

The Columbia River Protection Supplemental Technologies Quality Assurance Project Plan

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January 2007



Prepared for the U.S. Department of Energy under Contract DE-AC05-76RL01830

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Pacific Northwest National Laboratory Richland, Washington 99352

Summary

The U.S. Department of Energy (DOE) has conducted interim groundwater remedial activities on the Hanford Site since the mid-1990s for several groundwater contamination plumes. DOE established the Columbia River Protection Supplemental Technologies Project (Technologies Project) in 2006 to evaluate alternative treatment technologies. The objectives for the technology project are as follows: develop a 300 Area polyphosphate treatability test to immobilize uranium, design and test infiltration of a phosphate/apatite technology for Sr-90 at 100-N, perform carbon tetrachloride and chloroform attenuation parameter studies, perform vadose zone chromium characterization and geochemistry studies, perform in situ biostimulation of chromium studies for a reducing barrier at 100-D, and perform a treatability test for phytoremediation for Sr-90 at 100-N.

This document provides the quality assurance guidelines that will be followed by the Technologies Project. This Quality Assurance Project Plan is based on the quality assurance requirements of DOE Order 414.1C, *Quality Assurance*, and 10 CFR 830, Subpart A--*Quality Assurance Requirements* as delineated in Pacific Northwest National Laboratory's Standards-Based Management System. In addition, the technology project is subject to the *Environmental Protection Agency (EPA) Requirements for Quality Assurance Project Plans* (EPA/240/B-01/003, QA/R-5). The *Hanford Analytical Services Quality Assurance Requirements Documents* (HASQARD, DOE/RL-96-68) apply to portions of this project and to the subcontractors. HASQARD requirements are discussed within applicable sections of this plan.

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1.0 Quality Assurance Project Plan Distribution

Pacific Northwest National Laboratory (PNNL) Document Control will distribute this Quality Assurance Project Plan (QAPjP) internally to PNNL, the U.S. Department of Energy (DOE) Reading Room and Technical Library. The project manager will determine the distribution list. Also, the QAPjP will be published in accordance with the Standards-Based Management System (SBMS) subject area, *Publishing Scientific and Technical Information* (PNNL 2002a).

2.0 Introduction

2.1 Title

The Columbia River Protection Supplemental Technologies Quality Assurance Project Plan.

2.2 Client

U.S. Department of Energy, Richland Operations Office, Richland, Washington.

2.3 Authorizing Document

Work has been authorized by specified multi-year project work plans as shown in Table 2.1.

Table 2.1. Treatability Study Project Work Plans

Project Number	Project Work Plan Title	Author(s)
PNNL-SA-49953	100-N Area Strontium-90 Treatability	CC Ainsworth
	Demonstration Project: Phytoremediation Along	
	the 100-N Columbia River Riparian Zone	
PNNL-SA-49954	300 Area Uranium Plume Treatability	VR Vermeul, D.M Wellman, TG
	Demonstration Project: Uranium Stabilization	Naymik, MJ Nimmons
	Through Polyphosphate Injection	
PNNL-SA-50071	Sequestration of Strontium-90 Subsruface	JE Szecsody
	Contamination in the Hanford 100-N Area by	
	Surface Infiltration of an Apatite Solution	
PNNL-SA-50369	Hanford 100-D Area Treatability Demonstration:	JS Fruchter, MJ Truex, VR
	In Situ Biostimulation for a Reducing Barrier	Vermeul, PE Long
PNNL-SA-50254	Chromium Vadose Zone Characterization and	CC Ainsworth
	Geochemistry	
PNNL-SA-51843	Carbon Tetrachloride and Chloroform	JE Amonette, MJ Truex, JS
	Attenuation Parameter Studies: Heterogeneous	Fruchter
	Hydrolytic Reactions	

2.4 Quality Assurance Requirements

The Columbia River Protection Supplemental Technologies Project's Quality Assurance Program is based on the QA requirements of DOE Order 414.1C, *Quality Assurance*, and 10 CFR 830, Subpart A--Quality Assurance Requirements as delineated in PNNL's SBMS. The project is subject to the Environmental Protection Agency (EPA) Requirements for Quality Assurance Project Plans (EPA/240/B-01/003, QA/R-5) as required by the Tri-Party Agreement (TPA; Ecology et al. 1989). The project is subject to the Price Anderson Amendments Act (PAAA) as defined in the PNNL PAAA Program and implemented through SBMS (See Price-Anderson Amendments Act, [PNNL 2006a]). Additionally, the Technologies Project has determined that the Hanford Analytical Services Quality Assurance Requirements Documents (HASQARD, DOE/RL-96-68) apply to portions of this project and to the subcontractors. HASQARD requirements are discussed within applicable sections of this plan. The PNNL document for implementing HASQARD is Conducting Analytical Work in Support of Regulatory Programs (CAWSRP) located at http://etd.pnl.gov/docs/conducting-work/index.stm.

2.5 Special Requirements or Specifications

DOE Orders 435.1, *Radioactive Waste Management*; 5400.5, *Radiation Protection of the Public and Environment*; and 450.1, *Environmental Protection Program*, apply to the treatability studies to ensure that activities related to radioactive materials and samples are protective of human health and the environmental and stewardship requirements of PNNL.

The modeling projects shall comply with the software requirements as specified in the PNNL's SBMS *Safety Software* (PNNL 2006d) subject area. Specific safety software requirements are described in Section 17.

2.6 Project Scope

DOE has conducted interim groundwater remediation activities on the Hanford Site since the mid-1990s for several groundwater contamination plumes. DOE established the Columbia River Protection Supplemental Technologies Project (herein after referred to as the Technologies Project) in 2006 to evaluate alternative treatment technologies. The objectives for the Technologies Project are as follows: develop a 300 Area polyphosphate treatability test to immobilize uranium; design and test infiltration of a phosphate/apatite technology for strontium (Sr)-90 at 100-N Area; and perform a test for phytoremediation for Sr-90 at 100-N Area. Additional objectives include laboratory evaluation of carbon tetrachloride and chloroform attenuation parameters, evaluation of the geochemistry of chromium in the Hanford vadose zone, and evaluation of chromium degradation through in situ biostimulation using polylactate injection at 100-D Area. These six objectives comprise the six project tasks within the technology project.

The 300 Area polyphosphate treatability test will evaluate the efficacy of using polyphosphate injections to treat uranium-contaminated groundwater in situ. Data obtained from this study will be used to develop implementation cost estimates, identify implementation challenges, and investigate the ability of the technology to meet remedial objectives. This information will be used in the 300-FF-5 Phase III feasibility study during final evaluation of remedial alternatives.

The test of the 100-N Area phosphate/apatite technology for Sr-90 will inject an apatite-forming solution, which should result in sufficient removal capacity of Sr-90 for approximately 10 years followed by higher concentration injections to develop further capacity. Because most (50% to 70%) of the Sr-90 contamination is in the shallow, variably saturated Hanford formation, the most efficient means of treating this zone may be surface infiltration of the apatite-forming solution, but there has been no development of this technology for vadose zone application.

The phytoremediation test for Sr-90 will (1) determine the most efficient fertilization method for coyote willow that will generate the greatest biomass possible while protecting the Columbia River from excess nutrient runoff; and (2) demonstrate the efficacy of using coyote willow as a Sr-90 phytoremediation tool along the riparian zone associated with the 100-N Area of the Hanford Site. The initial effort will be in a "cold zone" outside of the contaminated area; follow-on work, if funded, will be conducted within a contaminated area.

The carbon tetrachloride/chloroform study will determine (1) the neutral and base-catalyzed homogeneous hydrolysis rates for chloroform under near-ambient temperatures, (2) the impact and mechanisms of representative Hanford mineral surfaces on the hydrolysis of carbon tetrachloride at near-ambient temperatures, and (3) the impact and mechanisms of representative Hanford mineral surfaces on the neutral and base-catalyzed hydrolysis of chloroform at near-ambient temperatures.

The chromium geochemistry project will (1) determine the leaching characteristics of Cr(VI) from contaminated sediments collected from 100 Area spill sites, (2) elucidate possible Cr(VI) mineral and/or chemical associations that may be responsible for Cr(VI) retention in the Hanford Site 100 Areas through the use of (i) macroscopic solubility studies and (ii) microscale characterization of contaminated sediments, and (3) from these data construct a conceptual model of Cr(VI) geochemistry in the Hanford 100 Area vadose zone.

The 100-D Area in situ biostimulation technology is intended to provide supplemental treatment upgradient of the In Situ Redox Manipulation (ISRM) barrier by directly treating chromium and other oxidizing species in groundwater (i.e., nitrate and dissolved oxygen). This thereby increases the longevity of the ISRM barrier and protects the ecological receptors and human health at the river boundary.

2.7 Change Control (Scope, Schedule, Budget)

The project scope, schedule, and budget baseline are compiled, tracked, and reported using a project control system in accordance with DOE direction.

Changes in work scope, schedule, or budget may be necessary during the year. Changes may be requested of subcontractors by PNNL that will result in a change to the statements of work (SOWs) due to revisions of work scope, schedule, and/or budget. These changes will be documented in revisions or addendums to the existing SOWs and a PNNL Subcontracts Supplement Form shall be completed.

Administrative changes requested of subcontractors that are approved by Task Leaders may be made by verbal or electronic message authorization. Written documentation of the verbal changes and electronic messages should be maintained in the permanent project files. These changes may only be made if technical work scope and budget are not affected significantly.

