Evaluation of Statistical Methods for CCS-Related Groundwater Monitoring Programs Based on Illinois Basin - Decatur Project Monitoring

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Introduction

The Midwest Geological Sequestration Consortium is conducting the Illinois Basin – Decatur Project (IBDP), a large-scale carbon capture and storage (CCS) project in Decatur, Illinois, USA. The IBDP study area (Figure 1) covers approximately 160 acres (0.65 km² / 0.25 mi²). As a part of an extensive Monitoring, Verification, and Accounting (MVA) program, shallow groundwater monitoring is being conducted to verify that project activities are protective of human health and the environment (Figure 2).

Shallow regulatory compliance wells were installed in thin sandstone of the Pennsylvanian-age bedrock that was designated by the regulatory agency as the lowermost underground source of drinking water (USDW). Carbon dioxide (CO_2) injection began at the IBDP site in November 2011 and terminated in November 2014 after 999,215 tonnes of CO_2 had been injected into the Mt. Simon Sandstone.

4 Regulatory Compliance Wells:

- Depths ~140 ft (43 m) deep
- Monthly sampling initiated August 2010
- 220 total samples from USDW through November 2014
  - 52 baseline, 168 during injection
- 11 compliance parameters:
  - pH, alkalinity, Ca, dissolved CO_2, Br, Cl, Na, specific conductance, dissolved oxygen, temperature, and water level (red = most sensitive to CO_2 interactions, blue = most sensitive to brine interactions)

Figure 2. Shallow groundwater monitoring scope in IBDP.

Objectives

The goal of this study was to: 1) compare statistical methods that can be used for CCS-related groundwater monitoring programs, and 2) determine statistically if CO_2 injection at the IBDP site has impacted shallow groundwater quality (Figure 3).

- **To evaluate if groundwater quality has been impacted;**
  - Establish baseline (i.e., pre-injection) data
  - Compare pre-injection, injection, and post-injection period geochemical data for out-of-bounds conditions
  - Identify and understand data outliers, if any
  - Interpret the cause of variability in data (natural variability vs. leak detection)

Figure 3. General process for IBDP groundwater quality evaluation.

Groundwater samples were analyzed for more than 30 constituents. However, the analytical results used for this study included only 13 analytes that were present in all samples: pH, specific conductance, alkalinity, bromide, calcium, chloride, iron, magnesium, potassium, sodium, sulfate, total dissolved CO_2, and total dissolved solids.

Statistical Approaches

Several bivariate and multivariate statistical techniques (Figure 4) were applied to the groundwater data set to determine if significant differences occurred in groundwater quality between the pre-injection and injection periods. Seasonality trends were not indicated in either period. When pre-injection shallow groundwater quality data were not normally distributed, non-parametric statistical techniques were required.

- **Bivariate Methods**
  - Outliers (EPA 1989)
  - Serial correlation (Rank Von Neumann)
  - Seasonality (Kruskall-Wallis)
  - Trend (Mann-Kendall)
  - Normality (Shapiro-Wilk/Francis)
  - Prediction limit, Tolerance limit, Control charts
  - Mann-Whitney test, Welch's t-test
- **Multi-Variate Methods**
  - Principal Component Analysis (PCA), Factor analysis

Figure 4. Statistical methods used.

Figure 1. Illinois Basin – Decatur Project (IBDP) shallow groundwater network.

Acceptable ranges of concentrations (e.g., limits) by three different statistical methods (prediction limit, tolerance limit, and control charts) were calculated (Table 1). When pre-injection data were not normally distributed, non-parametric prediction limits were used in lieu of control charts. When pre-injection data were not normally distributed, the highest value of a parameter (or lowest value in the case of pH) in the background data set was chosen for both prediction and tolerance limits. If applicable, the lowest and highest limit values were calculated by prediction limit and control charts respectively.

