Data Verification, Validation, and Usability Assessment at the DoD

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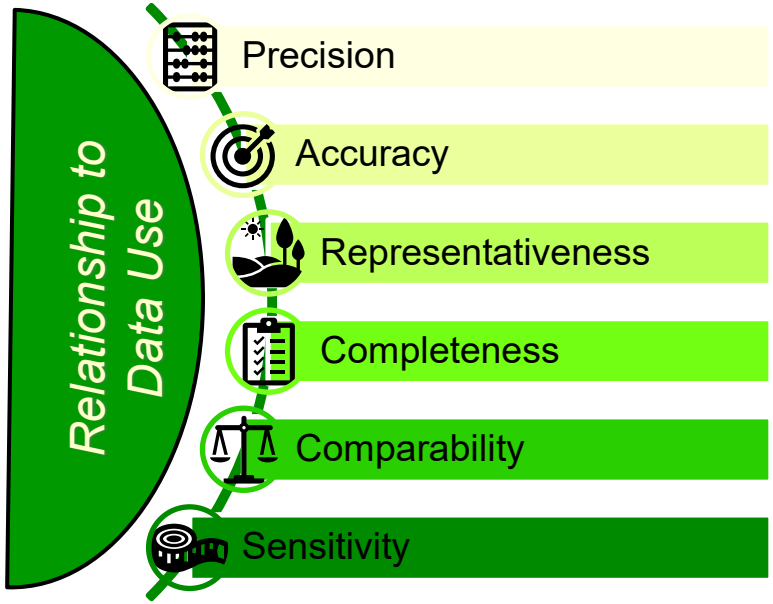
Outline

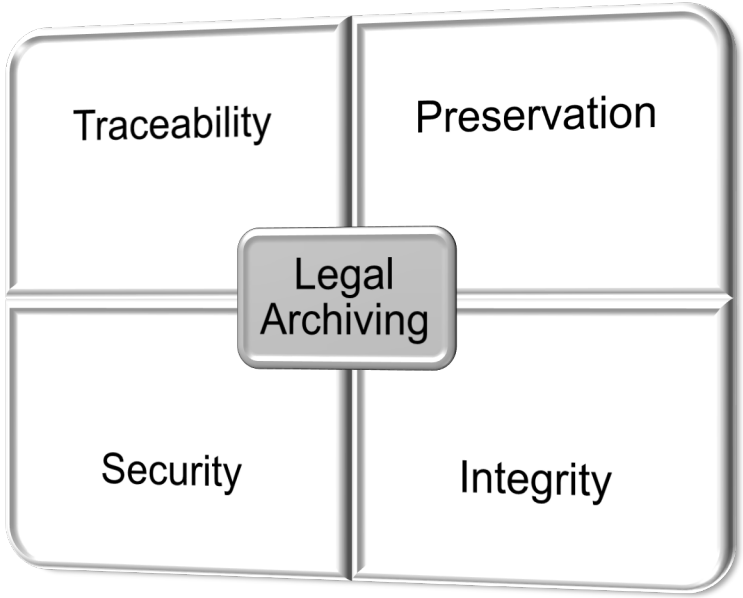
- **DoD Data Collection Process**
- **DoD Data Review Process**
  - Data Verification
  - Data Validation
  - Data Usability
- **Lessons Learned**

Data Collection and Review – Goals

Scientifically Valid



Legally Defensible



Data Collection

- Starts with Systematic Planning Process and the UFP-QAPP Worksheets
  - WS #1-8, Management: Background, PDT, Communication Pathways, Training Requirements, Proof of Review, and Approval Pages
  - WS #9, Planning Sessions: Documents ALL project meetings and agreements
  - WS #10-16, Project Objectives: CSM & DQO Development, and Performance Objectives
  - WS #17-30, Design and Data Collection: Sampling and Analysis Methods, and Quality Control Requirements
  - WS #31-33, Assessment and Oversight
  - WS #34-37, Data Review

Overview: EPA DQO 7-Step Process

1. State the problem
   - What is the problem we need to solve?
2. Identify the decision to be made
   - What are we trying to do about it?
3. Identify the inputs to the decision
   - What data do we need to address Question 1 and 2?
4. Define the boundaries of the study
   - What limitations are we working under?
5. Develop decision rules
   - How are we going to use the data to make our decisions?
6. Specify tolerable limits on decision errors
   - What confidence do we need?
   - How comfortable are we with data errors?
7. Optimize the design
   - Having worked out all the above, how are we going to do this?

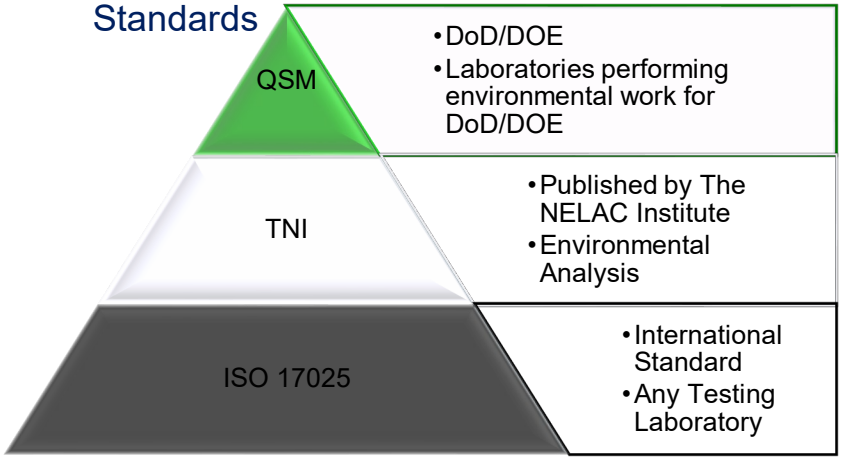
Guidance on Systematic Planning Using the Data Quality Objectives Process, U.S. EPA, EPA QA/G-4, February 2006.