3.0 Project Organization and Responsibilities

Line authority, quality assurance authority and support within PNNL, and client interfaces are shown organizationally in Figure 1. The responsibilities of key PNNL personnel are summarized in Section 3.1. Changes to organizational/interface structures shown in Figure 1 that do not reflect a change in the overall scope of the activities or a change of requirements will not require a QAPjP revision and will be incorporated into the next required revision of the QAPjP.

3.1 Responsibilities of Key Personnel

- Project Manager provides overall direction to task managers and project personnel within PNNL
 necessary to accomplish project objectives; coordinates and executes project controls associated with
 scope, schedule, and budget baselines; reports on project status; assures that the project is staffed
 with technically qualified personnel; serves as primary client interface to assure that customer
 expectations are met in terms of quality, cost, and schedule; assures the QAPjP is implemented.
- *Technology Task Leaders* oversees task-specific planning, control, communications, and progress reporting; prepares scope, resource needs, cost baseline, and deliverables; assures quality and timeliness of the work, in accordance to plans, policies, and procedures; provides monthly reports; interfaces with DOE, other contractors, subcontractors, and other Task Leaders.
- *Technology Principle Investigators* provides task-specific technical plans, communications, and progress reporting to the Task Leader; prepares technical details of the task plan; assures technical quality of the work; supports the Task Leader to assure work is performed on schedule, within budget, and in accordance to plans, policies, and procedures; assigns and directs work of project staff; interfaces with DOE, other contractors, subcontractors, and other Investigators.
- Project Quality Engineer provides guidance and direction to Project Manager, Task Leads, and
 project staff within PNNL on PNNL QA Program requirements; performs assessments to assure
 quality of the work; develops, updates, and approves QAPjP; reviews and approves appropriate work
 plans and procedures.
- *Other Project Staff* assures technical quality of the work and that it is performed on schedule, within budget, and in accordance to plans, policies, and procedures; reports concerns such as unsafe conditions and stops work as necessary.

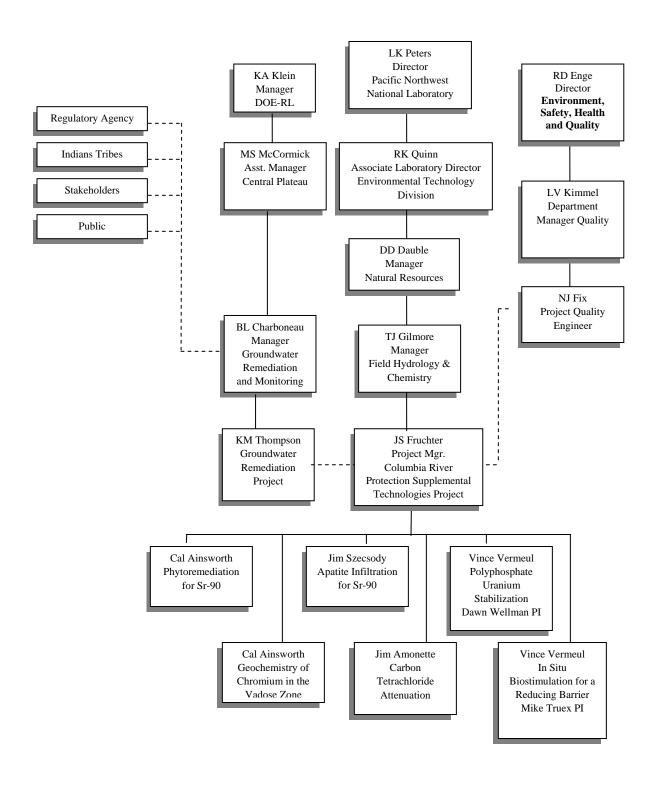


Figure 1. Project Interfaces

3.2 Other Work Services

Other work services for various portions of project work will be through the purchasing process. General scope of work, work requirements, specifications, and quality assurance requirements are communicated via a contracting mechanism to various subcontractors (see Section 14.0). Statements of Work (SOWs) to subcontractors used for groundwater and sediment sampling and analysis will require compliance with the HASQARD (DOE/RL-96-68) and/or the *EPA Requirements for Quality Assurance Project Plans* (EPA/240/B-01/003, QA/R-5), and will specify requirements to be achieved by appropriate quality documents. The SOW will include instructions for inspecting/accepting supplies and consumables used for this project.

Subcontracts for drilling, sediment sampling, groundwater sampling, and associated support activities will include the following:

- Fluor Hanford, Inc. (FHI) performs routine groundwater sampling and water-level measurements, purge water containment and disposal, radiological control technician support, and miscellaneous solid waste disposal.
- FHI also provides drilling, sediment and water sample collection related to drilling, and well
 construction services.

Subcontracts for analytical laboratory services will include the following:

- Severn Trent Laboratories
- Other subcontractors may provide civil surveys, special analytical services, or other services.

3.2.1 Analytical Services

The analytical laboratories including commercial, on-site, and other DOE national laboratories are responsible for preparing data reports that summarize the results of analyses and detailed data packages that include the following:

- Sample receipt and tracking documentation, including identification of the organization and individuals performing the analysis; names and signatures of the responsible analysts; sample holding time requirements; references to applicable chain-of-custody procedures; and dates of sample receipt, extraction (if applicable), and analysis.
- Quality control data, as appropriate for the methods used, including (as applicable) matrix spike/matrix spike duplicate data, recovery percentages, precision and accuracy data, laboratory blank data, and identification of any nonconformance that may have affected the laboratory's measurement system during the time period in which the analysis was performed.
- Analytical results or data deliverables, including reduced data and identification of data qualifiers and contractually defined reporting comments.

These requirements as well as QA and technical requirements are specified in the SOW to the analytical laboratories. Also, the requirements for the hard copy and electronic data received from the analytical laboratories are specified in respective analytical subcontractor SOWs.

3.2.2 Sampling Services

The sampling organization is responsible for (1) obtaining the samples; (2) delivering samples to the laboratory; and (3) delivering completed sampling and water-level paperwork to PNNL. Activities associated with the sample collection, sample handling, sample labeling, and custody of the samples in the field shall be consistent with the SOW.

3.2.3 Well Drilling, Sampling, and Construction Services

FHI provides well-drilling and construction subcontractors and oversight on the Hanford Site. FHI is responsible for (1) well drilling design specifications and contract management, (2) site preparation and documentation requirements, (3) sediment and water sample collection during drilling, (4) support of hydrologic tests conducted during drilling, and (5) well construction, development, and sample pump installation. Well construction will meet the requirements of WAC 173-160. Well drilling and construction, sediment and water sampling, testing support, and associated quality requirements will be specified in the SOW to FHI. FHI may subcontract work activities provided the requirements in the SOW and the FHI QA Program are met by subcontractor(s).

3.2.4 Other Services

Other subcontracted services received from FHI or other Hanford Site contractors may include construction of fences and enclosures, geophysical logging, etc.

3.3 Work Conducted by Project Staff

Analytical activities conducted by the project staff in support of the technology project shall be conducted in accordance with written standard operating procedures. Field measurements will be conducted in accordance with in-house operating procedures. The project staff members are responsible for preparing data reports that summarize the results of analyses, quality control data for the methods used, and identification of data qualifiers. The results and raw data will be included in the project records.

Project staff will perform sampling and measurements according to written and approved test plans (Section 5.1), written procedures, or other written direction.

3.4 Field Work

Field work is executed by the treatability study projects. Prior to executing field work, project-specific test plans are developed, as described in Section 5. If supplemental information or individual parameters are needed to perform a test, a test instruction will be developed. The test instruction shall be reviewed by a technical reviewer.

Field work associated with task activities is conducted in accordance with the *Surface Environmental Surveillance Procedures Manual* (PNL-MA-580, Rev. 4). The following procedures in PNL-MA-580 are used:

- Section 4.1 Grab Samples
- Section 4.6 Sampling Columbia River Riverbank Springs
- Section 4.8 Specific Conductance
- Section 4.9 pH Measurement
- Section 4.10 Water Filtration
- Section 8.1 Trip Sheets.

A specific procedure for sampling aquifer tubes is undergoing final review and will be included in the *Procedures for Ground-Water Investigation* Manual (PNL-MA-567) upon completion.

4.0 Data Quality Objectives

The QA objectives for measurements generally applicable to technology investigations under the purview of this QAPiP are primarily related to (1) the definition of appropriate methods and analytical precision and accuracy appropriate for chemical analysis of the analytes of interest; and (2) the definition of methods and limits and values for physical measurements associated with the investigation (e.g., column tests). Discussions of aqueous sample analytical objectives and analytical methods with corresponding target values for detection limits, precision, and accuracy are provided in the Groundwater Performance Assessment Project Quality Assurance Plan Appendix (QC Plan contained in PNNL-15014, current revision), the Environmental Sciences Laboratory QA Plan (QAP ESL, Rev. 0), individual test plans, and/or test procedures. The sediment analytical objectives and analytical methods with corresponding target values for detection limits, precision, and accuracy are provided in the Environmental Sciences Laboratory OA Plan, individual test plans, and/or test procedures. Other measurement objectives and methods with corresponding target values for detection limits, precision, and accuracy (as applicable) are provided in the specific work plans and/or the SOW for such activities. Specific data quality needs for individual investigations that are different than the requirements established herein shall be addressed within individual work plans. Other measurement considerations, accuracy requirements, units, and data recording and reporting protocols for instruments supporting stratigraphic characterization, aquifer testing, and other types of field investigations shall be as specified in the applicable plans and/or procedures.

