Statistical Analysis of Hanford Data to Determine Representative Groundwater Formulations

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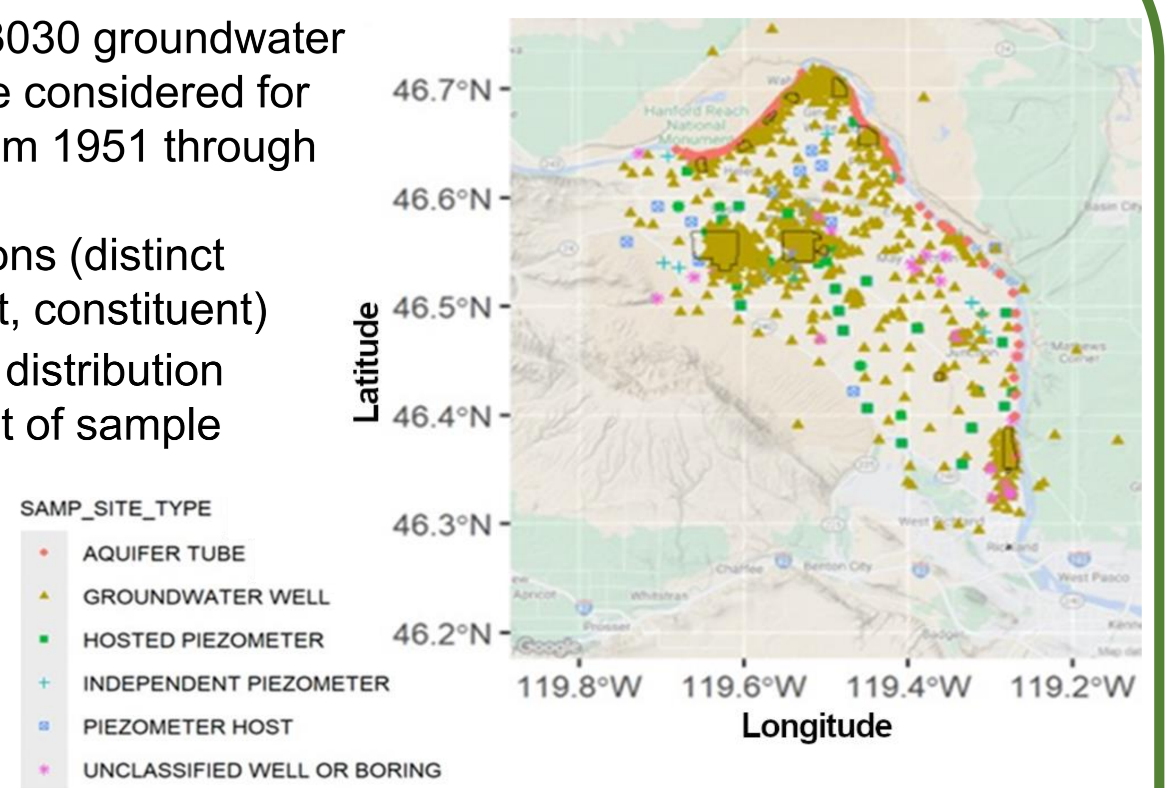
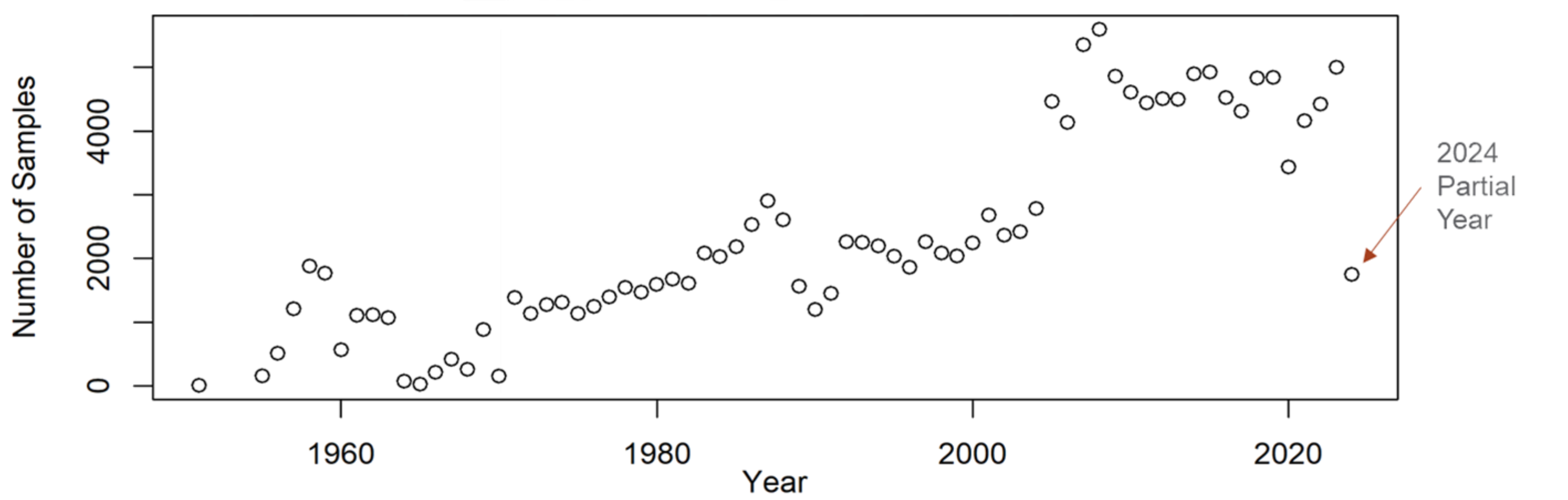
Introduction

