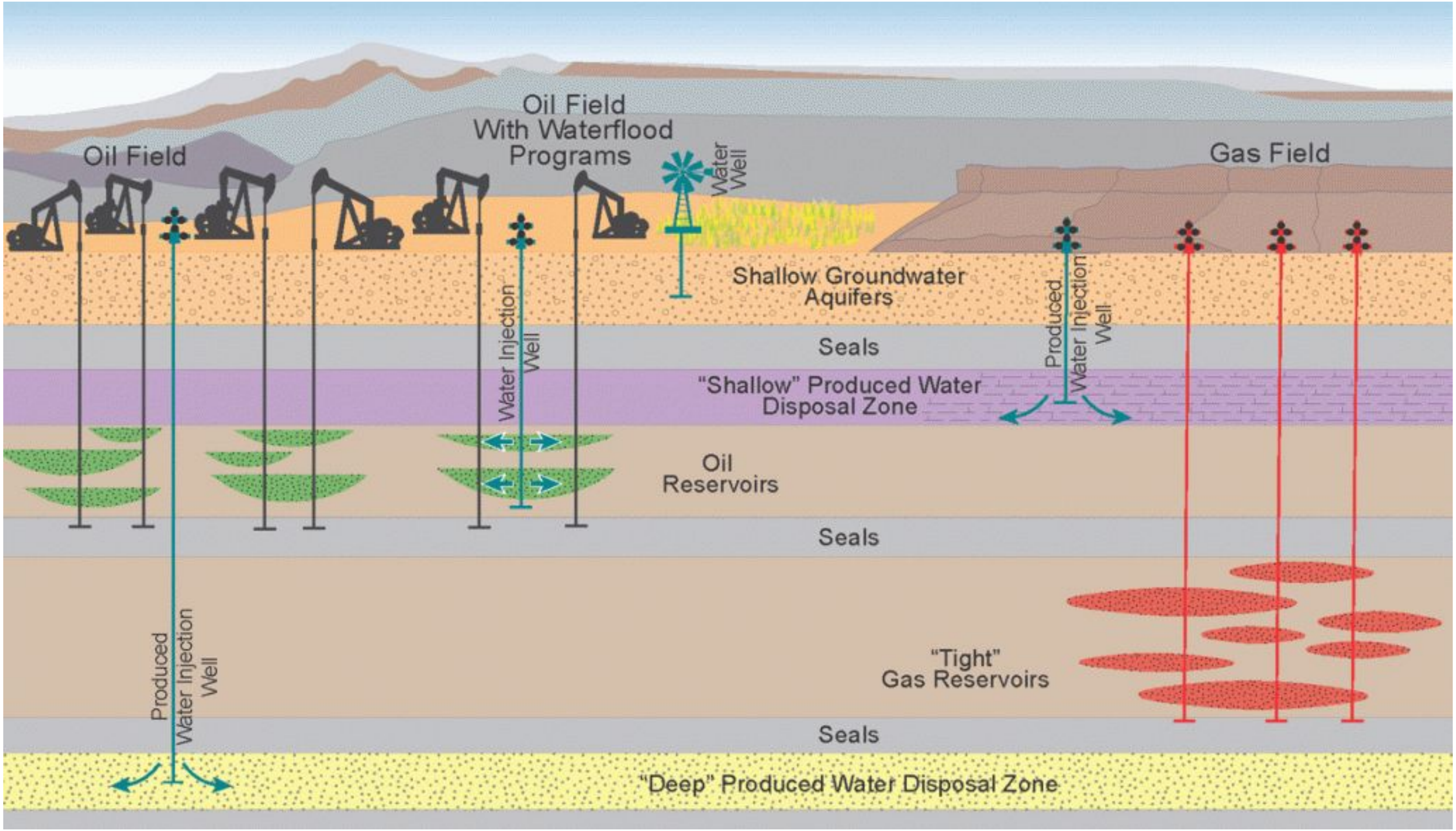
Scaling

When water has high levels of minerals (like Calcium Carbonate), that can build up on surfaces, this is called scaling. This can cause damage to appliances and pipes.

Critical Element

Elements that are high in demand yet have limited availability.

Elements that affect downstream treatment.