5.0 Test Plans and Procedures

Test plans and procedures are used to ensure that activities affecting quality are performed consistently and correctly. Test plans are prepared by PNNL staff to conduct a single experiment or test as identified below. Formal procedures will be developed for quality affecting work activities that are routinely performed.

5.1 Test Planning and Performance

Test plans will be used to document a single or related set of experiments or tests (e.g., hydrologic field tests, vertical sampling) of work activity.

5.1.1 Developing the Test Plan

The test plan shall contain the following information:

- A title and/or number including date or revision.
- Dated signatures of the Preparer, Technical Lead, Project Manager or Task Lead, and Quality Representative.
- Individual page identification (page ___ of ___).

The content of each test plan will depend on the scope of the test. The following is a brief description of mandatory and optional items to be considered in the preparation of the test plan:

• **Purpose/Description (mandatory)** – Provide a short narrative on the purpose of the experiment/test/activity.

Example: The purpose of this test is to provide hydrologic property data at polyphosphate treatability injection test wells.

• **Prerequisites** (mandatory) – List items, conditions, or other concerns that must be satisfied prior to beginning the test.

Example: Prior to beginning the work activity, the staff must complete special training on other plans or procedures that will be used in conjunction with the test plan, special handling or storage requirements, special access or permits, and required records that need to be generated as the result of the work activity.

- Safety (mandatory) Describe the hazards associated with the work such as physical agents (e.g., temperature, pressure, noise, electrical); hazardous environments (e.g., confined spaces, remote locations, heat/cold stress); and hazardous materials (e.g., flammables, corrosives, highly toxic, carcinogens). Describe the methods used to mitigate the hazards that were identified (e.g., personal protective equipment, time periods away from the hazard, alarms, location of nearest aid station).
- Materials and Equipment (optional) List the materials and equipment that are necessary to complete the work.
- Measuring and Test Equipment (mandatory) List the equipment that will be used to make the measurements; include the calibration requirements, system checks, and quality control checks in this section or in the work instructions section of the test plan.

- **Pretest Verification (mandatory)** Determine if certain items of a test require verification prior to their use and indicate how the verification will be done.
 - +Example: A tracer solution containing Br will be used throughout the test and the initial concentration shall be known. The solution shall be measured by the calibrated probe (as described above) and the concentration shall be recorded prior to injection.
- **Documentation and Reporting (mandatory)** Describe where the data collected during the test should be documented (e.g., field record forms, laboratory record books, entered into a computer, downloaded from computer to hardcopy) or entered into HEIS. Additionally, describe what will be reported, to whom, and the due date(s).
- Work Instructions (mandatory) Provide step-by-step instructions and/or non-sequential instructions (whichever is more appropriate to the activity). Each step or instruction shall be as simple as possible but with sufficient detail so that individuals experienced in the technology or activity involved can easily understand. The following types of information should be considered for inclusion: administrative control hold points (i.e., where safety, quality, radiological, or other approvals or actions are required before proceeding); cautions that indicate potentially hazardous situations which, if not avoided, may result in death, injury, or damage to facilities or equipment; and notes that call attention to supplemental information that assist the user in making decisions or improving work performance.

5.1.2 Test Performance

Tests will be performed in accordance with the test plans, which shall be available at the work location. The Technical Lead is responsible for assuring that the current version is used to perform the work.

If changes to the test plan are required during the execution of the work, the Technical Lead shall document the deviation and the justification or rationale for the change.

5.2 Procedures

Procedures will be developed in accordance with SBMS subject area, <u>Procedures, Permits, and Other Work Instructions</u> (PNNL 2004). Project staff will perform scheduling, data verification, data processing, and data management as described in Section 6 and by following the applicable internal technical procedures or instructions.

5.2.1 Analytical Procedures

The specific work plans and/or test plans identify the constituents to be analyzed. As applicable, a PNNL internal procedure generates the sampling package (e.g., chain-of-custody form), which identifies the analytical methods, sample identification, etc. on the chain-of-custody form. The chain-of-custody form and samples are provided to the appropriate analytical laboratory. Administrative quality assurance processes and procedures (e.g., chain of custody, custody logs, sample handling, storage and disposal, training) will be required of the onsite and offsite analytical laboratories and will be specified in the SOW. The analytical methods required may be contained within the following references:

- Test Methods for Evaluating Solid Waste (EPA/SW-846, as amended)
- *Methods for Chemical Analysis of Water and Wastes* (EPA-600/4-79-020)
- Methods for the Determination of Organic Compounds in Drinking Water (EPA-600/4-88-039)
- Prescribed Procedures for Measurement of Radioactivity in Drinking Water (EPA-600/4-80-032)
- Procedures for Radiochemical Analysis of Nuclear Reactor Aqueous Solutions (EPA-R4-73-014)
- Radiochemical Analytical Procedures for Analysis of Environmental Samples (EMSL-LV-0539-17).

Many radiochemical methods have not been standardized, but the procedures are documented in the laboratory-specific standard operating procedures. Aqueous sample chemical and radiological analytical methods and requirements for constituents are specified by the SOW, work plan, or other written direction. Most potential chemical constituents to be analyzed are provided in the *Groundwater Performance Assessment Project Quality Assurance Plan* Appendix (QC Plan; see PNNL-15014, current revision) and/or the *Environmental Sciences Laboratory QA Plan* (QAP ESL, Rev. 0). Sediment and other media constituents to be analyzed and corresponding analytical methods and procedures will be passed on to the analytical laboratory by a SOW, work plan, or other written direction.

Method detection limits (MDLs) shall be determined for all non-radiochemical methods required by the project. The laboratory provides MDL study results to PNNL as specified in the SOW. Required detection limits for radiochemical methods are provided in the SOW, work plan, or other written direction.

Technical procedures not previously documented will be developed and used as described in CAWSRP, Section 7, *Procedures*. If supplemental information or individual parameters are needed to perform a test, a test instruction will be developed. The test instruction shall be reviewed by a technical reviewer and must include the following information:

- A unique numerical designation
- Revision number
- Title
- Effective date
- Instructions operating parameters and specific test run information such as sample size and /or composition, temperature, pH, test duration, etc.
- Reference to controlling procedure or test plan
- Approval by author
- When well-established methods (e.g., ASTM, Soil Science Society of America, or EPA) are used, a PNNL cover page will not be provided unless there is a deviation from the established method.

Appendix B lists additional analyses and measurements with the respective procedures, methods, and other relevant information.

5.2.2 Calibration Procedures

The requirements for calibrating field and analytical laboratory instruments and maintaining traceability to national or international standard (e.g., National Institute of Standards and Technology) are in accordance with *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods*, EPA/SW-846 and HASQARD (DOE/RL-96-68). These requirements are passed to the subcontractors by a SOW.

PNNL will periodically assess the use and effectiveness of procedures and systems for calibration of equipment with the subcontractors.

Measuring and test equipment (M&TE) used by PNNL staff to collect quality affecting data that are calibrated by the user (Category 2 M&TE) or by an approved external or internal source (Category 1 M&TE) will be in accordance with SBMS subject area, *Calibration* (PNNL 2005b). Upon receiving calibrated equipment, staff must review the documentation for acceptability, verify the proper operation of the M&TE, and check the calibration label.

Measuring and test equipment shall be controlled as described in CAWSRP, Section 4, *Instrument Calibration*, and in accordance with the SBMS subject area *Calibration* (PNNL 2005b). Externally calibrated M&TE such as balances will be calibrated in accordance with manufacturer's tolerances unless other control limits are specified and justification is provided.

Data sheets and log book entries will be used to document pipette performance checks. Calibration reports and other calibration data will be maintained as project records.

Quality control requirements are described in CAWSRP, Section 5, *Quality Control*, and in Appendix C of this QAMP. A few exceptions to CAWSRP requirements are considered necessary for the project, as described in the following paragraphs.

5.2.3 Common Data Quality Calculations

Data quality parameters of precision, accuracy, measures of agreement, detection limits/sensitivity, and uncertainty will be calculated per the formulas in CAWSRP, Section 6, in the exhibit *Calculations for Assessing Data Quality*. For radiochemistry analyses, the minimum detectable activity (MDA) is reported as the detection limit.

CAWSRP Exhibit "Calculations for Assessing Data Quality" - Control charting is a tool used to monitor an ongoing/continuous process where there are sufficient data points to perform a representative statistical evaluation. The analyses performed within this project are performed as a research function in which instrumental operating parameters may be changed to accomplish many different objectives. The frequency of instrumental operating changes does not allow accumulation of sufficient data points to properly utilize control charting as a statistical analysis tool. In lieu of control charts, instrument performance is monitored daily by the use of fixed control limits.

5.2.4 Well Drilling and Construction Procedures

A SOW to FHI specifies well drilling, characterization (aquifer and sediment sampling, etc.), and construction requirements. These activities will be performed to FHI procedures and/or to subcontractor procedures (e.g., geophysical logging). FHI Health and Safety, QA procedures, and waste management procedures will be followed during the drilling activity.

5.2.5 Water and Sediment Sample Collection Procedures

Groundwater sampling of a routine nature will be done by Fluor Hanford Nuclear Chemical Operators (NCOs). Quality requirements for sampling activities, including requirements for procedures,

containers, transport, storage, chain of custody, and record requirements, are specified in a SOW. Non-routine sample collection may be performed by PNNL staff in order to meet specific conditions or requirements.

