

Produced Water Chemistry for Environmental & Agricultural Utilization

Roxana Darvari | Brittany Svab | John Cahill | Sarah Cain | Alejandro Juarez

Key Terms

Produced Water

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

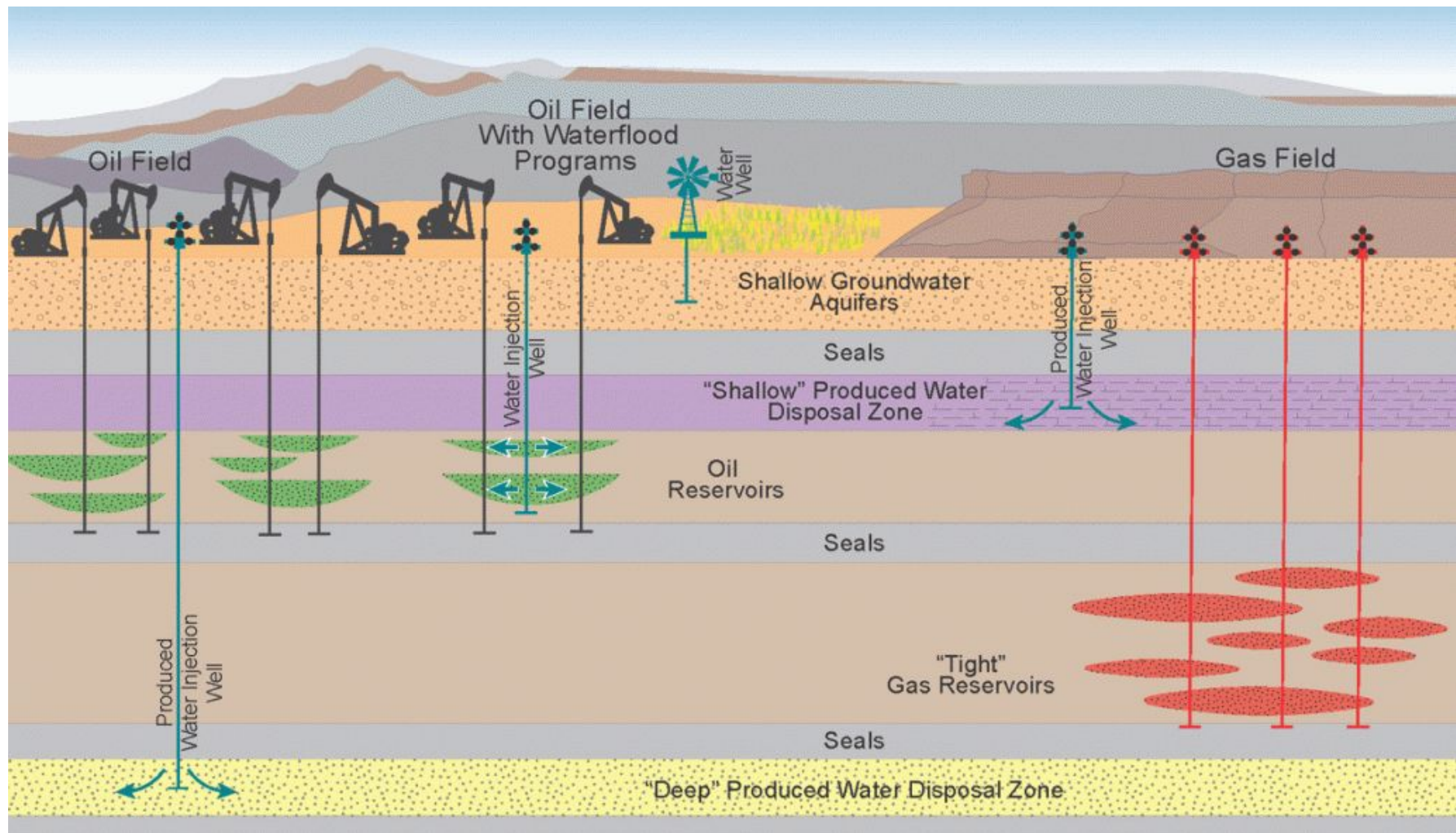
Scaling

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.