Oil Field
Oil Field
With Waterflood
Programs
Water
Well
Gas Field
Shallow Groundwater
Aquifers
Water Injection
Well
Produced
Water Injection
Well
Seals
"Shallow" Produced Water
Disposal Zone
Oil
Reservoirs
Seals
"Tight"
Gas Reservoirs
Produced
Water Injection
Well
Seals
"Deep" Produced Water Disposal Zone

Project Objectives

- To analyze the chemistry of produced water and identify elements that lead to scaling
- To identify lithium availability in produced water across basins in the United States

Data Cleaning & Filtering

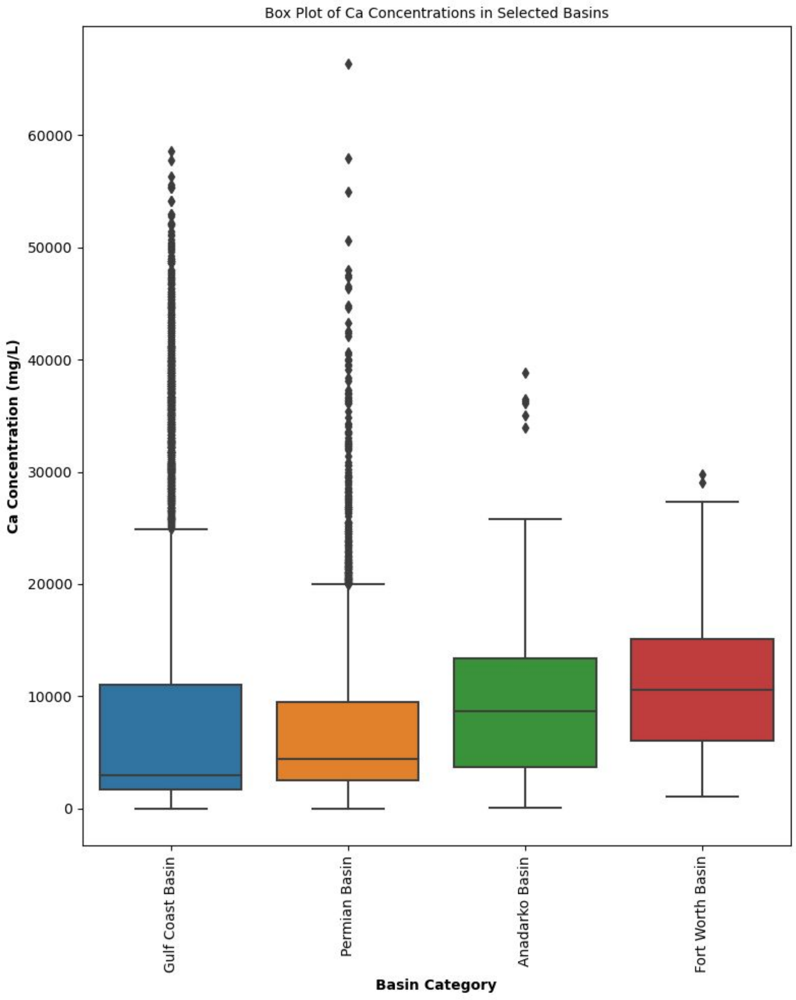
General Filtering

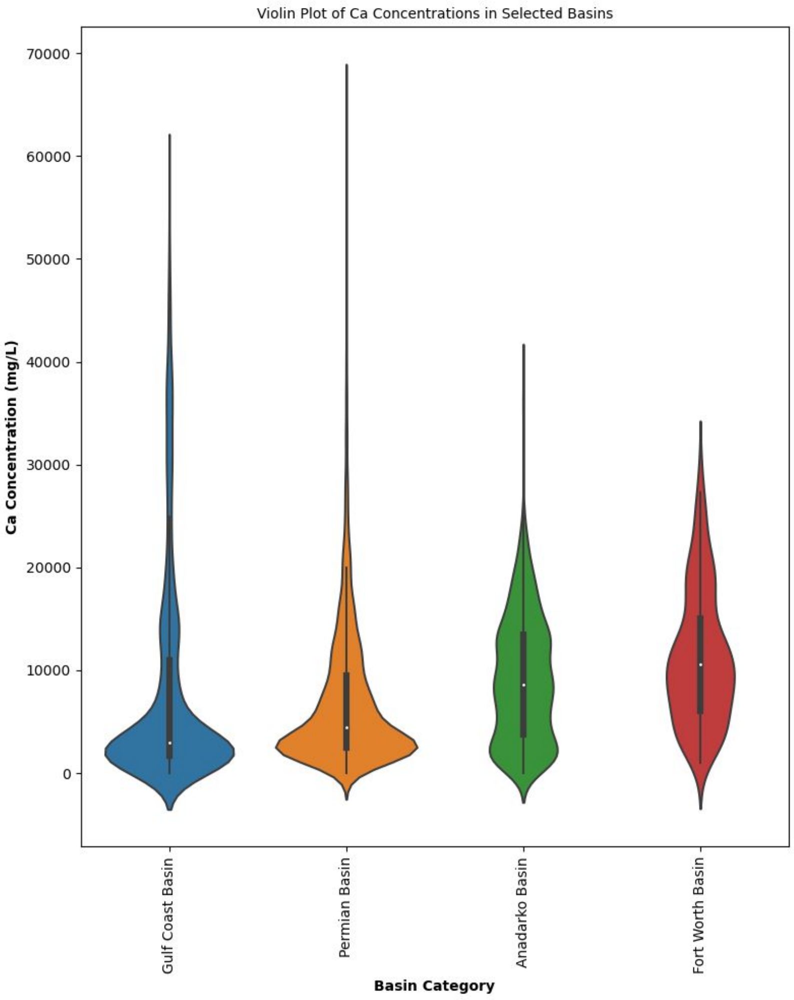
- Reduce columns
- Adjust for missing information
- Unit conversion

Technical Filtering

- Filter out samples for TDS less than 35,000
- Utilize industry accepted practices to adjust for missing concentrations
- Filter out unnatural chemical combinations