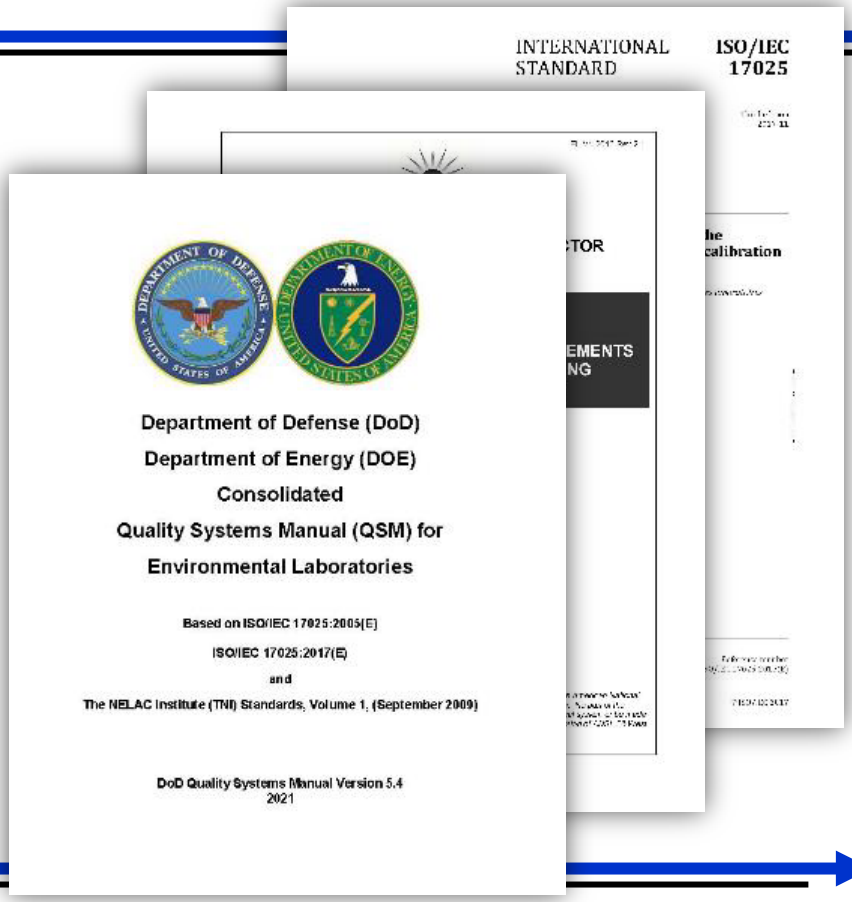
Key Worksheets for Data Collection

- WS #12:
  Measurement Performance Criteria
  - Criteria that collected data must meet in order to satisfy the DQOs
  - Failures may impact end uses of the data
- WS #14/16: Project Tasks & Schedule
- WS #17: Sampling Design & Rationale
  - Process flow
  - Activities to obtain data
    - Site preparation
    - Sampling and analysis
- WS #15: PALs & Lab-Specific Limits
  - Detection & quantitation limits
- WS #18: Sampling Locations/Methods
  - Cross references sample types, locations, and methods
- WS #29: Project Documents & Records
  - QC/QA records
  - Reports
  - Field records
- WS #34-37: Data Review
  - Data Verification
  - Data Validation
  - Data Usability Assessment

Analysis – Quality Systems Manual

- Published by EDQW, built upon ISO and TNI Standards



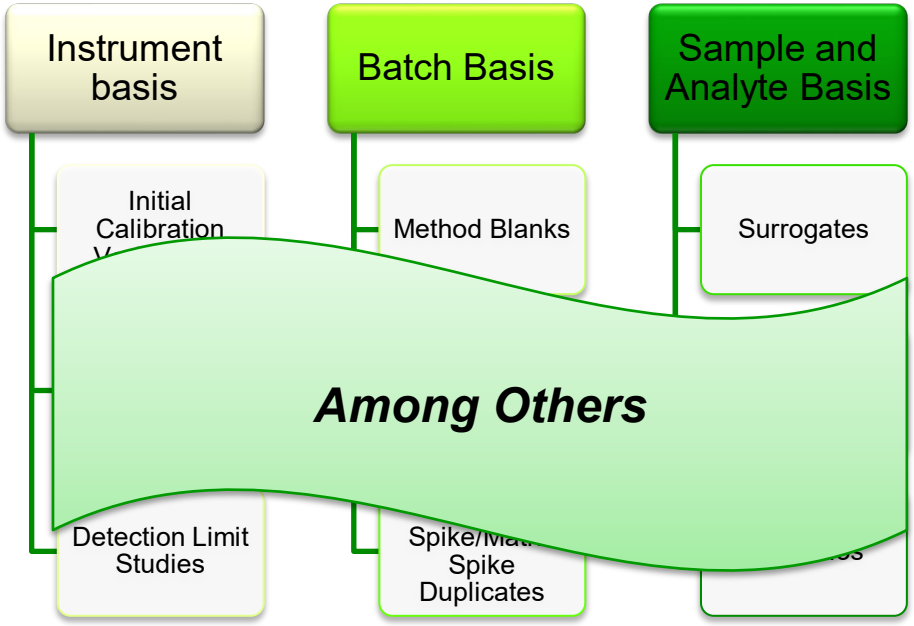


- Minimum quality requirements for laboratories performing environmental analysis for DoD/DOE
- Accreditation by approved third-party ABs
- Does **not** provide sampling requirements
- Does **not** ensure **specific data points** have met requirements or that data are usable for a project

Analysis – Measurement Performance

- Analytical SOPs ensure adherence to baseline method criteria
- Instrument Calibration and Maintenance ensure accuracy
- Measurement Performance is monitored on an:

Hmm… Could this be a basis for organizing data review?