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

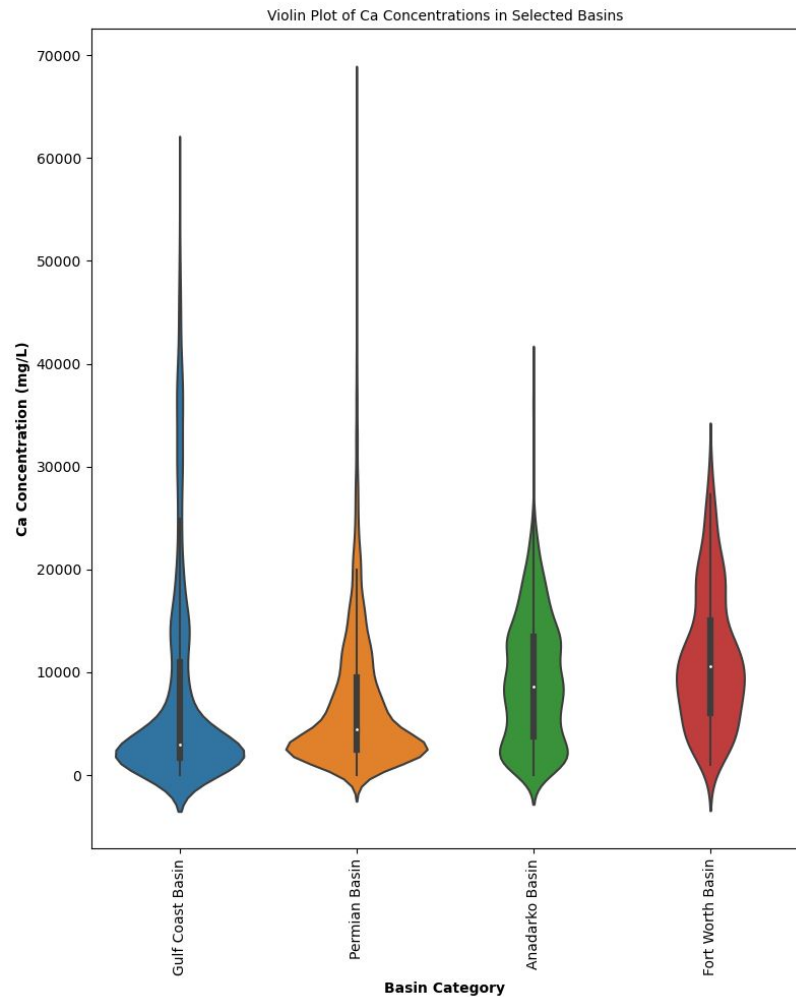
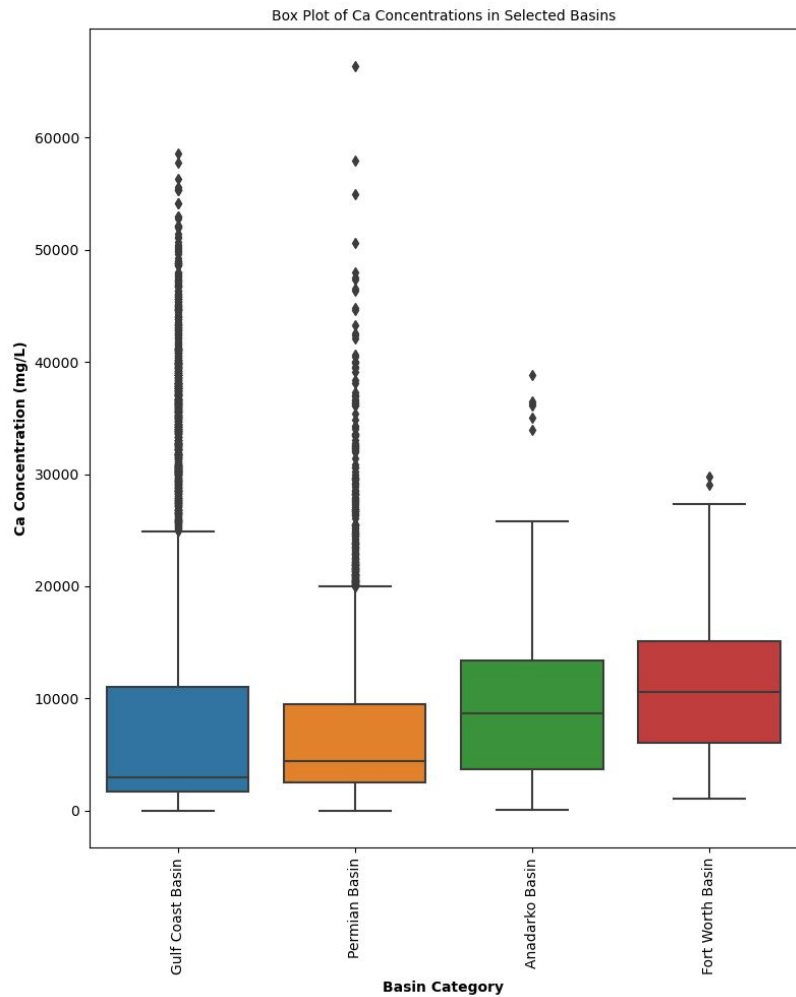
General Filtering