Box & Violin Plots

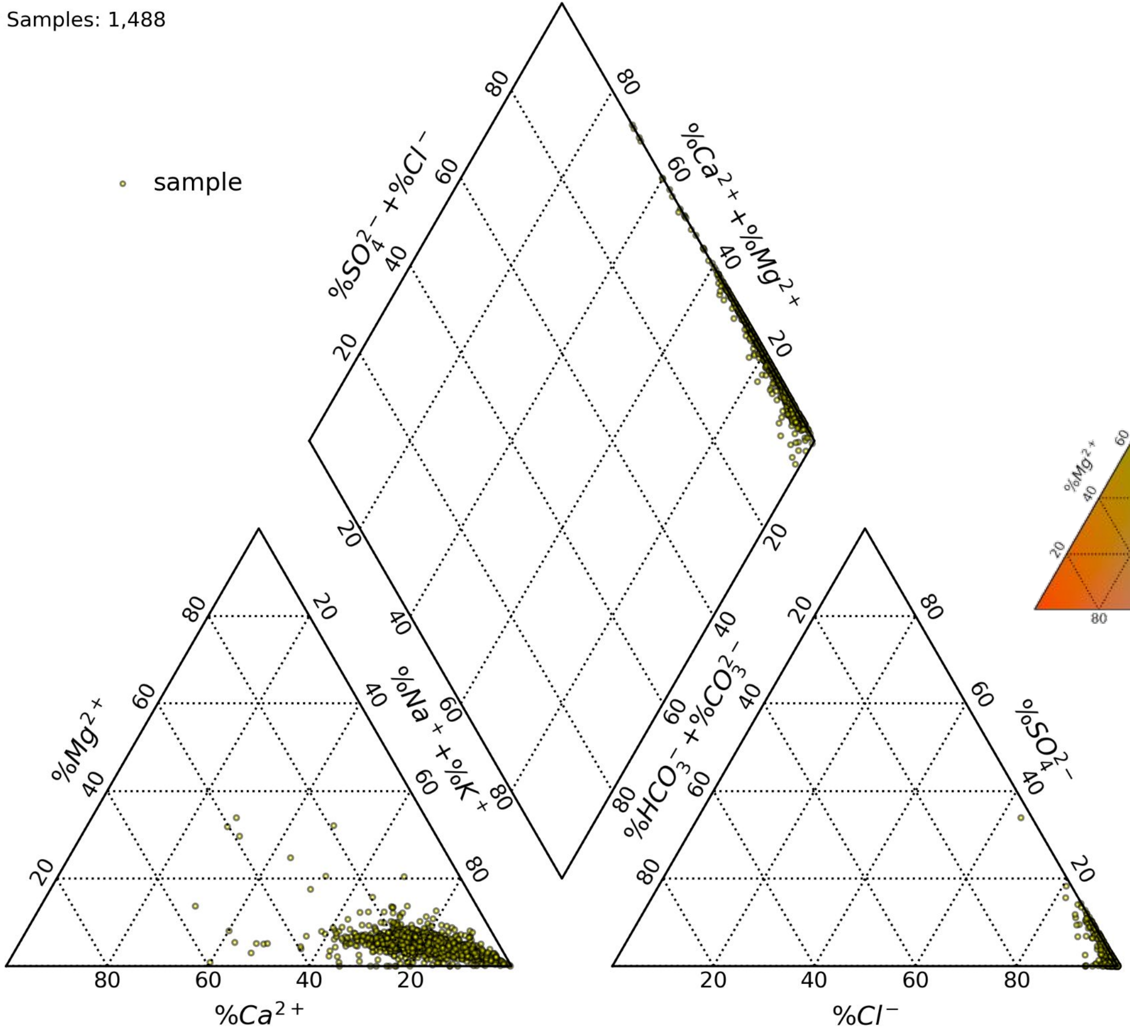


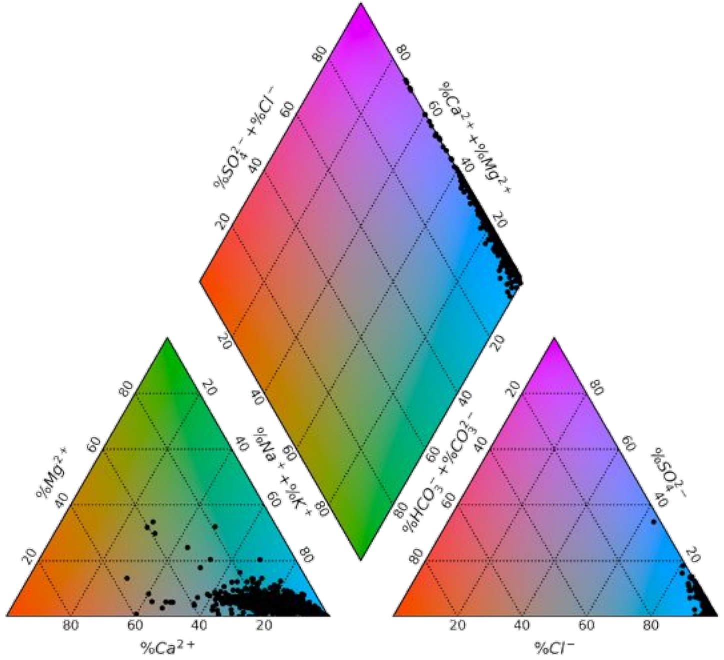


