



Considerations for Data Validation

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Presentation Overview

- **Define data validation**
- **Explain where it takes place in the process of establishing data usability**
- **Data integrity considerations prior to assessing project-specific data validation**
- **Example**

What is Data Validation?

- **As defined by the USEPA (QA/G-8)**
- **An analyte- and sample-specific process that extends the evaluation of the data beyond method, procedural, or contractual compliance (i.e., data verification) to determine the analytical quality of a specific data set.**

Where in the Usability Process?

- The step following data verification.
- The step prior to establishing data usability.
- USEPA QA/G-8:
 - The definitions and activities form a continuum.
 - Distinction between steps is somewhat artificial.

Ultimate Goal of the Process

- **To assess whether the final, qualified results support the decisions made with the data.**

Application to AFCEE Projects

- **Data verification includes the application of the AFCEE flags per the QAPP and a general assessment of the data presented in the analytical report.**
- **Data validation focuses on an evaluation of the flagged data and impact on results.**

Data Integrity Issues

- **Data Integrity: Are the analytical values accurately reported?**
- **Need to incorporate understanding of the laboratory's data reporting procedures via**
 - audit
 - performance evaluation samples
 - corrective action reports

Data Integrity: Audits

- Are data uploaded electronically or manually entered?
- Are there systems in place to adequately verify final reported data?
- Could there be discrepancies between the hard copy and EDD?

Data Integrity: PE Samples

- **Can identify potential isolated or systematic failures.**
- **Source of failures:**
 - Sample login problem (field or lab)
 - Standard preparation error
 - Dilution error

Data Integrity: CARs

- Is the laboratory responsive to client-identified discrepancies?
- Are out-of-control issues adequately described?
- Is a resolution identified?
- Is there follow-up on the selected resolution?

Example: Surrogate Failure

Data Quality Objective (DQO) Development

- **Considerations during development of the DQOs:**
 - TCE and other chlorinated solvents may have been released in the soil.
 - TCE may have migrated to groundwater.
 - The California risk-based derived Tap Water Preliminary Remediation Goal (PRG) for PCE, TCE, and VC in groundwater are lower than can be achieved by standard (full scan) SW8260B method.
 - Lower MDLs/RLs for these VOCs can be achieved using selected ion monitoring (SIM).

Field Sampling Design

- The field sampling design (Step 7 of the DQO Process) states that if groundwater is encountered, then a grab groundwater sample will be collected for VOCs by SW8260B and SW8260B SIM.
- The SIM sample will be placed on hold pending results of full scan analysis.
- If TCE, PCE, and VC are ND in full scan analysis, then sample will be analyzed for low-level VOCs by SIM.

Lab Results

Sample ID: 147-SB11-GW01					
	SW 8260B		SW 8260B SIM		
Compound	Sample	MDL	Sample	MDL	MB
TCE, µg/L	< 1	0.056	< 0.05	0.0040	< 0.05
PCE, µg/L	< 0.5	0.060	< 0.02	0.0023	< 0.02
VC, µg/L	< 1	0.1	< 0.02	0.0031	< 0.02
<i>Surrogate</i>	101%	--	77	--	79

- Results for all VOCs in full scan analysis were ND, so sample was analyzed for low-level VOCs.
- Surrogates in both the method blank and sample were recovered slightly below the lower control limit of 80%.

Communication Failure

- **Sample could not be reanalyzed because the other containers specified for VOC SIM were used for MS and MSD.**
- **Laboratory should have contacted project chemist for direction.**
- **Laboratory could have used remaining VOA vials designated for full scan VOCs to reanalyze.**
- **Sample should not have been run after failing method blank.**

Data Verification

Sample ID: 147-SB11-GW01							
	SW 8260B SIM						
Compound	Sample	MDL	MB	LCS	MS	MSD	CL
TCE, µg/L	< 0.05	0.0040	< 0.05	103%	89%	104%	75-125%
PCE, µg/L	< 0.02	0.0023	< 0.02	103%	85%	104%	75-125%
VC, µg/L	< 0.02	0.0031	< 0.02	114%	112%	116%	75-125%
<i>Surrogate</i>	77	--	79	85	86	82	80-120%

- **Surrogates in other QC samples (LCS, MS, MSD) were within control.**
- **IC, second-source ICV, and CCVs were in control.**

Data Verification Output

- All low-level VOC results were ND, so results for VOC SIM compounds were rejected because of surrogate failure.