To verify that samples of known quality are obtained, FHI and PNNL staff will be required to use controlled procedures based on standard methods for groundwater sampling whenever possible. Assessments will be performed by PNNL to further assure that procedures are followed to maintain sample quality and integrity (see Section 8).

Sediment and water samples collected during drilling will be collected by or under the direction of FHI, and in accordance with FHI or subcontractor procedures. The quality requirements for sampling activities, including chain of custody, storage, and records requirements are specified in the Statement of Work (or well data sheet). Scheduling sample bottle preparation, conducting sample analysis, and preparing associated paperwork are conducted by PNNL in accordance with PNNL internal procedures.

5.2.6 Receiving and Handling Samples

Directions for sample receipt, handling, and storage are provided in CAWSRP, Section 3, *Receiving and Handling Samples*, and in the SBMS subject area <u>Sample Handling, Archival, and Disposal</u> (PNNL 2006c).

Chain of custody for samples will be documented using a chain of custody form. An example of a chain of custody form is provided as an exhibit in CAWSRP. Each PNNL facility is a secured area, restricted to authorized personnel only. Chain of custody will be documented for moving samples from one facility to another, but not for moving samples within a secured facility.

The samples to be received from other PNNL groups are materials from various field investigations. Documentation of unique sample and sub-sample identifications will be maintained for samples received from other PNNL groups and for other samples generated from tests conducted by the project. The documentation may consist of entries in Laboratory Record Books or data sheets.

Disposition of unused materials may include returning the material to another group at PNNL, the client or disposal at PNNL. Material returned to the client will be documented by a chain of custody. Material disposed of at PNNL will be documented by standard waste paperwork (forms).

5.2.7 Sediment Physical Analysis Procedures

Sediment physical analyses including moisture content, particle-size distribution, hydraulic conductivity, water retention, water content, bulk density, particle density, and matric potential will be performed as directed in the test plan by PNNL staff. These procedures are contained in the internal *Procedures for Groundwater Investigations* (PNL-MA-567).

5.2.8 Sediment Core Analysis Procedures

Sediment core analyses and column experiments will be performed by PNNL staff as directed in the test plan. Procedures are contained in the individual test plans, which will either provide a procedure or reference an existing procedure.

6.0 Data Generation and Acquisition

6.1 Sampling Process Design (Experimental Design)

The experimental data generation and data collection designs for each of the treatability study projects are described in the individual work plans and sampling and analysis plans.

Routine sampling processes used to support the treatability studies will be in accordance with the waste management area sampling design, based on the regulatory requirements (e.g., RCRA or CERCLA) and applying the Data Quality Objectives Process in accordance with *Guidance on Systematic Planning Using the Data Quality Objectives Process* (EPA/240/B-06/001 [QA/G-4]). A description of these processes will be included in sampling and analysis plans along with the number of samples, when to sample, number of sample locations, number of quality control samples (field replicates, etc.), analysis methods and quality control criteria, and the groundwater level measurements.

6.2 Sampling Methods

The procedures for collecting samples and identifying the sampling methods and equipment, including any implementation requirements, sample preservation requirements, decontamination procedures, and materials needed for projects involving physical sampling, are described in the treatability study-specific work plans and procedures. Specific performance requirements for the methods are also described. If a failure in the sampling or measurement system occurs, documentation of and recovery from the failure will be documented in the project-specific laboratory record book. The treatability study principle investigator is responsible for ensuring that the corrective action is effective and documented.

The preparation and decontamination of sampling equipment, including the disposal of decontamination by-products; the selection and preparation of sample containers, sample volumes, and preservation methods; and maximum holding times to sample extraction and/or analysis are also treatability study topic-specific and will be managed in accordance with SW-846 or PNNL-specific procedures, as applicable. Waste generated as a result of the activities will be handled in accordance with SBMS subject areas, Treatability Studies (PNNL 1999) and Waste, Managing (PNNL 2006e).

Field sample collection, if applicable, will be done by Fluor Hanford Nuclear Chemical Operators (NCOs) under the direction of FHI and specific procedures. PNNL will prepare, integrate, and coordinate sample collection schedules and constituent analysis of groundwater samples in accordance with monitoring plans and a specific procedure. The paperwork and instructions provided to the field personnel will include Sample Authorization Forms, Chain of Custody forms, labels, and the Groundwater Sample Reports. PNNL will track, oversee, and interface with the sampling organization to ensure that the work is completed as specified.

6.3 Sample Handling and Custody

Water samples will be collected by NCOs under the direction of FH and in accordance with FH procedures. Custody of the samples in the field and receipt at the laboratory will be documented on the

Chain of Custody forms in accordance with FH procedures. Also, shipping and transporting of the samples will be handled by the NCOs under the direction of FH and in accordance with FH procedures.

6.4 Analytical Methods

The sampling and analysis plan for each site will identify the sample constituents and the analytical method. The sampling package (e.g., chain-of-custody form, groundwater sampling report) will be generated by an internal procedure, which identifies the analytical methods, sample identification, etc. on the chain-of-custody form. The chain-of-custody form and samples are provided to the appropriate analytical laboratory. The analytical methods required may be contained within the following references:

- Test Methods for Evaluating Solid Waste (EPA/SW-846, as amended)
- Methods for Chemical Analysis of Water and Wastes (EPA-600/4-79-020)
- Methods for the Determination of Organic Compounds in Drinking Water (EPA-600/4-88-039)
- Prescribed Procedures for Measurement of Radioactivity in Drinking Water (EPA-600/4-80-032)
- Procedures for Radiochemical Analysis of Nuclear Reactor Aqueous Solutions (EPA-R4-73-014)
- Radiochemical Analytical Procedures for Analysis of Environmental Samples (EMSL-LV-0539-17).

Many radiochemical methods have not been standardized, but the procedures are documented in the laboratory-specific standard operating procedures. These analytical methods requirements will be passed on to the analytical laboratory in their SOW.

Potential chemical constituents to be analyzed for, specific analytes of interest, and the corresponding standard analytical methods on which the primary analytical laboratory bases its procedures will be displayed in the Groundwater Monitoring and Reporting QA Plan. The contract to the analytical laboratories, which is administered by FHI, specifies the use of these procedures.

Method detection limits (MDLs) shall be determined for all non-radiochemical methods required by the project. Water MDLs shall be determined in accordance with 40 CFR 136, Appendix B -- Definition and Procedure for the Determination of the Method Detection Limit—Revision 1.11. The laboratory will provide the MDL study results to the PNNL Point of Contact when new MDLs have been determined. Required detection limits for radiochemical methods are provided in the analytical laboratory contract.

7.0 Data Reduction, Verification, and Reporting

7.1 Data Reduction

Data measured during technology project investigations are compiled, evaluated, and documented as described below. Samples and associated analyses will be scheduled and tracked to ensure successful sample collection. Selected data may be loaded into the Hanford Environmental Information System (HEIS) Database, as identified in the respective test plan. Tools in use by the Groundwater Performance Assessment Project may be utilized as appropriate for the data objectives and use.

Verification of analytical data provided by subcontracted laboratories is performed in accordance with the *Groundwater Performance Assessment Project Quality Assurance Plan* (PNNL-15014, current

revision), as appropriate. Results are reviewed to ensure the reliability and validity of the field and laboratory measurements based on accuracy, precision, and detection limits. Representativeness, completeness, and comparability may also be evaluated for overall quality. These parameters are evaluated through laboratory QC checks, replicate sampling and analyses, analysis of blind standards and blanks, and interlaboratory comparison. Acceptance criteria are established for each of these parameters in the *Groundwater Performance Assessment Project Quality Assurance Plan* Appendix (QC Plan), the *Environmental Sciences Laboratory QA Plan* (QAP ESL, Rev. 0), and/or in specific test plans. When a parameter is outside the criteria, corrective actions are taken to prevent a future occurrence and any data impacted is appropriately flagged. If appropriate, the review will take into account results of the quality control evaluation as defined in the internal procedure QC-5, *Groundwater Data Validation and Process* (see PNL-MA-567), and results of the review are documented as stated in the test plan.

When the data review identifies suspect data, those data are investigated to establish whether they reflect true conditions or an error. A RDR is initiated in accordance with the procedure DA-3, *Data Review Procedure* (see PNL-MA-567). If there are any limitations noted on the data, a flag will be added to the data in HEIS.

7.2 Sample Data and Tracking for Sediment and Other Media Samples

Completed data packages for sediment and other media samples will be verified by PNNL personnel prior to loading into HEIS (if applicable) or reported. Verification will consist of verifying required deliverables for completeness, required QC results, chain of custody forms, and case narrative that describes any issues related to the sample analyses. Verification may also include evaluating and qualifying results based on holding times, method blanks, matrix spikes, laboratory control samples, laboratory duplicates, and chemical and tracer recoveries, as appropriate to the methods used. No other verification/validation or calculation checks will be performed.

7.3 Data Reporting

Interpretative data, test results, and reports will be released through the information release process in accordance with the <u>Publishing Scientific and Technical Information</u> (PNNL 2002a) SBMS subject area.

8.0 Analytical Quality Control Checks

Analytical Quality Control (QC) checks are performed on internal and external samples. A summary of QC check samples is outlined in the *Groundwater Performance Assessment Project Quality Assurance Plan* Appendix (QC Plan; PNNL-15014, current revision), the *Environmental Sciences Laboratory QA Plan* (QAP ESL, revision 0), and/or in specific test plans. Internal QC data are generated when the analytical laboratory prepares QC samples to monitor the quality of their analyses.