Piper Plots

Anadarko Basin

Samples: 1,488





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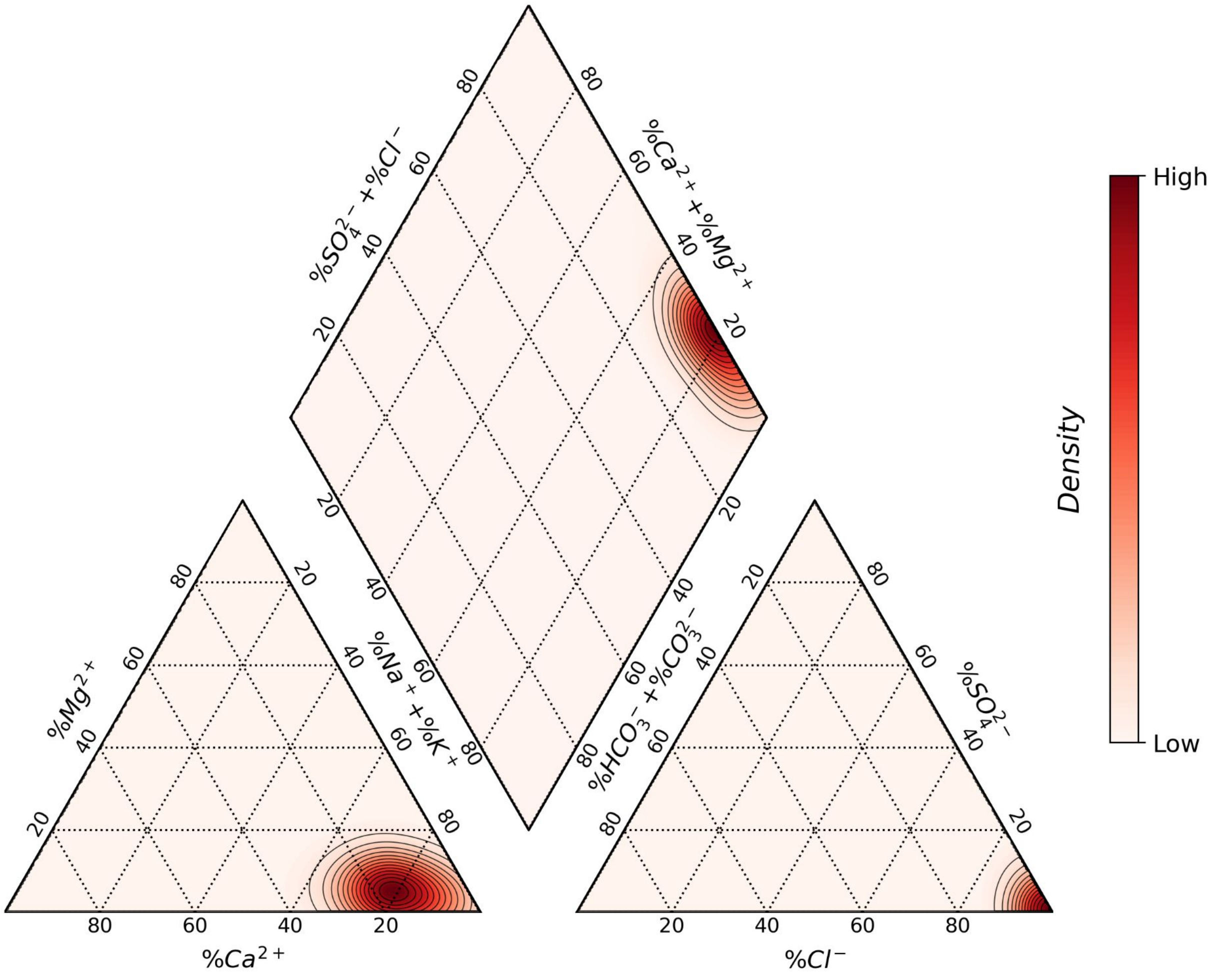
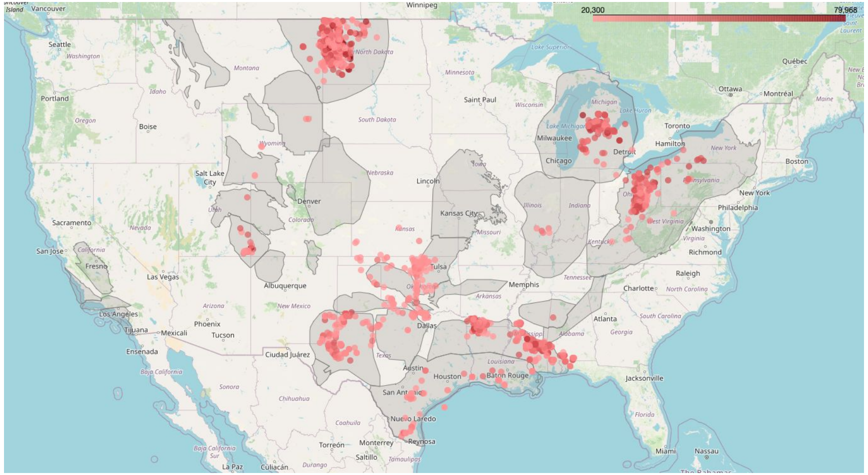
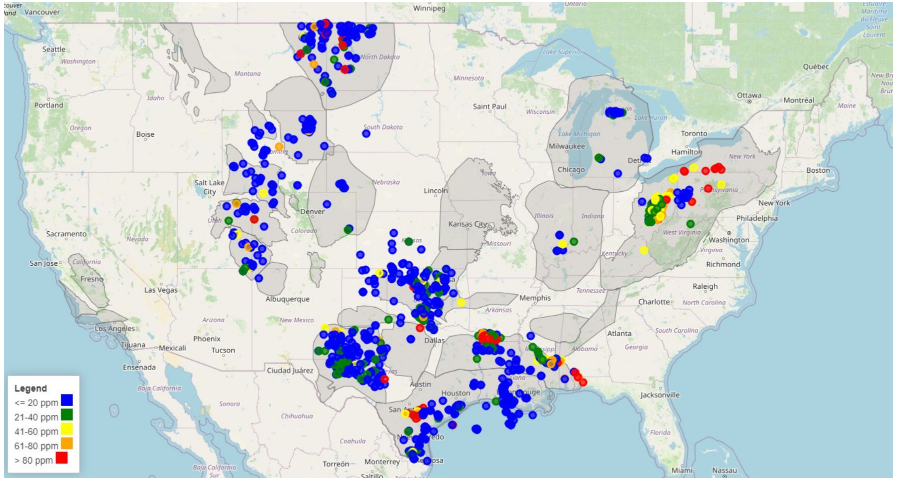