Data Validation

- The concern with a low surrogate recovery is that the ND results may be false negatives.
- Thus, the sample results may not be representative of actual site conditions.

Data Validation

Sample ID: 147-SB11-GW01			
			Tap Water
	SW 8260B SIM		PRG,
Compound	Sample	MDL	Cancer
TCE, $\mu\text{g/L}$	< 0.05	0.0040	0.028
PCE, $\mu\text{g/L}$	< 0.02	0.0023	0.66
VC, $\mu\text{g/L}$	< 0.02	0.0031	0.02

- **However, for each compound, the Tap Water PRG is approximately an order of magnitude greater than the MDL.**

Data Validation

Sample ID: 147-SB11-GW01			
			Tap Water
	SW 8260B SIM		PRG,
Compound	Sample	MDL	Cancer
TCE, $\mu\text{g/L}$	< 0.05	0.0040	0.028
PCE, $\mu\text{g/L}$	< 0.02	0.0023	0.66
VC, $\mu\text{g/L}$	< 0.02	0.0031	0.02

- **If the compound were present in the groundwater at a concentration equal to or greater than the Tap Water PRG, it would have been detected, even in the slightly biased low analytical environment.**

Data Validation

Sample ID: 147-SB11-GW01		
	Tap	If Present in Sample at
	Water	Concentrations Equal to PRG
	PRG,	(Adjusting for 79%
Compound	Cancer	Surrogate Recovery)
TCE, $\mu\text{g/L}$	0.028	$0.028 * 0.79 = 0.022$
PCE, $\mu\text{g/L}$	0.66	$0.66 * 0.79 = 0.52$
VC, $\mu\text{g/L}$	0.02	$0.02 * 0.79 = 0.016$

- **Worst-Case Scenario: Compounds are actually present in the groundwater at concentrations equal to the PRG but are not detected because of the low-bias analytical environment.**

Data Validation

Sample ID: 147-SB11-GW01				
	Tap	Hypothetical		
	Water	Reported Value		
	PRG,	in the Biased Low		
Compound	Cancer	Analytical Environment	RL	MDL
TCE, µg/L	0.028	0.022 F	< 0.05	0.0040
PCE, µg/L	0.66	0.52	< 0.02	0.0023
VC, µg/L	0.02	0.016 F	< 0.02	0.0031

- **If worst-case scenario were true, the laboratory would have been able to detect and report these values (and, had the compounds been in the groundwater at Tap Water PRG concentrations, these hypothetical results reported with the low surrogate would have been biased low).**

Data Validation Output

- **Qualifiers changed from “R” to “J” to denote the analytical non-conformance.**
- **The results were usable for the purpose of determining that the contaminants of concern have not impacted groundwater at concentrations above the Tap Water PRGs.**

Alternative Sampling Objective

- **Would likely not “un-reject” data if the sampling objective were as follows:**
 - **If it were a groundwater monitoring event, and the well were a boundary well located at the perimeter of the property.**
 - **In this scenario, need to know as soon as possible if any detectable amount of TCE were present.**

Alternative Sampling Objective

- **Would likely not “un-reject” data if the sampling objective were as follows:**
 - **If the groundwater sample were collected to establish multiple rounds of “ND” for the purposes of site closure.**

Conclusion

- **Data validation occurs after systematic data verification and prior to usability assessment.**
- **Need to incorporate understanding of the laboratory's data production procedures (data integrity).**
- **Project chemist has to be familiar with the DQOs of the project and the analytical data in order to perform data validation.**
- **Data validation is performed to assess whether the final data set is usable to support the decisions made with the data.**