Data Review Process

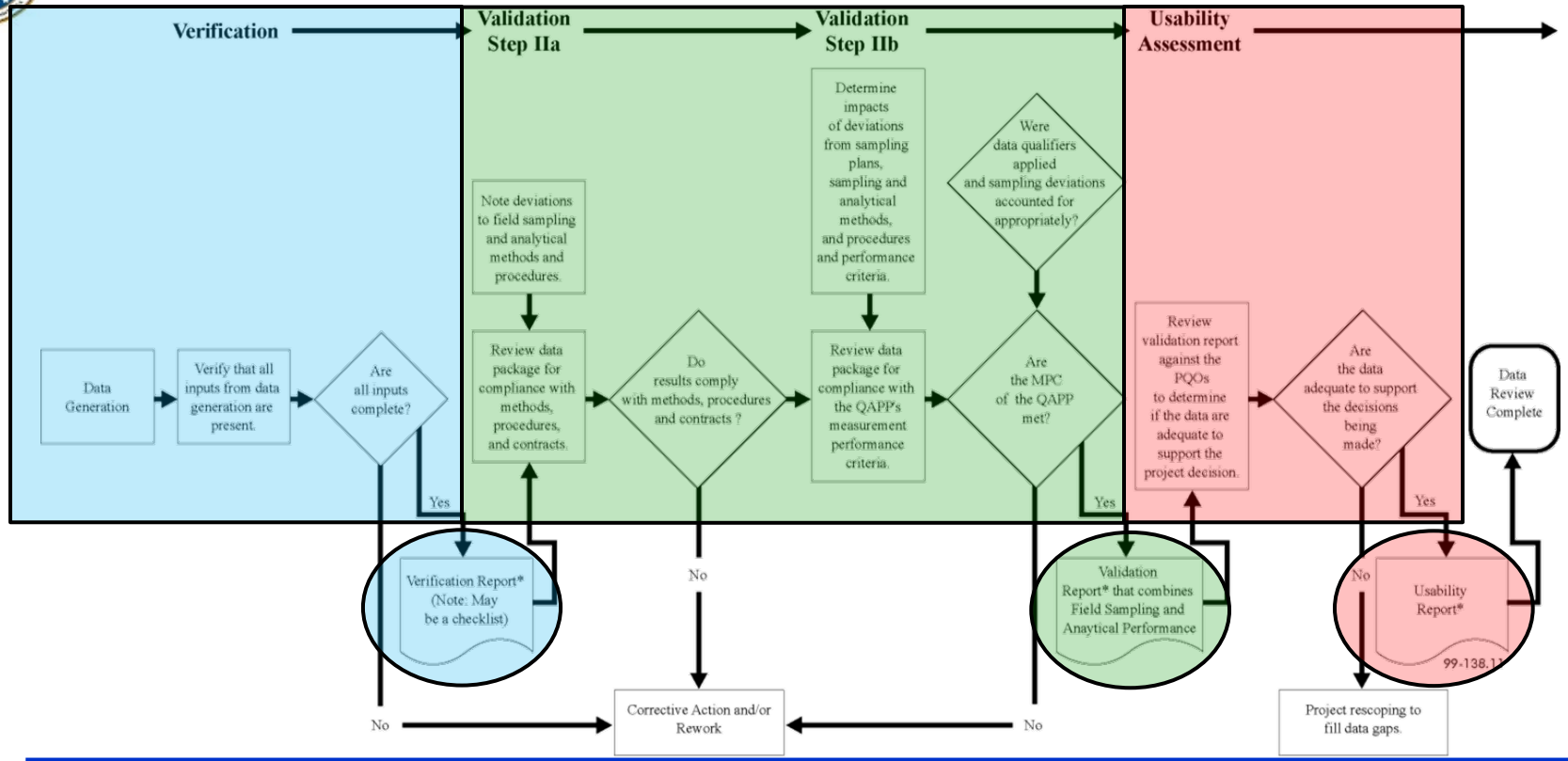


Figure from IDQTF, UFP-QAPP Manual V1, March 2005, Figure 37. Data Review Process.

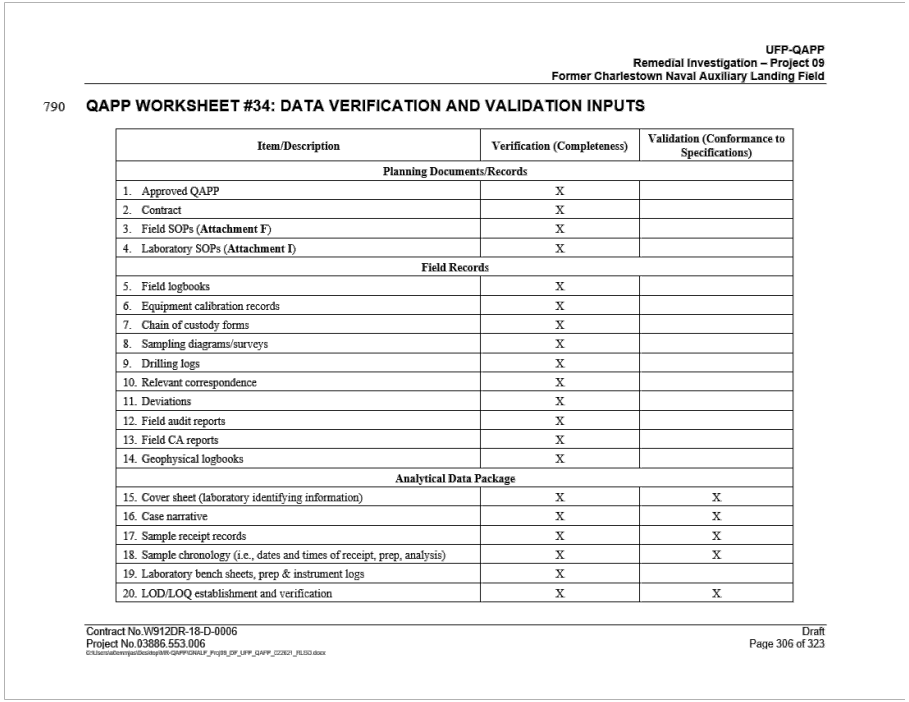
Comparison

	Verification	Validation	Usability Assessment
Purpose	Ensure presence and completeness	Ensure compliance with underlying specifications (e.g., SOPs, Methods, QSM)	Adequate quality and quantity for decisions (DQOs, PARCCS)
Responsible Party	Varies, usually contractor	3rd Party* Validators	Entire Project Team
Covers	Field records and laboratory data	Laboratory data	All project records and data
Timeline	Following collection	Following laboratory report issuance	End of sampling event, prior to decision making

Data Verification & Validation Inputs: Worksheet 34

- Describe which data needs to be
- Verified (i.e., do we have it?)
- Validated (i.e., is it of adequate quality?)
- List this for records included on WS #29
- Ones impacting project decisions
  - Is absence, or poor quality, of these data going to adversely impact the decision?