Geo Plots | Interactive HTML

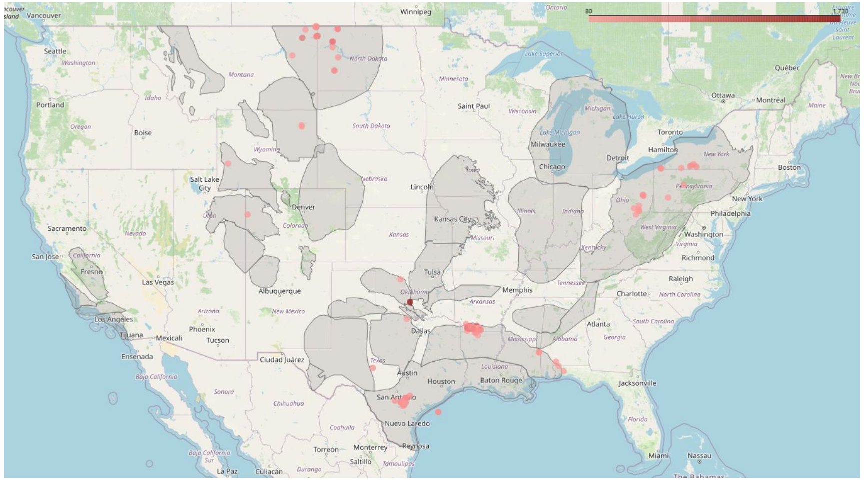
Scaling Elements (90th Percentile Gradient): Example Image Depicts Calcium