Calculated limits by different techniques based on the statistics of pre-injection data, 95% confidence level

Parameter	Unit	Maximum value (pre-injection)	Maximum value (injection)	Prediction[1] limit	Tolerance limit	Control chart	
						h	SCL
Alkalinity	mg/L	448	441	448	448	NA	NA
Br	mg/L	1.28	1.36	1.54	1.27	1.54	1.49
Ca	mg/L	45	123	45	45	NA	NA
Cl	mg/L	597	621	597	597	NA	NA
CO_2	mg/L	404	406	398.8	401.9	428.3	423.9
EC	µS/cm	3,215	2,647	2,729	2,971	4,144	3,930
Fe	mg/L	0.44	1.02	0.27	0.31	0.73	0.64
K	mg/L	4.85	4.78	4.65	4.79	5.75	5.61
Mg	mg/L	22.54	52.62	22.54	22.54	NA	NA
Na	mg/L	504	490	504	504	NA	NA
pH	units	7.71	8.05	7.71/6.78	7.71/6.78	NA	NA
SO_4	mg/L	17.9	196.2	12.8	14.82	41.16	35.44
TDS	mg/L	1,367	1,378	1,367	1,367	NA	NA

NA: Not Applicable [1]Non-parametric prediction limit used in lieu of interwell control chart

Table 1. Comparison of limits of statistical methods used.

Method Strength and Reliability

Statistical power curves illustrate how effective a method is able to correctly reject the null hypothesis while the alternative hypothesis is true.

Power curves for statistical tests such as prediction limit, tolerance limit and control charts, were prepared for monthly and quarterly background data (i.e. pre-injection data) and compared to the EPA Reference Power Curve (ERPC). Results indicated control charts and tolerance limits with the highest and lowest effective power respectively (Figure 5). Factors that affect statistical power include the sample size (Figure 6), the specification of the parameter(s) in the null and alternative hypothesis (i.e., how far they are from each other), the precision or uncertainty the researcher allows for the study (generally the confidence or significance level), and the distribution of the parameter to be estimated.

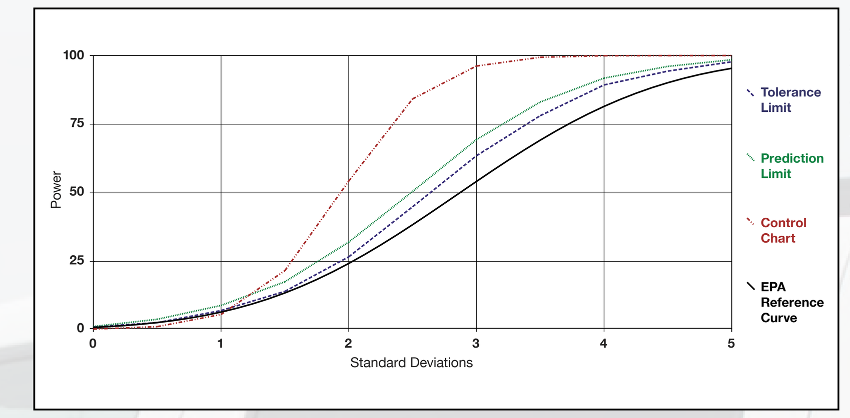

Figure 5. Power curve for different statistical techniques compared to ERPC, monthly data (n=13).

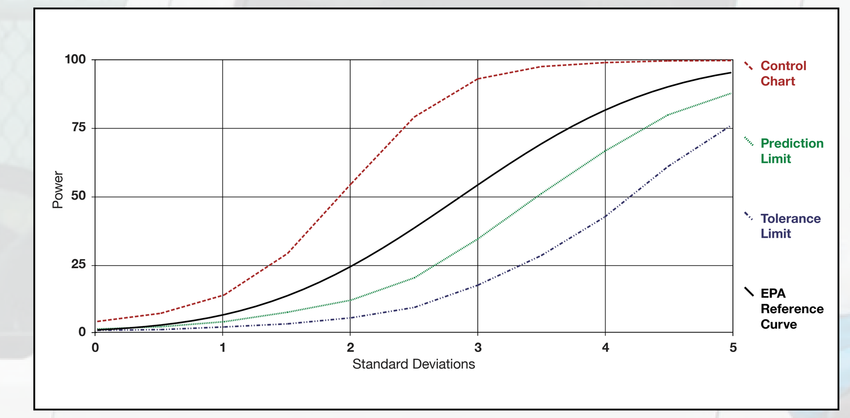

Figure 6. Sample size affects a test's power, quarterly data (n=5).