All inputs should be verified, but not everything will require validation



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790 **QAPP WORKSHEET #34: DATA VERIFICATION AND VALIDATION INPUTS**

Item/Description	Verification (Completeness)	Validation (Conformance to Specifications)
Planning Documents/Records		
1. Approved QAPP	X	
2. Contract	X	
3. Field SOPs (**Attachment F**)	X	
4. Laboratory SOPs (**Attachment I**)	X	
Field Records		
5. Field logbooks	X	
6. Equipment calibration records	X	
7. Chain of custody forms	X	
8. Sampling diagrams/surveys	X	
9. Drilling logs	X	
10. Relevant correspondence	X	
11. Deviations	X	
12. Field audit reports	X	
13. Field CA reports	X	
14. Geophysical logbooks	X	
Analytical Data Package		
15. Cover sheet (laboratory identifying information)	X	X
16. Case narrative	X	X
17. Sample receipt records	X	X
18. Sample chronology (i.e., dates and times of receipt, prep, analysis)	X	X
19. Laboratory bench sheets, prep & instrument logs	X	
20. LOD/LOQ establishment and verification	X	X

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Project No.03886.553.006
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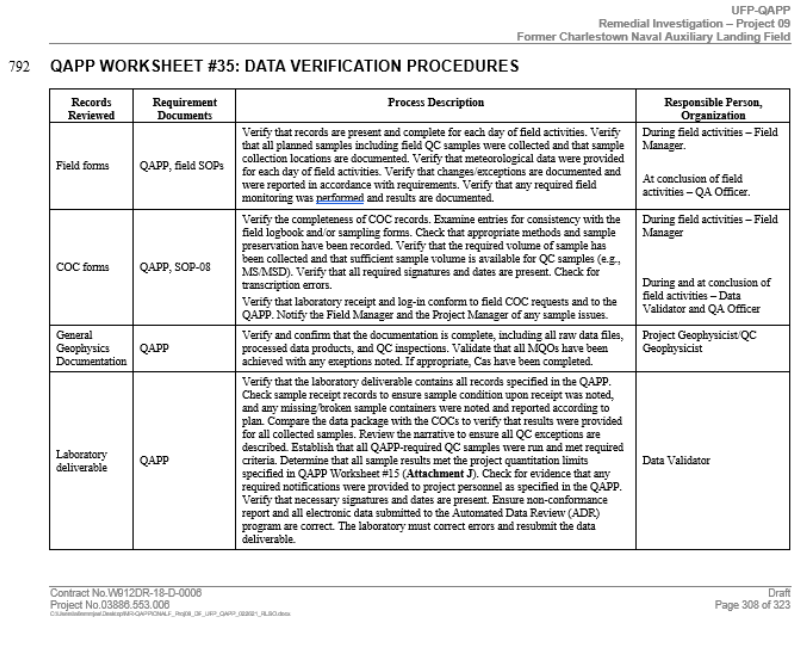
Figure adapted based upon UFP-QAPP Workbook.

Data Verification: Worksheet 35

- WS #35: Data Verification Procedures
  - Should confirm
    - Required activities were conducted
    - Specified records are present
    - Contents of records are complete
  - Describe verification process for each record or data deliverable
    - May be a multi-step process
    - May be performed at steps throughout project
    - May be performed by more than one person



792 **QAPP WORKSHEET #35: DATA VERIFICATION PROCEDURES**

Records Reviewed	Requirement Documents	Process Description	Responsible Person, Organization
Field forms	QAPP, field SOPs	Verify that records are present and complete for each day of field activities. Verify that all planned samples including field QC samples were collected and that sample collection locations are documented. Verify that meteorological data were provided for each day of field activities. Verify that changes/exceptions are documented and were reported in accordance with requirements. Verify that any required field monitoring was performed and results are documented.	During field activities – Field Manager. At conclusion of field activities – QA Officer.
COC forms	QAPP, SOP-08	Verify the completeness of COC records. Examine entries for consistency with the field logbook and/or sampling forms. Check that appropriate methods and sample preservation have been recorded. Verify that the required volume of sample has been collected and that sufficient sample volume is available for QC samples (e.g., MS/MSD). Verify that all required signatures and dates are present. Check for transcription errors. Verify that laboratory receipt and log-in conform to field COC requests and to the QAPP. Notify the Field Manager and the Project Manager of any sample issues.	During field activities – Field Manager During and at conclusion of field activities – Data Validator and QA Officer
General Geophysics Documentation	QAPP	Verify and confirm that the documentation is complete, including all raw data files, processed data products, and QC inspections. Validate that all MQOs have been achieved with any exceptions noted. If appropriate, Cas have been completed.	Project Geophysicist/QC Geophysicist
Laboratory deliverable	QAPP	Verify that the laboratory deliverable contains all records specified in the QAPP. Check sample receipt records to ensure sample condition upon receipt was noted, and any missing/broken sample containers were noted and reported according to plan. Compare the data package with the COCs to verify that results were provided for all collected samples. Review the narrative to ensure all QC exceptions are described. Establish that all QAPP-required QC samples were run and met required criteria. Determine that all sample results met the project quantitation limits specified in QAPP Worksheet #15 (**Attachment J**). Check for evidence that any required notifications were provided to project personnel as specified in the QAPP. Verify that necessary signatures and dates are present. Ensure non-conformance report and all electronic data submitted to the Automated Data Review (ADR) program are correct. The laboratory must correct errors and resubmit the data deliverable.	Data Validator

Data Validation – Definitions

Purpose

- An analyte- and sample-specific process that determines the analytical quality of a specific data set (EPA G-8).
- The systematic review of laboratory data deliverables which can help identify laboratory and field sample analytical uncertainty. … Evaluation of data with respect to the project measurement quality objectives (MQOs). (DoD General Data Validation Guidelines)

Scope

- Performed on Analytical Laboratory Data
- *Could and should* be performed on field data, (but usually is not).