The QC activities needed for sampling, laboratory (internal and external) and field analysis, and measurement techniques will be defined in the appropriate treatability study test plans. For each required QC activity, the associated method, acceptance criteria, and corrective action will be listed. Also required for the field and laboratory QC activities are blanks, duplicates, matrix spikes, laboratory control samples,

and surrogates in the plans. The project-specific QA Plans also identify the procedure, formulae, or references for calculating the percent recovery, bias, and precision.

9.0 Assessments

Assessments are performed to gather results that can be evaluated to measure the effectiveness of the quality systems and processes implemented by the project. Assessments will be performed periodically during the year. The following types of assessments may be used at varying frequencies during the year:

- Management self assessment an assessment performed by those immediately responsible for overseeing and/or performing the work to establish whether policies, practices, and procedures are adequate for ensuring results needed.
- Management independent assessment an assessment performed by an individual or group independent of the work performed to ensure that policies, practices, and procedures are adequate for obtaining the needed.
- Technical independent assessment an assessment performed by an individual or group technically
 competent to do the work but independent of the work being performed to assure qualitative and
 quantitative aspects of the work are accomplished according to documented specifications.

9.1 Assessment Planning and Documentation

Assessment planning is done by the project management team (including Project Manager, Task Leaders, PI, and appropriate staff) in consultation with the project Quality Engineer. Assessments are in accordance with the SBMS subject area, <u>Planning, Assessment, and Analysis</u>, Section 2 <u>Performance Assessment</u> (PNNL 2005c). The assessor plans the assessment on a Self-Assessment Planning Form (Figure 2) where the scope of the assessment, topic, and supporting references are documented on the plan. A unique identification number is assigned to the plan and entered on an Assessment Log Sheet.

Results of assessments will be documented on a Self-Assessment Results form (Figure 3). The corrective action and action owner will be documented on the assessment report. The Task Manager will assign the action owners, and the Project Manager will prioritize the corrective actions. An action item log will be maintained by the project Quality Engineer to track and close out actions, and to finally verify the corrective actions. The Project Manager will sign the assessment report when the corrective actions have been closed. The assessment plan and report will distributed to the appropriate Task Managers, Project Manager, and project records.

Scope & Location: (General: Maintenance, Operations,	I.D. Number: (ATS Number or other Unique Tracking	
(Centerum Mannetonice, operanous,	Number)	
Topic: (Describe what will be assessed)	Date: (Date planning form is prepared)	
References: (Cite Source Documents for Performance Expec	<u> </u>	
A-Manual, Standards Based Management System [SBMS], Re	equirements, Procedures and Guidelines [RPG]).	
Performance Exp		
Criteria developed from Source Documents that will be applie	_	
have the reference enclosed in parenthesis at the end of the cri	1	
RPG). Performance expectations should be limited to six max		
Planning Forms can be completed to expand the scope of a par	ticular assessment.	
1.		
2.		
3.		
4.		
5.		
6.		
Procedure: (Perform the following as applicable for the asses	sment)	
Review assessment planning form		
• Review applicable procedure/requirements. (references)		
Conduct performance tests and data validation.		
Observe the activity controlled by the procedure.		
• Interview appropriate personnel about requirements and practice.	etices.	
Record observations based on comparison to plan.		
Document the results after receiving final information on the	Self-Assessment Results form.	
Basics for the [] Planned [] Lessons Learned	1	
Assessment: [] Responsive [] Other		
Assessment. [] Responsive [] Outer		
Work Package Number (optional):		
Assessment Requestor/Authorizing Person:		
Assessment Requestor/Authorizing Ferson:		
Assessor(s):		

Figure 2. Self-Assessment Planning Form

Assessor:	I.D. Number:		
Assessment Location:	Date: (Date assessment perform	Date: (Date assessment performed)	
	esults Performance Expectations)		
(<i>Use additional pages if necessary.</i>) Concise and object the end and must be based upon a series of facts that sup opportunities. Include date the information is obtained a	ive statements are the goal. Subjective ports the comments. Include strengths	and improvement	
Summary			
1.			
2.			
3.			
4.			
5.			
-	nent Actions ssociated Results)		
Assigned Action	Action Owner	Due Date	
1.			
2.			
3.			
4.			
Actions Assigned By:		Date:	
Completion (To be signed by Lead Assessor when asses Signature: Date:	ssment is completed.)		
Completion (To be signed by Manager when assessment Signature: Date:	t is completed and all actions have been	n entered into ATS)	

Figure 3. Self-Assessment Results

9.2 Subcontractor Assessments

If PNNL passes work on to subcontractors, periodic assessments of analytical subcontractors are performed as an oversight function or prior to contract award in accordance with the internal acquisition quality procedures. Provisions are made in the SOW for oversight assessment activities to be performed as necessary.

The results of all subcontractors' assessments (including surveillances and audits) will be made available to project and line management, individuals contacted, and the client as requested. The corrective action tracking, corrective action, and closure response will be in accordance with the internal acquisition quality procedures. The official assessment report files and responses (audits and surveillances) are maintained in the PNNL Suppliers History File by the Quality Assurance Services group.

Periodic assessments of the well drilling and construction, drilling and sampling-related activities, and the analytical laboratory may also be performed in accordance with the requirements discussed above.

10.0 Preventive Equipment Maintenance

Subcontracted organizations will be required to implement preventive maintenance on their equipment to mitigate the possibility of down time affecting cost and schedule. This will be specified in the SOW to the respective organizations.

11.0 Specific Routine Procedures Used to Assess Data Precision, Accuracy, and Completeness

The evaluation of laboratory precision, accuracy, and completeness is accomplished during the verification process performed upon receipt of data (see Section 7 of this plan).

12.0 Corrective Action

12.1 Project Corrective Actions Resulting from Assessments

As part of the continuous improvement processes initiated by the project management team, assessments will be tracked and improvement actions identified and prioritized. The Assessment Tracking System (ATS) is the process used by this master project for tracking and managing assessments, including determining Conditions and the development of actions. ATS supports the identification, control, and correction of items, services, and processes that do not meet established requirements. The SBMS Assessment Management (PNNL 2005a) subject area documents this corrective action management process for handling and documenting events and assessments, including those that must be tracked in ATS such as formal project reviews or audits performed by the client or

their representative; management-initiated assessments; etc. If immediate corrective action is required, the quality problem will be directly entered into the ATS and actions taken as specified in Section 12.2.

12.2 Unplanned Deviations

Corrective action must be initiated by the Project Manager or cognizant Task Leader when <u>unplanned</u> deviations from procedural, contractual, regulatory requirements, or construction specifications occur. These deviations will be documented by documenting the quality problem information directly into the ATS in accordance with SBMS subject area, <u>Quality Problem Reporting</u> (PNNL 2005e). The assessment must describe the problem, the cause of the deviation, the impact of the problem, and the corrective action needed to remedy the immediate problem and to prevent recurrence.

Subcontractors will be required to have a system in place to identify, correct, and prevent recurrence of contractual, procedural, or regulatory requirement deviations, and to notify the PNNL point-of-contact specified when such an event occurs. These requirements will be passed on in a SOW to the subcontractors.

12.3 Planned Deviations

Planned deviations from procedure, documented (including justification) and approved by the Project Manager or Task Leader **in advance**, do not constitute a deficiency and do not require generation of an assessment item. Documentation may consist of a hard copy e-mail or memo to the Project Manager or Task Leader. This documentation must include either an approval signature if on a memo or electronic approval via a reply to the e-mail indicating such approval.

12.4 Measuring and Test Equipment Calibration Discrepancies

Subcontractors will be required to maintain a system for identifying calibration discrepancies and tracing data or samples that may have been affected. Subcontractors will be required, via a SOW, to notify the PNNL point-of-contact as soon as possible when such an incident occurs. PNNL will perform periodic assessments to assess the effectiveness of subcontractor procedures and processes for calibration control.

Project staff must investigate instruments or equipment found to be operating outside acceptable operating ranges (as specified in the applicable technical procedure or manufacturer's instructions) and issues must be addressed in accordance with SBMS subject area Quality Problem Reporting (PNNL 2005e). If data on an instrument's calibration report are found to be "Out of Tolerance" during the review and acceptance process, an "Out-of-Tolerance Notification will be generated using the ATS in accordance with the SBMS subject area, Assessment Management (PNNL 2005a). Then the project staff must determine if there is any impact on data. If it is determined from calibration verification that Category 1 or 2 Measuring and Test Equipment is out of tolerance, the project staff will proceed with the evaluation to determine impact on data and document the results with justification.

13.0 Quality Assurance Reports to Management

Quality activities such as project improvement efforts, identification of significant deficiencies and associated corrective actions, and summary of assessment results will be reported to the Project Manager. When major quality problems are identified, they shall be reported to the Project Manager. Surveillance plans and results of the surveillances are provided to the Project Manager and Task Manager after a surveillance event.

Quality-related problems identified by project personnel must be reported to project management immediately for resolution. Any problems involving data quality, sample integrity, or test measurements will be thoroughly documented by a request for data review (RDR) and/or a *Problem and Discrepancies* form and communicated to the appropriate Task Leader and Project Manager for resolution.

Significant quality-related problems that may affect customer satisfaction shall be communicated to the Product Line Manager by the Project Manager.