Test of Hypothesis

Mann-Whitney and Welch's t-test were used to determine if the median of individual parameters in pre-injection and injection data sets are equal. Overall results provided by these methods show no significant differences in shallow groundwater quality between the pre-injection and injection phases (Table 2).

The hypothesis statements were:

H_0: The quality of shallow groundwater in IBDP project area ***has not been changed*** over injection period.

H_A: The quality of shallow groundwater in IBDP project area ***has been changed*** over injection period.

Test of Hypotheses for shallow groundwater quality data in IBDP, 95% of confidence level

Parameter	Unit	Mann-Whitney (Wilcoxon Rank Sum)		Welch's t-test[1]	
		Variation indicated	Hypothesis accepted	Variation indicated	Hypothesis accepted
Alkalinity	mg/L	-	✓	NA	NA
Br	mg/L	-	✓	-	✓
Ca	mg/L	-	✓	NA	NA
Cl	mg/L	-	✓	NA	NA
CO_2	mg/L	-	✓	-	✓
EC	µS/cm	-	✓	-	✓
Fe	mg/L	✓	-	-	✓
K	mg/L	-	✓	-	✓
Mg	mg/L	-	✓	NA	NA
Na	mg/L	-	✓	NA	NA
pH	units	-	✓	NA	NA
SO_4	mg/L	-	✓	-	✓
TDS	mg/L	-	✓	NA	NA

✓ Significant - Not Significant NA: Not Applicable

[1]The Welch's t-test requires the normality of background data distribution.

Table 2. Statistical evaluation of groundwater data verifies the acceptance of the null hypothesis (H_0).

Multivariate Statistical Evaluation of Groundwater Chemistry Data

Principal Component Analysis (PCA), was used for a more comprehensive evaluation of groundwater data collected from October 2010 to November 2014 (Figure 7). The goal of this assesment was to use multivariate statistics to understand the mechanisms potentially affecting groundwater quality and evaluate whether CO_2 injection activities were impacting shallow groundwater quality.

- 13 parameters were used: Alkalinity, Br, Ca, Cl, CO_2, EC, Fe, K, Mg, Na, pH, SO_4, and TDS
- 52 pre-injection and 168 injection samples
- 14 months of pre-injection data from August 2010 to October 2011 and 36 months of injection data from November 2011 to November 2014
- 676 (13*52) pre-injection and 2,184 (13*168) injection values

Figure 7. Parameters used for PCA assessment.

Principal Component Analysis Interpretation

Thirteen principal components were defined for the pre-injection and injection period data sets. The first three principal components in each case explained 80 and 88 percent of the variance of the pre-injection and injection data sets, respectively (Figure 8). PCA interpretation for both the pre-injection and injection data sets show strong correlation between the components and eight constituents (chloride, sodium, magnesium, potassium, calcium, total dissolved solids, specific conductance, and pH). Other investigators who have used PCA to analyze groundwater data have observed similar relationships and have attributed them to a "salinity factor," which is directly related to constituents affected by natural processes of water-rock interactions.

Pre-injection Period

- Three first components explained 80% of total geochemical variations and indicated natural:
  - Salinity
  - Oxidation-reduction
  - Acidity

Injection Period

- Three first components explained 80% of total geochemical variations and indicated natural:
  - Salinity
  - Dissolution
  - Acidity

Interpretation: Natural water-rock interactions were the primary mechanism governing groundwater quality during both periods.

Figure 8. Interpretation of component principal analysis.

PCA Score Plots

To inspect similarities and differences in the composition of groundwater samples, their component scores were calculated and plotted. The scores were plotted in relation to PC1 and PC2 because these components account for the majority of the variability associated with the samples. Score plots for PC1 and PC2 for both pre-injection and injection periods indicate that scores for data from each of the wells (G101–G104) group tightly together (Figure 9). This tight grouping of score data for individual wells indicated the similarity of the groundwater quality between all the sampling times and periods. Only a few data from well G104 fall outside of this range. Investigations suggest this abnormality related to periodic recharge from shallower aquifers.