Responsibilities

- 3rd Party – a definition

  "It is anticipated that data validation is performed by a party independent of the laboratory. Project teams may identify a government quality assurance validation as necessary. A government quality assurance validation is defined as being independent of the prime contractor and performed by a government representative or services directly contracted by the government agency independent of the prime contractor." (DoD General Data Validation Guidelines)

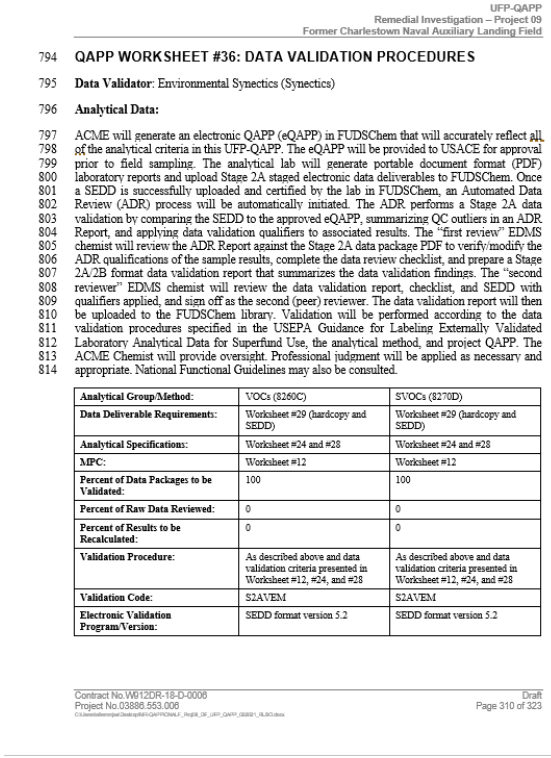
Independent of the Laboratory
Contractor Chemists
Validators Subcontracted to Prime
Government Project Chemist

Independent of the Prime Contractor
Validators Contracted to Government
Government Project Chemist

Data Validation Procedures: WS #36

Describe validation process for each record or data deliverable

- Analyte & sample-specific
- **Stage** of data validation must be defined during project planning
  - *Affects type & level of records required for both field & laboratory*
- Specify **percentage of recalculation** needed at Stages 3 and 4



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QAPP WORKSHEET #36: DATA VALIDATION PROCEDURES

Data Validator: Environmental Synectics (Synectics)

Analytical Data:

ACME will generate an electronic QAPP (eQAPP) in FUDSChem that will accurately reflect all of the analytical criteria in this UFP-QAPP. The eQAPP will be provided to USACE for approval prior to field sampling. The analytical lab will generate portable document format (PDF) laboratory reports and upload Stage 2A staged electronic data deliverables to FUDSChem. Once a SEDD is successfully uploaded and certified by the lab in FUDSChem, an Automated Data Review (ADR) process will be automatically initiated. The ADR performs a Stage 2A data validation by comparing the SEDD to the approved eQAPP, summarizing QC outliers in an ADR Report, and applying data validation qualifiers to associated results. The "first review" EDMS chemist will review the ADR Report against the Stage 2A data package PDF to verify/modify the ADR qualifications of the sample results, complete the data review checklist, and prepare a Stage 2A/2B format data validation report that summarizes the data validation findings. The "second reviewer" EDMS chemist will review the data validation report, checklist, and SEDD with qualifiers applied, and sign off as the second (peer) reviewer. The data validation report will then be uploaded to the FUDSChem library. Validation will be performed according to the data validation procedures specified in the USEPA Guidance for Labeling Externally Validated Laboratory Analytical Data for Superfund Use, the analytical method, and project QAPP. The ACME Chemist will provide oversight. Professional judgment will be applied as necessary and appropriate. National Functional Guidelines may also be consulted.

Analytical Group/Method:	VOCs (8260C)	SVOCs (8270D)
Data Deliverable Requirements:	Worksheet #29 (hardcopy and SEDD)	Worksheet #29 (hardcopy and SEDD)
Analytical Specifications:	Worksheet #24 and #28	Worksheet #24 and #28
MPC:	Worksheet #12	Worksheet #12
Percent of Data Packages to be Validated:	100	100
Percent of Raw Data Reviewed:	0	0
Percent of Results to be Recalculated:	0	0
Validation Procedure:	As described above and data validation criteria presented in Worksheet #12, #24, and #28	As described above and data validation criteria presented in Worksheet #12, #24, and #28
Validation Code:	S2AVEM	S2AVEM
Electronic Validation Program/Version:	SEDD format version 5.2	SEDD format version 5.2

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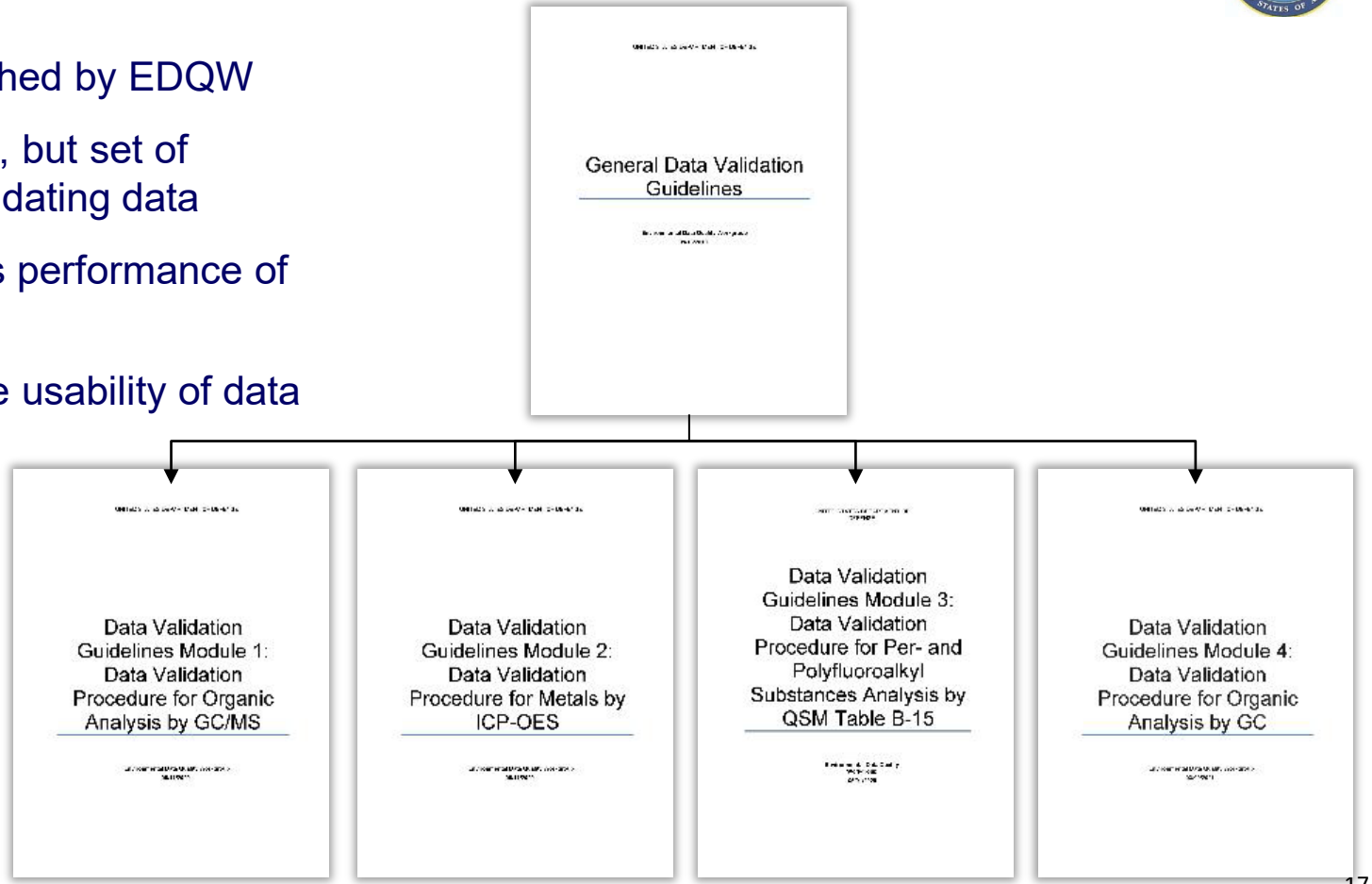
Guidelines