- 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

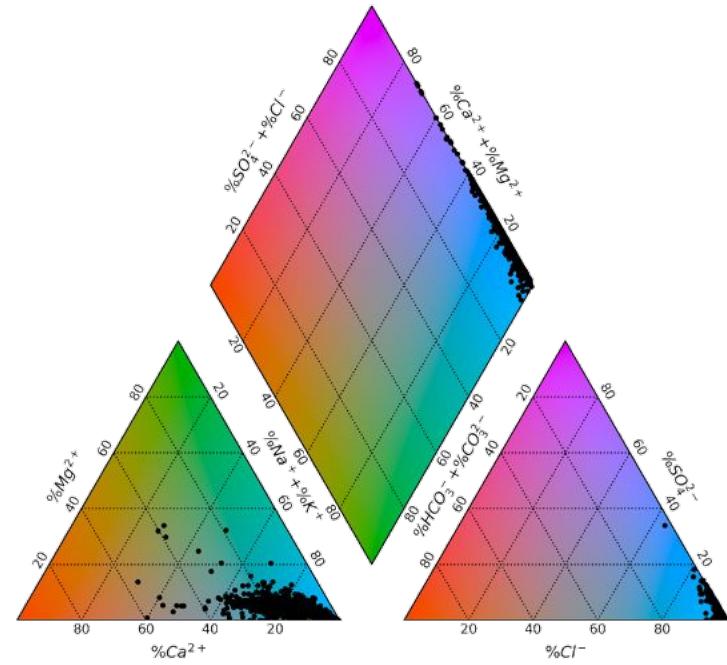