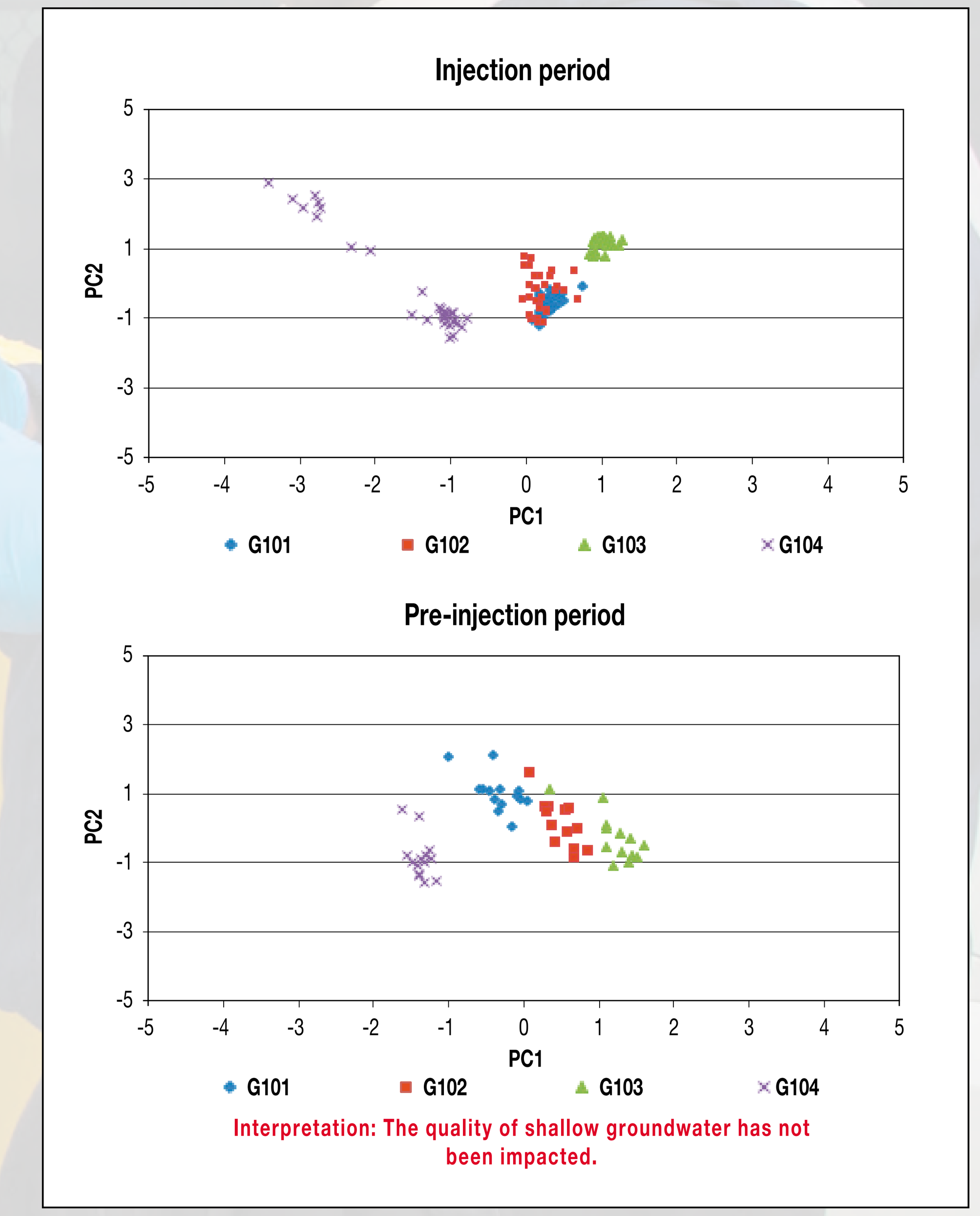

Figure 9. Score plots of principal components.

Conclusions

Statistical Considerations Based on Groundwater Quality Datasets at IBDP:

- Distribution (i.e., normal distribution) of pre-injection data sets is a main factor to choose a statistical method.
- Acceptable range of concentrations (e.g., limits) vary based on statistical methods used.
- Increasing the sample size generally improves a test's power.
- Multivariate statistics are needed to perform integrated assessments of large datasets with many variables.

Project:

- Water-rock interactions were the primary mechanism that controlled water quality in the Pennsylvanian bedrock.
- Bivariate and multivariate statistical assessments showed CO_2 injection activities have not impacted shallow groundwater quality.

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