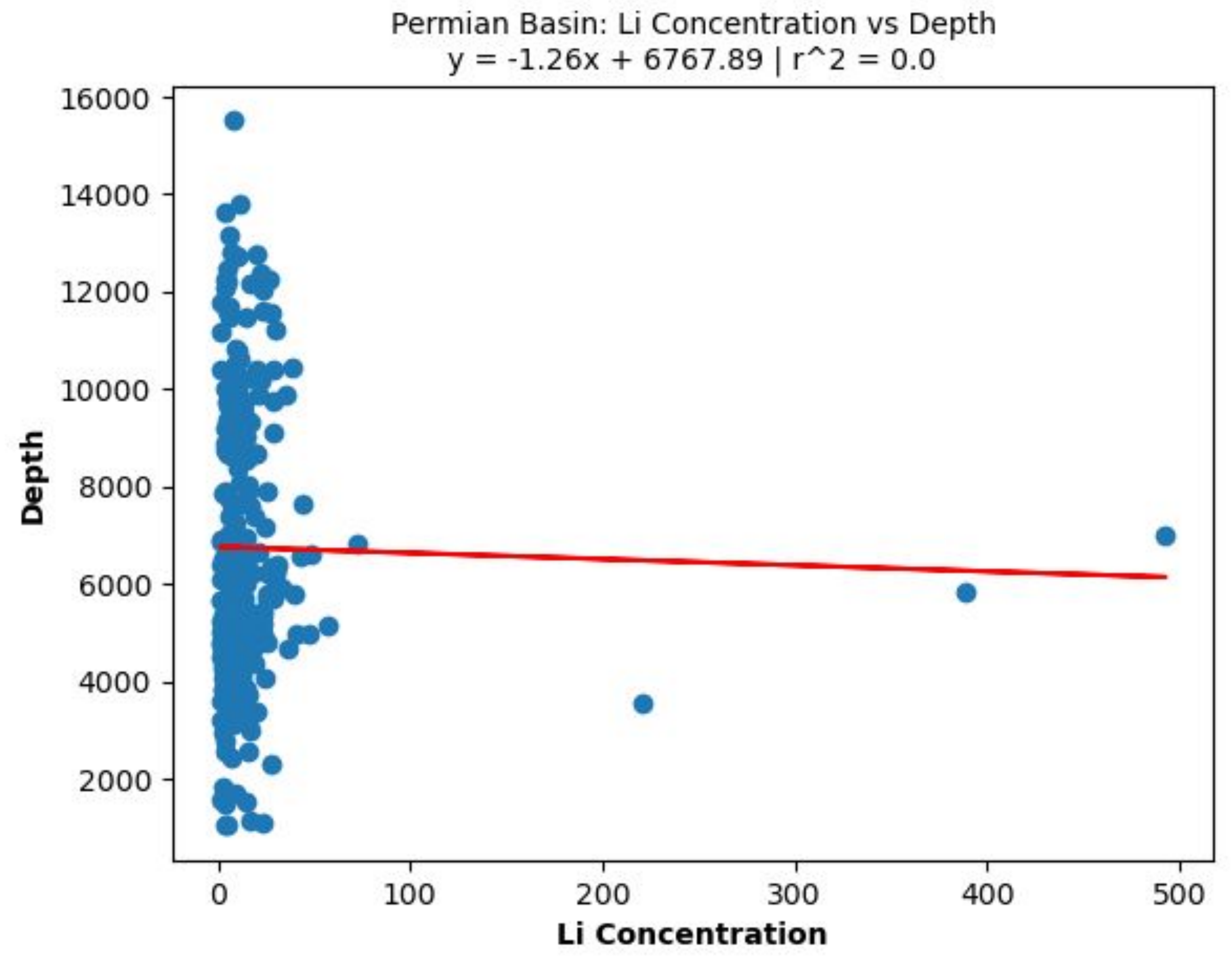
Lithium Availability (All Samples)



Lithium Availability (>80 ppm Gradient)



Linear Regression | Li Concentration vs Depth



Conclusion

Detailed Analysis of Produced Water

Understand the concentration of the primary elements affecting scaling to support implementing better management and treatment strategies.

Lithium Extraction Potential

Identify the areas to explore lithium extraction from produced water, turning a problem into a valuable resource.

Alignment with DOE Goals

This study aligns with the Department of Energy's objectives, supplying research that could lead to more sustainable industry practices.

Next Steps

Practical Methodologies

The approach taken in this study could be replicated in similar studies and applied in real-world scenarios.

Support for Better Water Management

The findings help support more sustainable water management practices, helping companies reduce environmental impacts.

Open Doors for Resource Recovery

The study encourages further exploration into recovering resources from produced water.

Questions?

Appendix

Database Utilization

The raw dataset for this study was sourced from the United States Geological Survey (USGS) website, available: https://data.usgs.gov/datacatalog/data/USGS:59d25d63e4b05fe04cc235f9 . This dataset contains extensive information on the chemistry of produced water from various sites. Due to the considerable size of the dataset, it was split into three separate CSV files to facilitate easier handling and uploading.

The individual CSV files were loaded into Pandas DataFrames. These separate DataFrames were then concatenated to form a single, comprehensive DataFrame representing the entire dataset. This step was crucial for ensuring a unified analysis across all data points.

Appendix - Data Cleaning and Filtering

Column Removal

Identify repeat samples from the same location at different dates, keeping only the most recent information

Data Filtering

Eliminate samples with Total Dissolved Solids (TDS) below seawater concentration (35,000 ppm)

Analyze and list elements causing scaling in water treatment (calcium, magnesium, carbonate, bicarbonate, silica, iron, barium, strontium), and assess lithium (Li) availability

Applying Conditions for Filtering

- Dataset is further refined
    - Focus on Molar Concentration relationships between elements
- The criteria are based on natural chemical balances

Appendix

Different strategies were employed to address missing values in various chemical constituents of the produced water.