- Available Guidelines
  - NFG
    - Organics
    - Inorganics
  - DoD Data Validation Guidelines by EDQW
    - General Guidelines
    - Modules (currently 1-6)

Data Validation

Guidelines published by EDQW

- Not requirements, but set of guidelines for validating data
- Does not address performance of field work
- Cannot determine usability of data



Modules – how they work

- Modules are technology or method specific
  - Module 1: GC/MS
  - Module 2: ICP-OES
  - Module 3: PFAS by B-15
  - Module 4: GC
  - Module 5: ICP-MS
  - Module 6: PFAS by Draft EPA Method 1633
- Give detailed, step-by-step instructions for validation at each stage
- Include QC criteria and resulting qualifiers

Stages of Validation

- Stage 1:
  - Review of sample results forms, sample receipt summaries (chain of custody), and field QC data (field blank, field duplicates)
- Stages 2A and 2B:
  - Review of summary forms
- Stages 3 and 4
  - Review of summary forms and raw data with some recalculation

- Required for all stages:
  - Cover Sheet
  - Table of Contents
  - Laboratory Case Narrative
  - Results Summary

Stage 1

Purpose and Scope

- Ensure analytical method outlined in QAPP were performed
- Verify sampling and reporting completeness
- Evaluate field QC
- Verify compliance with project sensitivity needs

Documents Reviewed

- Sample results forms
- Chain of custody and supporting records (such as ground courier documents)
- Laboratory receipt checklist,
- Field QC records
- Holding times

Stage 2A

Purpose and Scope

- All of stage 1
- Validation of preparation batch specific QC data

Documents Reviewed

- Method blanks
- Matrix Spikes and Matrix Spike Duplicates
- Surrogates
- Serial Dilutions
- LCS
- Post Digestion Spikes
- QC frequency

Stage 2B

Purpose and Scope

- All of stage 1 and 2A
- Validation of instrument specific QC

Documents Reviewed

- Sequence and Preparation Logs
- Initial calibration summaries
- Initial and continuing calibration verification summaries
- Instrument blanks
- Tune and interference check summaries
- Internal standard summaries

Stage 3

Purpose and Scope

- All of stage 1, 2A, and 2B
- Recalculation and re-quantification of selected samples, method and instrument QC
- Define percentage of recalculation and re-quantitation

Documents Reviewed

- Raw Data
  - Laboratory forms
  - Instrument outputs
  - Spreadsheets
  - Handwritten calculations
- Standards Traceability forms and worksheets
- Detection Limit Studies (optional)

Stage 4

Purpose and Scope

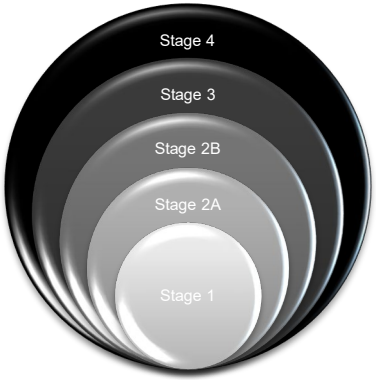
- All of stage 1, 2A, 2B, and 3
- Qualitative and quantitative review of detected and non-detected results from instrument outputs
- Requires professional judgment

Documents Reviewed

- Instrument chromatograms and spectra
- Tentatively identified compound searches
- Manual integration summaries with reasons

Which Stage is Right for me?

- Higher stage of validation does not necessarily result in higher data quality.
- However, quality of analytical data becomes more transparent.
- Depends on project DQOs!



Relationship of data to intended use is better understood

Validation Reports

- Prepared by validator following completion of validation
- Identifies laboratory SDGs, analyses included
- Includes cross reference between field sample identification and laboratory sample identification
- Specifies procedures followed including validation stage and percent recalculation
- Data is associated with a “validation qualifier”

Data Validation Report

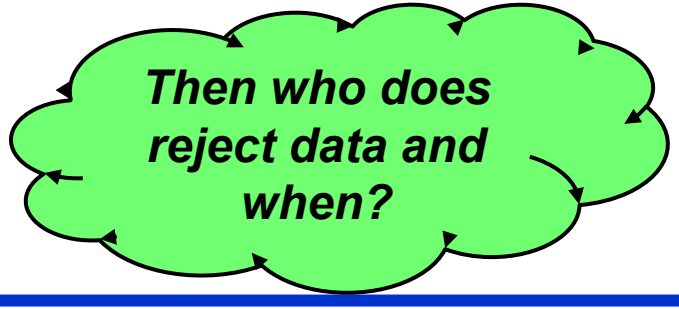
- **Cover Letter and Introduction**
- **Findings**
- **Checklists**
- **Documentation of recalculations**
- **Annotated Laboratory Reports**
- **Acronyms and Abbreviations**
- **Data Qualifiers Reference Table**
- **EDDs**

Validation Data Qualifiers

Qualifier	Definition
U	The analyte was not detected above the associate value (e.g., 5 U is synonymous with <5).
J	The reported result is an estimated value with unknown bias.
J+	The reported result is an estimated value and may be biased high.
J-	The reported result is an estimated value and may be biased low.
N	The analysis indicates the presence of an analyte for which there was presumptive evidence to make a tentative identification.
NJ	The analyte has been “tentatively identified” or “presumptively” as present and the associated numerical value is estimated.
UJ	The analyte was not detected; however, the associated numerical value is approximate.
X	The sample results were affected by serious deficiencies. Presence or absence of the analyte cannot be substantiated by data provided. Exclusion of data is recommended.