14.0 Records

14.1 Records Control

Records that document the subcontractor activities, analytical results, verification and compliance checks, test plans, and associated results will be maintained as project records. Individual test plans and work plans may identify other records requirements. Project records will be legible, identifiable, and maintained in accordance with PNNL SBMS subject area Records Management (PNNL 2005f).

The Project Records Specialist prepares and submits a Records Inventory and Disposition Schedule (RIDS) File Index for review and approval by the records management representative and Quality Engineer. The records custodian reviews and updates the RIDS annually at a minimum, or during any major change to the program. Records retention schedules shall be based on the requirements of TPA (Ecology et al. 1989), which requires the retention of records for 10 years after termination of the TPA.

14.2 Records Transfer to Storage

Within 90 days of project completion or termination, records shall be transferred to storage and/or the client. The PNNL project staff member originating the transfer should complete the appropriate internal form (e.g., Records Transfer Data Input (RTDI) Form). The records management representative will sign the RTDI form as acknowledging receipt of the records and return a copy of this form to the records custodian. The RTDI form is then placed in project records.

15.0 Procurement Control

For this project, the majority of procurements will result in purchases of services such as drilling, sampling, and analytical. All procurements will be obtained in accordance with SBMS subject area

<u>Purchasing Goods and Services</u> (PNNL 2006b). SOWs for purchasing services shall be reviewed and signed by the project Quality Engineer to assure consistency of quality assurance requirements specified to subcontractors with project quality standards in this plan.

15.1 Groundwater Sampling

Purchase orders (POs) shall be used to obtain sample collection and water level measurements. An electronic requisition will be prepared by project staff accompanied by a work authorization document (letter of Instruction (LOI) or SOW). The work authorization document will include requirements for sample collection, sample handling, sample labeling, custody of the samples in the field to delivery to the analytical laboratory or shipper, and water level measurements. The SOW will pass on the requirements of the *EPA Requirements for Quality Assurance Project Plans* (EPA/240/B-01/003, QA/R-5) and HASQARD to the subcontractor. A review must be performed by the Quality Engineer during the planning stages and preparation of the SOW/LOI.

15.2 Groundwater Analytical Services

Work package authorizations (WPAs), work orders (WOs), or POs, as applicable, shall be used to obtain analytical services. A letter of instruction or SOW must accompany each WO, WP, or PO. A review must be performed by the Quality Engineer during the planning stages and preparation of the SOW/LOI. The work authorization document must define the data quality and any additional project requirements associated with the service requested. The data quality requirements should include a description of the QC samples for each analysis for determining the level of possible contamination from preparation and analysis. The project requirements should include information on analysis method, calibration standards traceable to the National Institute of Standards and Technology, sample turnaround time and reporting requirements, and disposal requirements for remaining sample material and the waste from the process. The SOW will pass on the requirements of the EPA Requirements for Quality Assurance Project Plans (EPA-600/R-02/009, QA/R-5) and HASQARD to the subcontractor.

15.3 Other Hanford Contractor Services

Other Hanford contractor services (e.g., well drilling and construction) will be obtained using the procurement process. An electronic requisition will be generated by project staff accompanied by a work authorization document (LOI or SOW). The work authorization document will describe the requirements for the requised services. The SOW will pass on the requirements of the *EPA Requirements for Quality Assurance Project Plans* (EPA-600/R-02/009, QA/R-5) and HASQARD to the subcontractor. A review must be performed by the Quality Engineer during the planning stages and preparation of the SOW/LOI.

15.4 Sediment Analytical Services

Analytical services will be procured by using a work authorization document (LOI or SOW) accompanied by a WPA or WO. A review must be performed by the Quality Engineer during the planning stages and preparation of the SOW/LOI. The work authorization document must define the data quality and any additional project requirements associated with the service requested. The data quality requirements should include a description of the QC samples for each analysis for determining the level of possible contamination from preparation and analysis. The project requirements should include

information on analysis method, calibration standards traceable to the National Institute of Standards and Technology, sample turnaround time and reporting requirements, and disposal requirements for remaining sample material and the waste from the process. The SOW will pass on the requirements stated in the *EPA Requirements for Quality Assurance Project Plans* (EPA-600/R-02/009, QA/R-5) and HASQARD to the subcontractor.

16.0 Staff Training

Staff performing activities affecting quality shall be issued documented training assignments including applicable project administrative and technical procedures and this plan.

- 1. Task Leaders and staff members will assess project-specific training needs. The assessment will include evaluating cumulative training records of the staff.
- 2. Task Leaders will assign reading and/or briefings of procedures as needed. If training is assessed and the need for formalized training identified, the staff member will be scheduled to attend a formal training class.
- 3. Task Leaders and staff will document training on a Briefing Document, an individual On-the-Job Training (OJT) or Reading Assignment Documentation form, or a Group OJT or Reading Assignment Documentation form. These forms are available internally to PNNL staff. Documentation shall be sent to the PNNL Laboratory Training Coordinator for input into the training database. The training database will contain the record copy of project staff training.

Subcontractors are responsible for special training of their staff in accordance with the respective SOW.

The project shall utilize personnel who are knowledgeable and possess adequate technical, managerial, or professional skills to perform all their assigned tasks. The project manager will identify any additional specific project-related processes that will require project staff training and will identify who will be responsible for ensuring that the project-specific training will be developed, delivered, and changes managed in accordance with the Training Design, Development, Implementation and Evaluation SBMS subject area (PNNL 2002b). The project shall maintain training documentation for project-required coursework or on-the-job training taken by staff that is not capable of being tracked in the Laboratory's training database in accordance with the Training and Qualification for Staff and Non-Staff SBMS subject area (PNNL 2005g).

The project manager, or his/her delegate, shall inform the immediate manager of the project staff of the staff member's need for project-required training and will ensure that the training has been completed prior to project staff conducting work that requires the training. The immediate manager of project staff, or their delegate, shall record the need for identified project-required training and ensuring training and retraining records (for both Lab-level and project -specific training) are maintained in accordance with the Training and Qualification for Staff and Non-Staff (PNNL 2005g) subject area.

The development of software products that require complex or unfamiliar interactions with users and operators should include a comprehensive plan for training. The training plan should include the following:

- a) a description of the populations to be trained, the training objectives for each population, and the content to be covered in the training
- b) an estimate of the amount of resources necessary for training development, delivery, and time expenditures
- c) procedures for evaluating the effectiveness of the training and for making modifications to the training.

The master project shall utilize personnel who are knowledgeable and possess adequate technical, managerial, or professional skills to perform all their assigned tasks. The master project manager has identified the following project-specific training requirements:

Project core team members will have been briefed on

- the Project Management Plan
- the appropriate QA plan; PNNL-SA-40114, Rev. 2. *The Groundwater Performance Assessment Project Quality Assurance Plan.*

The individual projects shall maintain training documentation for project-required coursework, and on-the-job training taken by staff, which is not capable of being tracked in the Laboratory's training database in accordance with the <u>Training and Qualification for Staff and Non-Staff</u> SBMS subject area (PNNL 2005g).

17.0 Software Control

Various tasks of the project require the use of databases and software, which are managed, controlled, and operated by entities that are outside PNNL. The project also requires the use of databases and software that are developed, managed, controlled, and operated by PNNL. A graded approach is used to establish software quality assurance requirements based on identified risk. Software QA at PNNL is based on DOE Order 414.1C, *Quality Assurance*. This order establishes specific requirements for software related to safety and nuclear facilities.

The project uses databases, custom applications, and configurable software to support various activities. These databases, custom applications, and configurable software (spreadsheets and queries) used to generate reportable results shall be documented in accordance with the SBMS subject area, Software (PNNL 2005f). This documentation is maintained in project files.

17.1 Safety Software and Software Applications

For the purpose of design activities covered by the projects identified in the plan, "Software" is defined as computer programs – including computer programs embedded in firmware (see <u>Safety Software</u> [PNNL 2006c] or <u>Software</u> [PNNL 2005f] SBMS subject area). Excluded is software that is an integral part of firmware or equipment, where all software maintenance is performed by the vendor and

the software is verified as an integral part of the system (e.g., calibration with known standard materials). Any vendor will be required to follow the NQA-1-2000 (Quality Assurance Requirements for Nuclear Facility Applications) standards for software when the software that is part of firmware is identified as Safety Software. The Safety Software clause (QA-197a) will be passed down in any statements of work, at a minimum, and possibly with additional clarification, when requested by the vendor.

All Software applications used for the projects under this plan will be reviewed and identified as Safety Software or Software. The grading process for Safety Software will be recorded and copies for each application will be maintained as project records for each project that falls under this plan. Software applications that will follow this plan have the potential to be identified as Safety Software and when graded as such, will follow the <u>Safety Software</u> (PNNL 2006c) Level C requirements, at a minimum as identified in SBMS. The <u>Safety Software</u> subject area within SBMS is based on DOE Order 414.1C, which includes the NQA-1-2000 standard.

If applications are not identified as Safety Software then they will be documented as Software and the documentation will be maintained as project records for each project. Safety Software and Software applications identified for the projects in this plan will perform the work activities identified below that pertain to Custom Developed, Configurable, Acquired/Legacy, Utility Calcs and Commercial Design and Analysis Software.