- Decades of plutonium production operations at the Hanford Site in southeastern Washington State have resulted in soil and groundwater contamination.
- Understanding site groundwater chemistry is critical for evaluating contaminant transport, predicting plume behavior, and designing effective treatments.
- This work supports implementation and design of environmental remedies with technically defensible, site-specific synthetic groundwater formulations.

Groundwater Monitoring Data

- 42 constituents and 3030 groundwater monitoring wells were considered for samples collected from 1951 through mid-2024
  - 165866 observations (distinct well, sample event, constituent)
- Looked at the spatial distribution of wells and the count of sample events over time
- Focused on 2022-2023 data (more data, reflects recent conditions)





Hanford Aqueous Chemistry Synthetic Formulations

- Data for synthetic groundwater, perched water, and porewater used in laboratory testing

	Concentration (mg/L)						
Constituent	**SPW[1]**	**SPW + NO3[2]**	**200W-GW[3]**	**H-SGW[4]**	**VZPW[5]**	**IFRC 300ASGW-1[6]**	**Lysimeter Porewater[7]**
Na	402.5	698.4	36.5	5.9	126.4	33.1	32.9
CO_3	661.5	661.5	102.6	99.2	24.0	96.0	91.0
K	12.1	12.1	4.8	4.3	27.4	6.2	3.4
Mg	65.7	65.7	14.9	3.7	121.5	12.4	6.3
SO_4	481.4	481.4	35.2	47.3	1402.6	49.0	53.8
Ca	22.6	22.6	42.9	79.8	481.0	39.1	30.5
Cl[8]	117.1	117.1	93.4	13.0	255.2	46.1	4.3
NO_3	0.0	798.1	0.0	0.0	210.8	28.5	49.6
Si	0.0	0.0	0.0	2.0	0.0	0.0	13.8

[1] Synthetic Perched Water, (Saslow et al., 2018)
[2] Synthetic Perched Water + NO3, (Saslow et al., 2018)
[3] 200 West Area Groundwater, (Lawter et al., 2021)
[4] Hanford Simulated Groundwater, (Truex et al., 2017)
[5] Table 2.8, VZ Pore Water Simulant, in (Serne et al., 2015)
[6] (Zachara et al., 2010), (Zachara et al., 2009, PNNL-SA-64785)
[7] Data adapted from (Meyer et al., 2024)
[8] Does not include Cl from HCl added for pH adjustment

Parameters of Interest

- Parameters of interest are shaded in the table (including multiple synonyms for carbonate); those highlighted in **bold red** were selected for statistical analysis.
- Not all constituents are assayed for every sample; the table shows the percent of samples for the 522 wells sampled in 2022-2023 that have analytical results