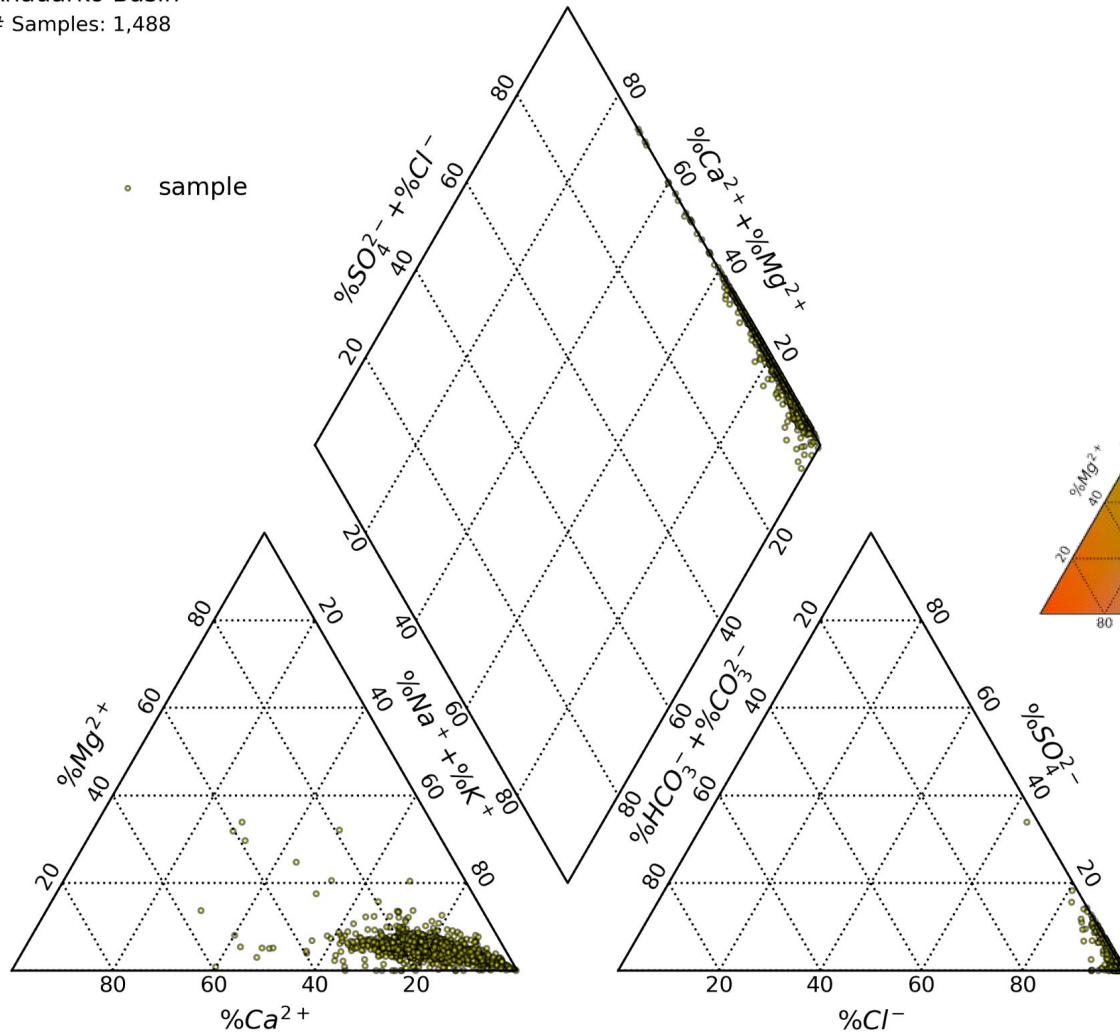
Box & Violin Plots