All Safety Software applications are required to be identified in the Information Resource Inventory (IRI). All Safety Software will be identified as Safety System Software, Safety and Hazard Analysis Software and Design Software, or Safety Management and Administrative Controls Software. The following will additionally be identified for each software application in the IRI: Type of software, Graded Level and the scope of the software, for the intended use with the project. The owner and point of contact information will also be identified in the IRI.

17.1.1 Minimum Documentation Requirements

To ensure that the implementation of the software satisfies requirements, the following documentation is required as a minimum for all Safety Software applications. These document requirements must be reviewed and processed through ERICA for software code being developed as a deliverable (e.g., Hanford Soil Inventory Model (SIM) software). The rigor of the documentation will be decided based on the grading of the safety software application. Refer to the Document Content Guidance Matrix, in the Safety Software (PNNL 2005d) subject area of SBMS, for the rigor needed for the documentation requirements. The rigor requirements will be one of three categories (Detailed and Specific, Functional, or Summary level) for each document identified below:

- a) Software Requirements Specifications (SRS)
- b) Software Design Description (SDD)
- c) Verification and Validation Plan (VVP)
- d) Verification and Validation Report (VVR)
- e) Configuration Management Plan (CMP)
 - 1) A problem reporting and corrective action tracking system will be identified with CMP documentation.
 - 2) Data management processes will also be identified, when applicable

f) Procurement Contractual documentation, when applicable.

17.1.2 Software Requirements Specification (SRS)

The SRS shall clearly and precisely describe each of the essential requirements (functions, performances, design constraints, and attributes) of the software and the external interfaces. Each requirement shall be defined such that its achievement is capable of being objectively verified and validated by a prescribed method (for example: inspection, analysis, demonstration, or test).

The SRS is subject to the Software Requirements Review (SRR), identified in applicable CMPs when needed, which identifies the QA organizational element's QA activities.

17.1.3 Software Design Description (SDD)

The SDD shall depict how the software will be structured to satisfy the requirements in the SRS. The SDD shall describe the components and subcomponents of the software design, including data bases and internal interfaces. The SDD is a technical description of how the software will meet the requirements set forth in the SRS. Its most important function is to describe a decomposition of the whole system into components (subsystems, segments, etc.) that are complete and well-bounded. In addition, it should document the rationale for the more important design decisions in order to facilitate the understanding of the system structure.

The SDD will describe major system features such as data bases, diagnostics, external and internal interfaces, as well as the overall structure of the design. It involves descriptions of the operating environment, timing, system throughput, tables, sizing, centralized or distributed processing, extent of parallelism, client/server, reusable objects library, program design language (PDL), prototypes, modeling, simulation, etc. The SDD will also describe any input and output data that may be required.

If prototyping, modeling, or simulations are used, the QA organizational element could observe a demonstration, which is a more efficient way to review and assess written design documentation.

The SDD will be baselined after each significant review. A new version containing a more detailed design description is developed for each subsequent review.

17.1.4 Verification and Validation Plan (VVP)

The VVP shall identify and describe the methods (for example, inspection, analysis, demonstration, or test) to be used:

- (1) To verify that:
 - the requirements in the SRS have been approved by an appropriate authority,
 - the requirements in the SRS are implemented in the design expressed in the SDD; and
 - the design expressed in the SDD is implemented in the code.
- (2) To validate that the code, when executed, complies with the requirements expressed in the SRS.

The VVP describes the overall plan for the verification and validation of the software/modeling and will be produced and reviewed incrementally, for Safety Software applications. The tasks, methods, and criteria for verification and validation will be described in the appropriate VVPs for each application.

The VVP will be used for documentation of the testing standards and practices as they are defined in each application VVP. The VVP will explain the scope of the validation testing to ensure the baseline requirements and explain the stages of development that require customer review and the extent of the verification that will precede such a review.

The VVP will specify minimum test documentation requirements for each test performed. Additionally, a section of the VVP will identify a verification matrix where the requirements are listed with their corresponding test identified in the VVP. A matrix will be maintained during the life of the software and will be used to verify all the requirements have been met, identified, and tested.

The contents of the VVP will be evaluated at the Verification and Validation Plan Review (V&VPR) prior to testing. A V&VPR will be conducted when significant changes are made to the baseline. The V&VPR will be used to identify all changes to be tested and to pass on pertinent information to the appropriate testing staff.

17.1.5 Verification and Validation Report (VVR)

The VVR shall describe the results of the execution of the V&VP. The VVR summarizes the observed status of the software as a result of the execution of the VVP. The VVR should include the following information:

- a) Summary of all life cycle V&V tasks.
- b) Summary of task results.
- c) Summary of anomalies and resolutions.
- d) Assessment of overall software quality.
- e) Summary from the verification matrix.
- f) Recommendations such as whether the software is, or is not, ready for operational use.

The report may be a full report or a summary (depending upon the grading of the software).

17.1.6 User Documentation

User documentation will be developed for applications where the code is part of the deliverable (e.g., the Hanford Soil Inventory Model (SIM)).

17.1.7 Configuration Management Plan (CMP)

The CMP shall document methods to be used for identifying software items, controlling and implementing changes, and recording and reporting change implementation status. The CMP should describe the tasks, methodology, and tools required to ensure that adequate Configuration Management (CM) procedures and controls are documented and are being implemented correctly. If the CMP is not a stand-alone document, and is included in the QAjP or PMP, it is not necessary that the QA organizational

element prepare the Configuration Management Plan (CMP); however, it is essential that one exist for each project or set of applications under each project.

The CMP should describe the methods to be used for

- Identifying all the configuration items (to determine whether or not each software item will be identified as Safety Software; if identified as Safety Software, the level will be identified as well.)
- b) Controlling and implementing changes.
- c) Recording and reporting change and problem reports implementation status.
- d) Conducting configuration audits.
- e) Identifying review and approval cycle as well as signature authority.
- f) Identifying the personnel responsible for maintaining the baselines and distributing the CMP.

The CMP shall contain the information identified in the Safety Software subject area of SBMS for the appropriate level of software to which the application was graded. Most software applications for the work under these projects will be graded at Level C.

17.2 Other Documentation

Other specific project plans for each project under this plan may include the following:

- Project Management Plan
- o Quality Assurance Plan
- o Security Plan.

17.2.1 Project Management Plan (PMP)

The PMP can be used as the highest-level planning document governing a project or could be subordinate within a larger set of plans. The PMP should identify all technical and managerial activities associated with the project. The PMP should specify the items, to be reviewed and assessed by the QE.

17.2.2 Security Plan

A Security Plan is only required if any of the software tools are going to be installed on the internal PNNL sites.

17.3 Software Use in Analysis

This refers to the use of software of any kind by this project to conduct analyses delivered, or in support of a deliverable, to the customer. Included in this definition are data analysis tools including spreadsheets and statistical analysis software, databases, modeling, and simulation tools. Excluded are software productivity tools such as word processors and spreadsheets when no automated calculations, macros, or scripts are used. The projects under this plan shall conduct work in accord with requirements for the control of software used in analyses as defined in the Safety Software (PNNL 2006d) or Software (PNNL 2006d) SBMS subject area based on how the software being used is graded.

18.0 Nonconformances and Deficiencies

For procured materials found to be in nonconformance with specifications or where the quality of an activity is found not to be in compliance, the quality problem will be documented in the ATS in accordance with the SBMS subject area, Quality Problem Reporting (PNNL 2005d). Corrective actions are documented in ATS in accordance with the SBMS subject area, Assessment Management (PNNL 2005a).

If a deficiency is found where a procedure or process is not followed or the activity is not in compliance with a procedure or process, the deficiency will be documented in the ATS in accordance with the SBMS subject area, <u>Quality Problem Reporting</u> (PNNL 2005d). Corrective actions will be documented using ATS in accordance with the SBMS subject area, <u>Assessment Management</u> (PNNL 2005a).

Subcontractors will be required to have a system to identify and disposition nonconforming items, procedure deficiencies, processes not followed, or activities not in compliance with a procedure or a process. This requirement will be specified in a SOW.

19.0 Document Control

19.1 Quality Assurance Project Plan Control

Distribution and control of this QAPjP shall be performed in accordance with SBMS subject area *Publishing Scientific and Technical Information* (PNNL 2002a). Modifications to this plan shall be made either by revision or by issuing an Interim Change Notice (ICN). See Figure 4 for the ICN form and instructions. This plan will be revised after four (4) ICNs or a major change in project scope or requirements. Any PNNL staff member may request a change to this QAPjP by submitting the requested change in writing to the Project Manager and Quality Engineer. All reviewers listed on the signature page and affected by the change will approve the revision. The ICN will be placed in front of the signature page and the individual pages will be replaced or the necessary correction will be lined out and correction added with initial and date. The QAPjP will be reviewed at least every two (2) years.

19.2 Technical Procedure Control

Technical procedures referenced by this QAPjP and used by PNNL staff will be contained in a PNNL internal procedure manual, *Procedures for Ground-Water Investigations* (PNL-MA-567) or other procedure manual as appropriate. Technical procedures will be distributed and controlled in accordance with SBMS subject area, *Document Control* (PNNL 2001). Modifications to any of the internal procedures shall be made either by revision or by issue of an ICN.