Some comments on the X-qualifier

"It should be re-emphasized that it is not the role of data validation to determine if project goals have been met or to provide the decisions to be made. Data validation provides the overall appraisal of a data set and the project team should use this appraisal along with their own judgment when making decisions. It is not the role of data validation to accept or reject data. As such, the conventional R (reject) flag has been removed from this document. The project team should make the decision to accept or reject qualified data during the Data Usability stage, in accordance with the QAPP (for example, using the process described in UFP-QAPP Worksheet #37)."



Time to talk about Data Usability

Data Usability Assessment: WS #37

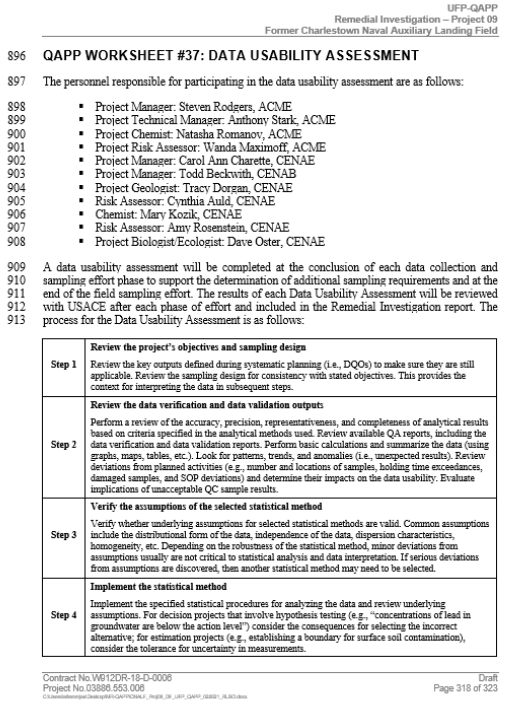
Usability Assessment is performed after data collection activities

- Uses data verification and validation outputs
- Also uses field records and other data sources
- Involves qualitative & quantitative data evaluation

Are project data of the right type, quality, and quantity to support project decisions?

Data Usability Assessment: WS #37

- WS #37: Data Usability Assessment, continued
  - Identify personnel responsible/involved
    - NOT just the chemist!
  - Summarize process
  - Document the Data Usability Assessment



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QAPP WORKSHEET #37: DATA USABILITY ASSESSMENT

The personnel responsible for participating in the data usability assessment are as follows:

- Project Manager: Steven Rodgers, ACME
- Project Technical Manager: Anthony Stark, ACME
- Project Chemist: Natasha Romanov, ACME
- Project Risk Assessor: Wanda Maximoff, ACME
- Project Manager: Carol Ann Charette, CENAE
- Project Manager: Todd Beckwith, CENAB
- Project Geologist: Tracy Dorgan, CENAE
- Risk Assessor: Cynthia Auld, CENAE
- Chemist: Mary Kozik, CENAE
- Risk Assessor: Amy Rosenstein, CENAE
- Project Biologist/Ecologist: Dave Oster, CENAE

A data usability assessment will be completed at the conclusion of each data collection and sampling effort phase to support the determination of additional sampling requirements and at the end of the field sampling effort. The results of each Data Usability Assessment will be reviewed with USACE after each phase of effort and included in the Remedial Investigation report. The process for the Data Usability Assessment is as follows:

Step 1	**Review the project's objectives and sampling design** Review the key outputs defined during systematic planning (i.e., DQOs) to make sure they are still applicable. Review the sampling design for consistency with stated objectives. This provides the context for interpreting the data in subsequent steps.
Step 2	**Review the data verification and data validation outputs** Perform a review of the accuracy, precision, representativeness, and completeness of analytical results based on criteria specified in the analytical methods used. Review available QA reports, including the data verification and data validation reports. Perform basic calculations and summarize the data (using graphs, maps, tables, etc.). Look for patterns, trends, and anomalies (i.e., unexpected results). Review deviations from planned activities (e.g., number and locations of samples, holding time exceedances, damaged samples, and SOP deviations) and determine their impacts on the data usability. Evaluate implications of unacceptable QC sample results.
Step 3	**Verify the assumptions of the selected statistical method** Verify whether underlying assumptions for selected statistical methods are valid. Common assumptions include the distributional form of the data, independence of the data, dispersion characteristics, homogeneity, etc. Depending on the robustness of the statistical method, minor deviations from assumptions usually are not critical to statistical analysis and data interpretation. If serious deviations from assumptions are discovered, then another statistical method may need to be selected.
Step 4	**Implement the statistical method** Implement the specified statistical procedures for analyzing the data and review underlying assumptions. For decision projects that involve hypothesis testing (e.g., "concentrations of lead in groundwater are below the action level") consider the consequences for selecting the incorrect alternative; for estimation projects (e.g., establishing a boundary for surface soil contamination), consider the tolerance for uncertainty in measurements.