Percent Data Completeness for 2022-2023 Data from 522 Wells

Constituent	% Data	Constituent	% Data	Constituent	% Data
Alkalinity	**100**	Carbonate_ion	0	pH_Measurement	99.9
Aluminum	28.1	**Chloride**	**100**	Phosphate	40.3
Ammonia	6.0	Copper	73.4	Selenium	67.9
Ammonium_ion	0	Cyanide	27.5	Silicon	0
Arsenic	67.9	Dissolved_organic_carbon	0	**Sodium**	**100**
Arsenic_filtered	0	Dissolved_oxygen	98.2	Strontium_90	41.5
Barium	67.6	**Fluoride**	**100**	**Sulfate**	**100**
Bi_carbonate_alkalinity	14.1	Hexavalent_Chromium	50.1	Technetium_99	37.2
Bicarbonate	9.4	Iodine_129	24.2	Total_dissolved_solids	3.6
Calcium	**100**	**Iron**	**100**	Trichloroethene	44.7
Calcium_Carbonate	0	Manganese	73.5	Tritium	47.4
Carbon_14	24.5	**Nitrate**	**100**	Turbidity	99.9
Carbon_tetrachloride	44.7	Nitrite	100	Uranium	73.6
Carbonate_alkalinity	21.0	Oxidation_Reduction_Potential	6.15	Zinc	100

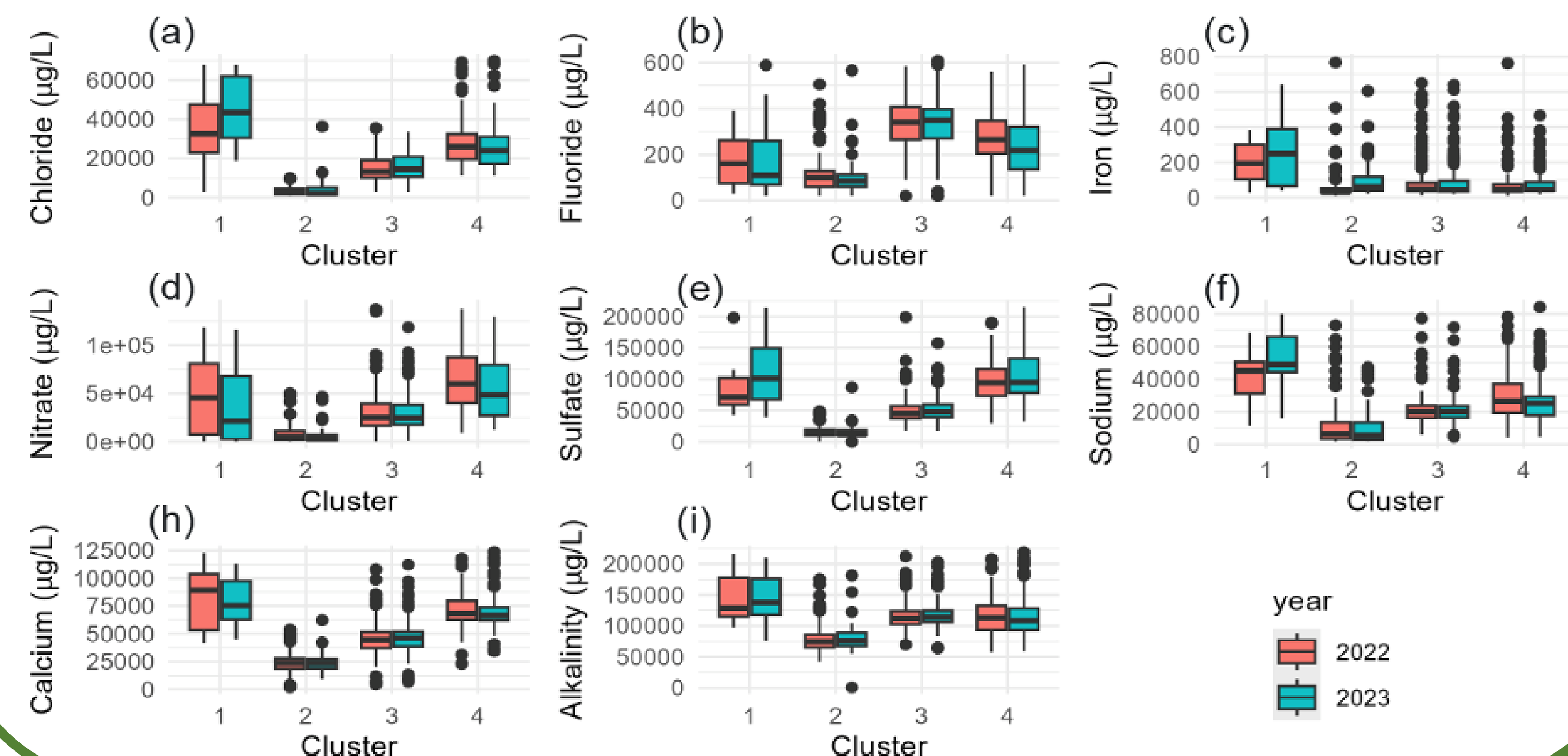
K-Means Clustering & Principal Component Analysis