Piper Plots

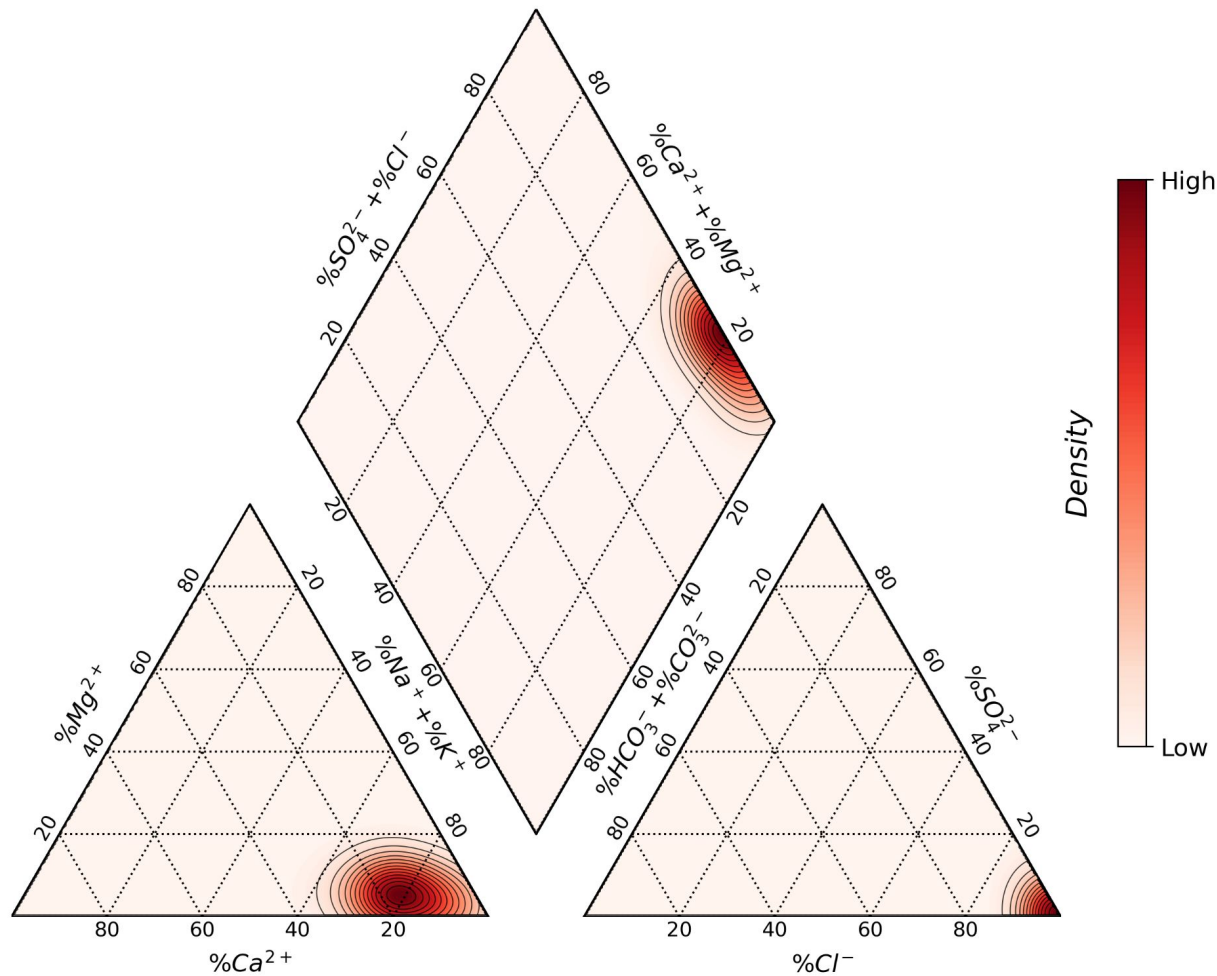
Anadarko Basin
Samples: 1,488

• sample

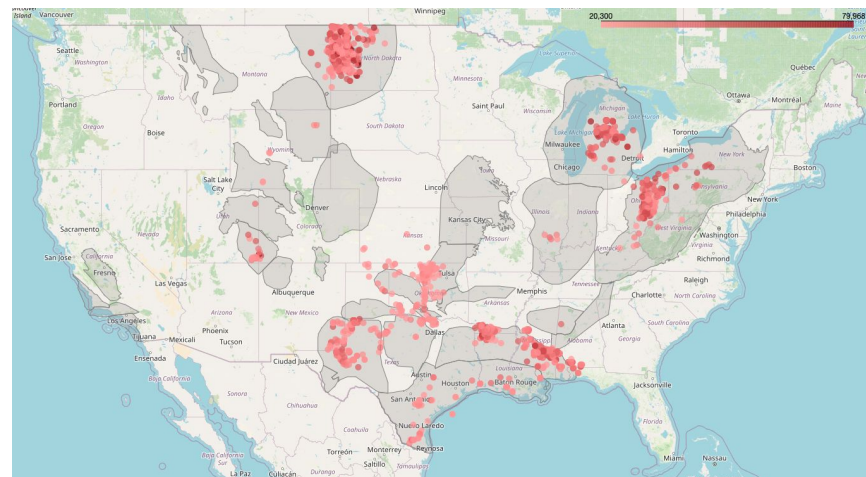


Piper Plots

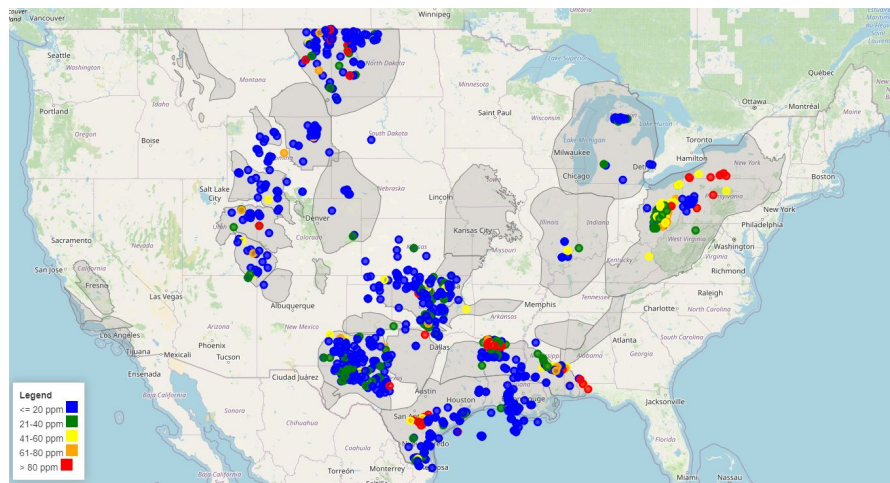