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Personnel Involved

Entities

Lead Organization

Stakeholders/Regulators

Contractor

Subcontractors

Each entity brings their own personnel and subject matter experts (SMEs) to the table

Personnel

Project Managers	*Risk Assessor*
Technical Managers	*Chemist*
Resource Managers	*Statisticians*
Geologist	*Analysts*
Hydrogeologist	*Field Samplers*
Geophysicist	*Safety Personnel*

Logistics of DUA Meeting

In Person	Virtual – Real Time	Virtual – Asynchronous
• Government PM with contractor schedules, hosts, and facilitates DUA meeting • Recorder documents responses to questions and distributes draft for review	• Government PM with contractor schedules, hosts, and facilitates teleconference • Recorder documents responses to questions and distributes draft for review	• Designated POC may send out email request for feedback on DUA Steps/ Questions • POC assembles responses and distributes draft for review

Process-Oriented

4-Step Process

- Step 1: Review the project's objectives and sampling design
- Step 2: Review the data verification/validation outputs
- Step 3: Document data usability, update CSM, apply decision rules, and draw conclusions
- Step 4: Document lessons learned and make recommendations

DUA Report

- Details of Who, What, When, etc. DUA was performed
- Detail to adequately explain impact of deviations from SOPs or MPCs
- Conclusions clearly stated and scientifically justified
- Lessons learned are communicated for future action
- Included as appendix in final reports

Data Review Process

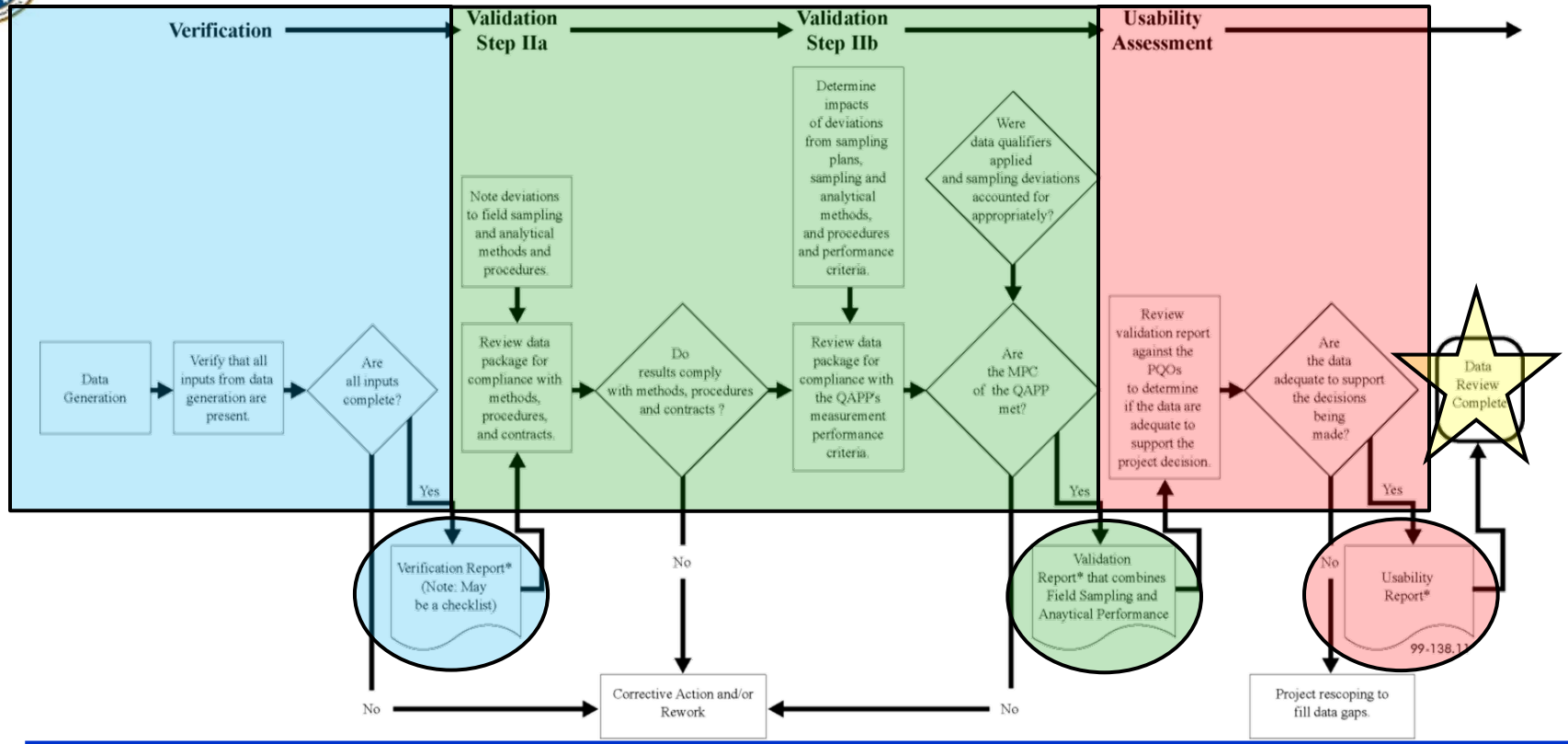

Figure from IDQTF, UFP-QAPP Manual V1, March 2005, Figure 37. Data Review Process.

Lessons Learned

- **What is DoD doing right?**
  - Data review planned in advance
  - Systematic and consistent procedures for analytical data validation
  - Thorough documentation of data quality from validation
  - Increasing adoption of comprehensive DUA
- **What is still challenging for DoD?**
  - Consistent incorporation of field and other records into data review
  - DUA process inconsistent across projects and programs
  - Difficulties in DUA decisions often reveal incomplete DQOs

References – Process and Planning

- Process and Planning
  - IDQTF, UFP-QAPP Part 1: UFP-QAPP Manual, March 2005
  - IDQTF, UFP-QAPP Optimized UFP-QAPP Worksheets, March 2012
  - IDQTF, UFP-QAPP Munitions Response QAPP Toolkit Module 1, April 2020
- Validation and Verification
  - EPA Guidance on Environmental Data Verification and Data Validation, EPA QA/G-8, November 2002
  - EDQW, General Data Validation Guidelines, September 16, 2019
  - EDQW, Data Validation Guidelines Module 1: Data Validation Procedure for Organic Analysis by GC/MS, May 11, 2020
  - EDQW, Data Validation Guidelines Module 2: Data Validation Procedure for Metals by ICP-OES, May 11, 2020
  - EDQW, Data Validation Guidelines Module 3: Data Validation Procedure for Per- and Polyfluoroalkyl Substances Analysis by QSM Table B-15, May 1, 2020
  - EDQW, Data Validation Guidelines Module 4: Data Validation Procedure for Organic Analysis by GC, March 9, 2021
  - EDQW, Data Validation Guidelines Module 5: Data Validation Procedure for Metals by ICP-MS, November 09, 2022
  - EDQW, Data Validation Guidelines Module 6: Data Validation Procedure for Per- and Polyfluoroalkyl Substances Analysis by QSM Table B-24, October 18, 2022
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