- K-means clustering was used to group the wells based on similarities in groundwater chemistry; four clusters was the optimal number to capture variance.
- Principal component analysis (PCA) was applied to reduce dimensionality and highlight the main patterns in the data.
- Concentrations for the selected constituents were compared in boxplots by parameter for each cluster to understand geochemical variability.
- Insights from clustering help explain geochemical variations. 2022 and 2023 follow similar patterns in each cluster, though there are some year-over-year variations.

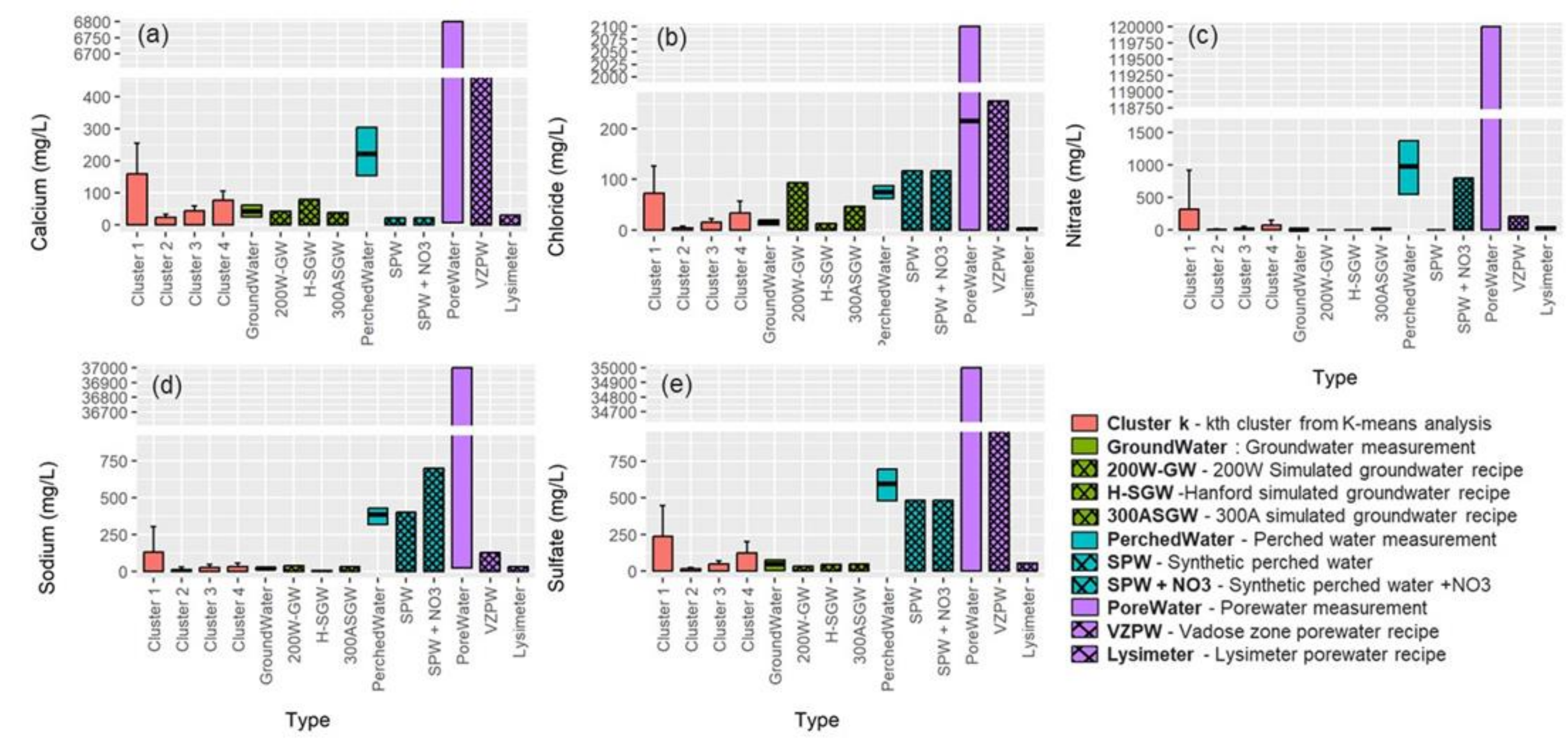
Wells per Cluster by Year

Year	Number of Wells			
	Cluster1	Cluster2	Cluster3	Cluster4
2022	17	96	196	123
2023	25	60	206	171

Boxplots Showing the Concentration Distributions of the Eight Selected Constituents across the Four Clusters for the Years 2022 and 2023

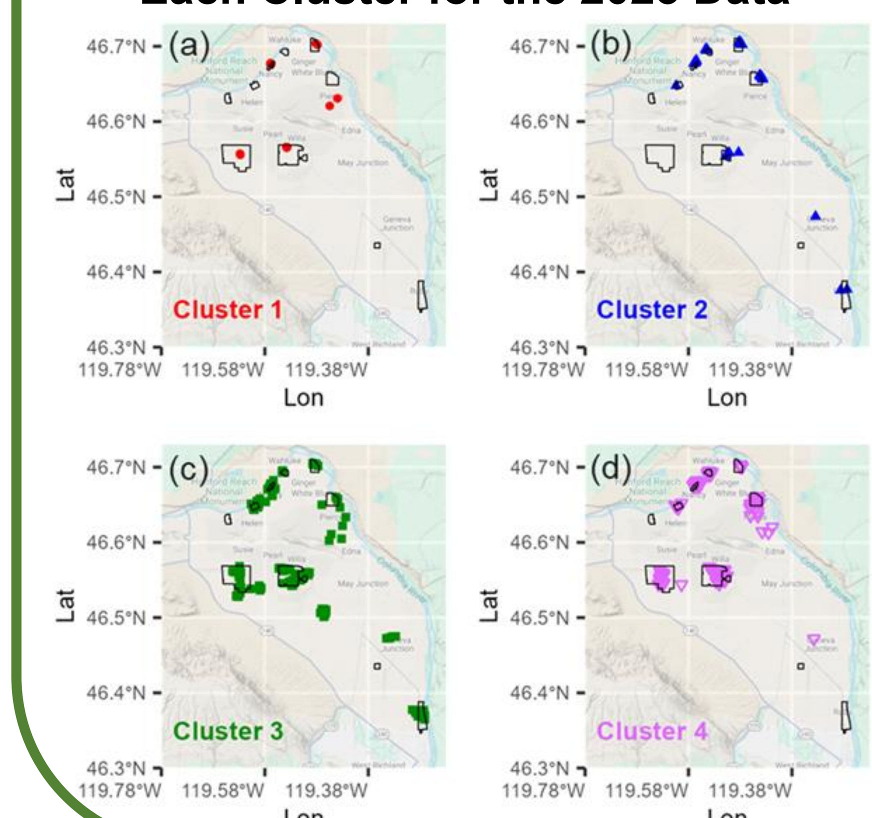


Comparison of Clusters versus Synthetic Formulations and Data from Other Sources



- Cluster 1 has the highest constituent concentrations, suggesting wells most impacted by natural or anthropogenic processes.
- Cluster 2 has the lowest constituent concentrations, corresponding to wells located along river (see spatial distribution), showing dilution effects.
- The synthetic groundwater formulations more closely resemble Cluster 1, representing worst-case scenarios of higher constituent concentrations, supporting use for conservative testing of groundwater remediation technologies.

Spatial Distribution of Wells for Each Cluster for the 2023 Data



Conclusions

- Statistical analysis of groundwater data from 2022-2023 provides a defensible technical basis for data-driven synthetic groundwater formulations for Hanford remediation technology treatability testing.
- High ion strength perched water chemistry is adequately represented by existing synthetic formulations, but calcium impacts need investigation.
- Porewater chemistry is waste-site specific; need to assess sensitivity of remediation technology performance to different constituent concentrations.

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