Anadarko Basin
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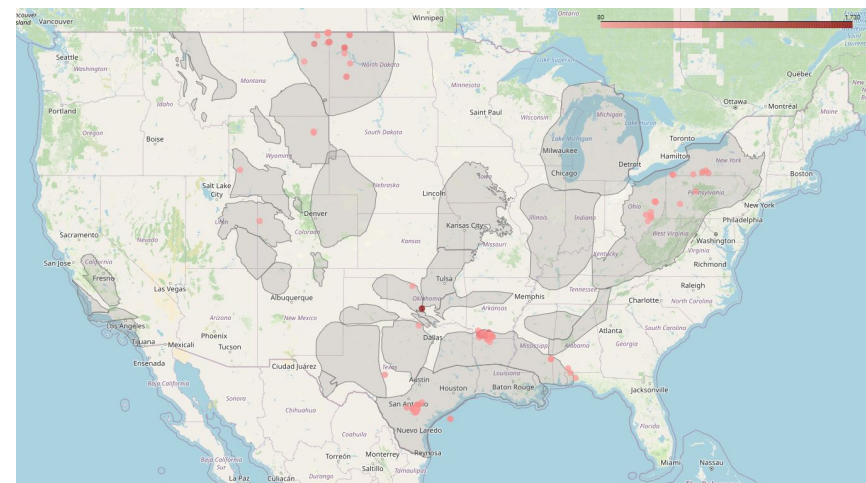
Scaling Elements (90th Percentile Gradient): Example Image Depicts Calcium