Filling NaN Values for Basic Elements

For key elements such as Potassium and Sodium (KNa), Potassium (K), Sodium (Na), Calcium (Ca), Chlorine (Cl), Sulfate (SO4), and Magnesium (Mg), missing values (NaN) were filled with zeros. This approach was necessary for calculation purposes, allowing for further processing and analysis without data loss.

Calculating Sodium (Na) Values Where Missing

A more nuanced approach was taken for Sodium (Na) due to its importance and relationship with other elements. The calculation for Na was based on the presence or absence of KNa and K:

- If Na was missing but both KNa and K were present, Na was populated with the difference between KNa and K.
- If Na was missing, KNa was present, but K was not, Na was set equal to KNa. This conditional approach ensured a more accurate representation of the Na values in the dataset. Rows where Na or Cl were still missing after these calculations were removed from the dataset, as these elements are crucial for the study.

Appendix

Handling Carbonates

For Carbonate (CO_3) and Bicarbonate (HCO_3), missing values were also treated with specific strategies:

- Missing CO_3 values were replaced with zeros.
- Missing HCO_3 values were replaced with available Alkalinity as HCO_3 (ALKHCO3) values where possible.
- In cases where both HCO_3 and ALKHCO3 were missing, HCO_3 was calculated based on the difference between cations and anions, divided by the molar mass of HCO_3.

These steps were essential to maintain the chemical balance in the dataset and to ensure that carbonate chemistry was accurately represented.

Each of these strategies for handling missing data was chosen to respect the chemical properties and interactions of the elements involved, ensuring that the dataset remained scientifically valid and robust for subsequent analyses. The updated datasets, post these cleaning steps, were saved as df_filtered_Na_Cl.csv and df_filtered_estimated_HCO3.csv for further use in the study.

Appendix

Natural Conditions for Produced Water

A sample is considered representative of natural produced water if it typically meets the following conditions:

Molar Sodium (Na) greater than Molar Calcium (Ca): Reflecting the ion balance in natural water bodies where sodium is often more concentrated than calcium.

Molar Chlorine (Cl) greater than Molar Sulfate (SO_4): Based on the common occurrence of chloride as a dominant anion in many natural waters, particularly those associated with oil and gas production.

Molar Calcium (Ca) greater than half of Molar Magnesium (Mg): Indicative of the natural geochemical processes affecting water composition.

Applying these conditions helps filter the dataset to focus on samples that reflect the expected natural chemical composition of produced water. This step is crucial for ensuring the accuracy and reliability of the subsequent analyses.

The dataset, post-application of these conditions, offers a more accurate representation of natural produced water chemistry, essential for the objectives of the study.

Appendix - Applying Conditions for Filtering

The molar concentration of each element is calculated using its concentration in ppm and its molar mass. The formula used is:

$$Molarity(M) = \frac{Concentration(\frac{mg}{L})}{MolarMass(\frac{g}{mol})}$$

For the analysis, the following molar masses were used:
Sodium (Na): 22.99 g/mol
Calcium (Ca): 40.08 g/mol
Chlorine (Cl): 35.45 g/mol
Sulfate (SO4): 96.06 g/mol
Magnesium (Mg): 24.305 g/mol

Dividing the concentration of each element by its respective molar mass provides the molarity, which is a basis for comparison across different water samples.

Appendix - Methodology for Box and Violin Plots

- Basins are presented to the user
- User selects basin of interest
- Elements are chosen for a concentration analysis and a box plot is generated
- The plots display the distribution of the element’s concentration across the basins selected

Appendix - Methodology for Piper Plots

- Piper plots - graphical representations that help visualize and interpret the results of water chemical analyses
    a. Use ternary diagrams, a triangular graph that represents the relative proportions of three components (cations and anions) in a water sample.
    b. The three vertices of the triangle represent the three major components
- In Hydrogeochemistry, Piper plots are used to classify water types based on the concentrations of major ions.
- Helps to identify the dominant ions in the water and categorize it into different types
- A modified version of the available WQChartPy library was utilized to generate the piper plots for this data. The basic steps are as follows:
    a. Read in the concentrations of Ca, Mg, Na, K, HCO3, CO3, Cl, and SO4 in mg/L.
    b. Normalize the concentrations to 100% by dividing each ion concentration by the total ion concentration.
    c. Calculate the percentage contribution of each ion to the total ion concentration for each sample.
    d. Plot the points.