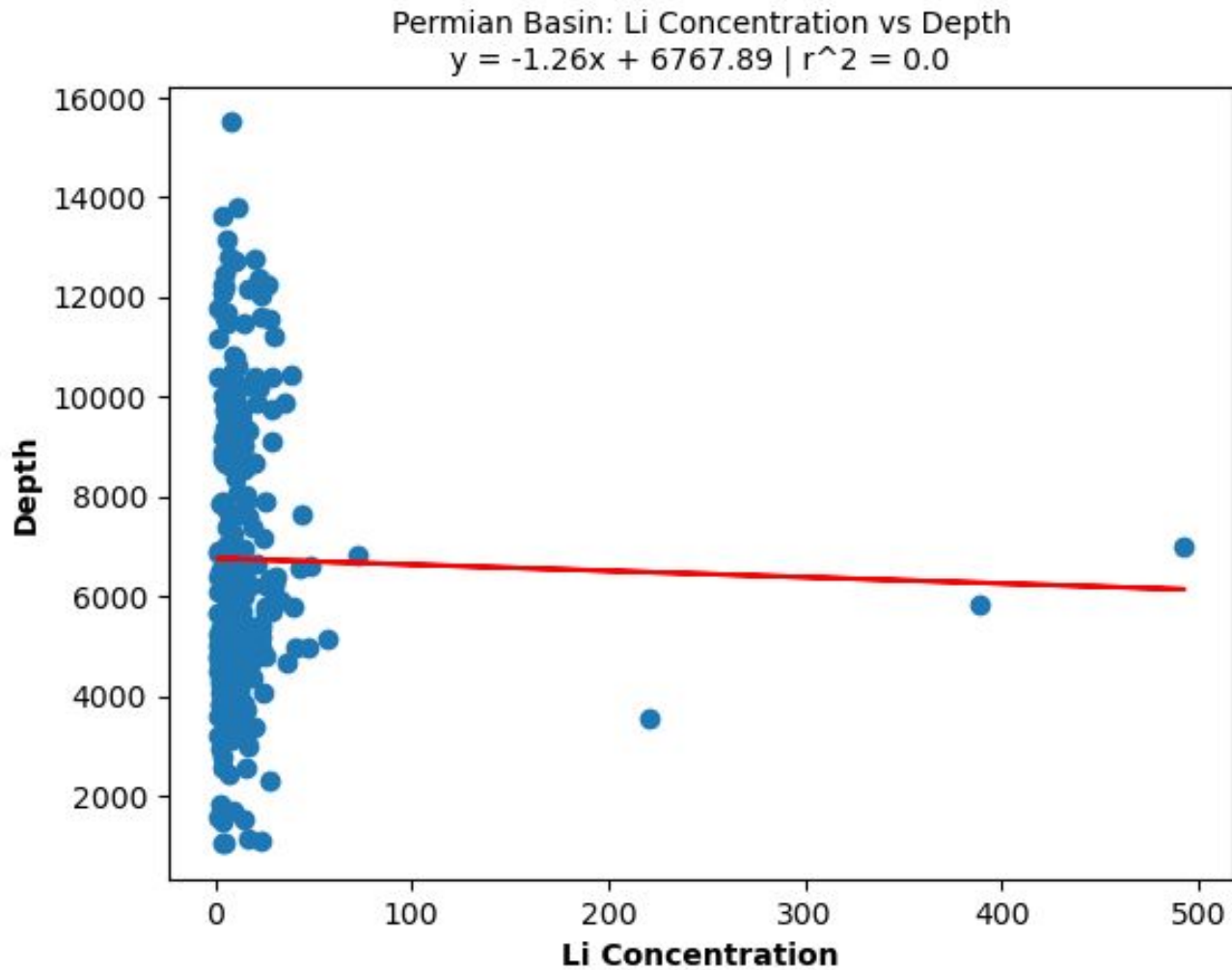


Lithium Availability (All Samples)



Lithium Availability (>80 ppm Gradient)





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



Natural Conditions for Produced Water

- Molar Sodium > Molar Calcium
 - Molar Chlorine > Molar Sulfate
 - Molar Calcium > Molar Magnesium
 - This ensures the samples reflect the natural chemical composition of produced water
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Database Utilization

Using data from the United States Geological Survey (USGS) and the Internal Bureau of Economic Geology (BEG) databases

Missing Data

Filling NaN Values for Basic Elements

- Missing values were filled with zeros
 - This was necessary for calculation purposes

Calculating Missing Sodium Values

- The calculation for Sodium is based on the absence/presence of KNa and K
 - If Na is missing and KNa and K are present, Na is populated with the difference between KNa and K
 - If Na and K are missing and KNa is not, a conditional approach is used

Handling Carbonates

- Missing Values for Carbonate and Bicarbonate were treated with specific strategies
 - Missing CO₃ replaced with zeroes
 - Missing HCO₃ were replaced with ALKHCO₃ where possible
 - With both missing, HCO₃ were calculated with cations, anions, and the molar mass

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

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:

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

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

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



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



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, HCO_3 , CO_3 , Cl, and SO_4 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.
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