Procedures will be revised after two major ICNs or if the procedure format has changed. Any PNNL staff member may request a change to procedures at any time by submitting the requested change in writing to the author. The author, technical reviewer, groundwater project Task Manager, and project Quality Engineer will review and approve the ICN. The ICN will be placed in front of the signature page and the individual pages will be replaced or the necessary correction will be lined out and correction

added with initial and date. Contact the Project Quality Engineer for the electronic copy of the ICN. New or revised technical procedures, whether they will be included in the internal procedures manual or not, must be developed in accordance with SBMS subject area, *Procedures, Permits, and Other Work Instructions* (PNNL 2004). The procedure owner is required to review the procedure at least every three (3) years.

19.3 Administrative Procedure/Instruction Preparation and Control

Administrative procedures/instructions used by PNNL staff will be developed, approved, and controlled to ensure consistent application by those staff performing the defined task(s). These procedures/instructions will be developed, approved, and controlled in a manner that has been approved by appropriate project management and the Quality Engineer.

19.4 Test Plans and Other Work Documents

Test Plans and other work instructions used by PNNL staff will be developed, approved, and controlled to ensure consistent application by those staff performing the defined task(s). These procedures/instructions will be developed, approved, and controlled in a manner that has been approved by appropriate project management and the Quality Engineer. Distribution and control of test plans and other plans shall be performed in accordance with SBMS subject area Publishing Scientific and Technical Information (PNNL 2002a).

INSTRUCTIONS FOR ICN FORM

TILL ID LIC.		

The ICN number is identified as ICN No.-____.

For a published groundwater monitoring plan, each page of the ICN shall have a header on the right upper corner that includes the report number, the date and the pagination. The number of the ICN must be placed after the PNNL number. The second line of the header should show the date and pagination. The cover sheet needs to identify how many pages are in the ICN packet.

Example header: PNNL-xxxxx-ICN-x

Month, day, year; Page x of xx

SECTION A.

HEADER.

Self-explanatory.

SECTION B.

Include all actions that the document holder must take to update the procedure or instruction. Possible actions include: replacing pages of the document with pages that are distributed with the ICN and marking up the document (in ink) to reflect the changes identified on the ICN or attaching the ICN cover sheet to the front of the document.

For a "Published" groundwater monitoring plan, include the following statement: "Attach this ICN to the front of the document, just before the title page."

SECTION C.

Identify, by title, all personnel whose job functions will be affected by the change and include a brief description of the effect. If there is no effect on personnel (e.g., the change was made to clarify the intent of the procedure or to correct a typographical error) this block should be marked "N/A."

SECTION D.

State the reason for the change followed by a description of the change (including the affected paragraph, information that is deleted, and the actual wording of any replacement test) for each change included on the ICN.

SECTION E.

The Cognizant Manager shall document the reason for not obtaining original reviewers' approval and/or any other decisions that must be documented. Additionally, list the individuals who will receive the document (distribution list).

SECTION F.

Identify type of change and document required approvals.

Figure 4. Interim Change Notice

INTERIM CHANGE NOTICE (ICN)

A. Document No.: Revision No.: Document Title: Document Title: Document S Original Author: Change Requested By:		Page of
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(Please Sign and Date) Project Quality Engineer Approval:	F. Groundwater Monitoring Task Manager Approval Signatures	
Author Approval:Date:		
	Project Quality Engineer Approval:	Date:
	Author Approval:	Date:
	Other Approvals:	Date:

Figure 4. (contd)

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Appendix A

The Columbia River Protection Supplemental Technologies Project Quality Control Plan

Appendix A

The Columbia River Protection Supplemental Technologies Project Quality Control Plan

A.1 Introduction

The quality control (QC) practices and analytical performance requirements described in the Groundwater Performance Assessment Project Quality Assurance Plan Appendix (QC Plan) and/or the Environmental Sciences Laboratory QA Plan are applied to most groundwater samples collected for the Technology Project. If the specific analyses, performance requirements, and/or QC requirements differ from those provided in the Groundwater Performance Assessment Project QA Plan, they will be documented in the specific test plans.

A.2 Requirements for Sediment and other Non-Aqueous Media Samples

The Technology Project will have sediment samples, insect samples, vegetation samples, and other media samples analyzed. The wide variety of sample media and diverse nature of this work precludes specification of many of the requirements in this QA Plan. Therefore, the types, quantities, and acceptance criteria for field and/or laboratory QC samples are specified in test plans and/or the laboratory statement of work.

Appendix B

Additional Analyses and Measurements to be Employed for the Treatability Studies

Appendix B

Additional Analyses and Measurements to be Employed for the Treatability Studies

Method	Analysis	Document Number	Procedure Title
Conduct of Routine Laboratory Operations	General	RPL-OP-001	Routine Research Operations Section 31 tab 3 of RPL Laboratory Handbook
Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES)*	Ca, Fe, K, Mg, Mn, Na, P, S, Si	PNNL-AGG-ICP-AES*	Inductively Couple Plasma – Optical Emission Spectrometry (ICP-OES) Analysis
Inductively Coupled Plasma-Mass Spectroscopy (ICP-MS)	Re, Tc	PNNL-AGG-415	Inductively Coupled Plasma Mass Spectrometric (ICP-MS) Analysis
Ion Chromatography (IC)	Cl, F	AGG-IC-001	Determinations by Ion Chromatography (IC)
Solid-State pH Electrode and Meter	рН	AGG-PH-001	pH Measurement
X-Ray Diffraction (XRD)	Mineralogy	RPL-XRD-PIP	Operation of Scintag Pad-V X-Ray Diffractor (RGD #62)
Scanning Electron Microscopy/Energy- Dispersive X-ray Spectrometry (SEM/EDS)	Particle morphology, size, and qualitative elemental analysis	PNL-SP-3	Scanning Electron Microscopy/Energy Dispersive Spectrometry
Particle Size Distribution		PNL-MA-567, SA-3	Particle-size analysis (pipette or hydrometer method); Wet sieve analysis will be used to remove sand-size particle
Hydraulic Conductivity		PNL-MA-567, SA-5	Falling head hydraulic conductivity
Water Retention		UFA-SK-01	Determination of water retention as a function of water content using open-flow centrifugation techniques
Water Content		PNL-MA-567, SA-7	Water content
Bulk Density		PNL-MA-567, SA-8	Clod density/bulk density
Particle Density		PNL-MA-567, SA-9	Determining particle density; necessary for constant head hydraulic conductivity
Column Packing		WHC-IP-0635, GEL-3 Rev.3	Moisture relationships of soils; necessary for constant head hydraulic conductivity
pH/EC		PNL-G-5-pH/EC	Measuring pH/EC of low-level radioactive solutions
Saturated column		AGG-SAT-COL-001	Conducting saturated column

Method	Analysis	Document Number	Procedure Title
experiments			experiments
Batch experiments		AGG-BSE-001	Batch sorption experiments
Surface Area		AGG-SA-001	Measuring Surface area

^{*} The document number states ICP-AES, but the instrument in use is an ICP-OES. ICP-AES and ICP-OES are equivalent and refer to the same analytical technique.

Appendix C

Experimental and Modeling Procedures for Subsurface Science Representative Sites Task

Appendix C

Experimental and Modeling Procedures for Subsurface Science Representative Sites Task

Method/ Instrument	Analyses/Calculations	Procedures
ICP/AES	Ca, K, Mg, P, Sr, Na, Si, Cu, Fe, Mn, S, and Ti in water in ppb or moles/L	*PNNL-AGG-ICP-AES
ICP/MS	Cu, Fe in water in ppb or moles/L	PNL-SAND-3.1 (needs updated)
Ion Chromatograp hy	F, Cl, NO ₂ , NO ₃ , CO ₃ , SO ₄ , PO ₄ , PO ₄ in water in ppm or moles/L	*PNNL-AGG-IC-001
KPA	U in water in ppb or moles/L	Liu et al. 2004
Spectrophotom eter	Fe(II) and total Fe in ppb	Kukkadapu et al. 2004
LSC	Sr90, Tc99, I129, in dpm/mL	*PNNL-AGG-RRL-002; Procedures vary slightly for different radioisotopes; McKinley et al.(2006) for Sr90 (PNNL- AGG procedures are from PNNL's Applied Geochemistry Group)
Potentiometric	pH, Bromide	*PNNL-AGG-pH-001
TIC/TOC	Inorganic C, organic C, total C	*PNNL-AGG-TOC-001
X-ray Fluorescence	Total analyses of sediments including Al, Si, K, Ca, Mg, Sr, Ti, Fe, Mn, Cu, Ni, Cr, Cs, U, and others.	*PNNL-AGG-OP-RGD74-001
Conventional Powder X-ray Diffraction	Mineral identity (% distribution)	Qafoku et al. 2005
Digital Autoradiograp hy	Identify locations of radioactivity in sediment thin section and mixtures of sand and silt-sized particles.	Zeissler et al 2001; McKinley et al. 2001
Scanning Electron Microscopy with WDS	High resolution imaging of particle morphology and atomic mass generally in sediment thin section; semi quantitative imaging of chemical distribution.	McKinley et al, 2005
Transmission Electron Microscopy with Selected Area Diffraction (SAED)	Very high resolution of single mineral grains in cross section; local morphology, structure and atomic arrangement.	Zachara et al. 2006. Selected area diffraction patterns are interpreted using the JADE software (see below) using x-ray powder diffraction data (PDF) retrieved from a standards library (ICDD, 2003)
Electron microprobe	Quantitative, intermediate sensitivity chemical mapping in thin sections. Chemical transects across grain/particle boundaries.	Wang et al. 2005b; Catalano et al. 2006
X-ray fluorescence microprobe	High sensitivity, semi quantitative mapping of element distributions in sediment thin sections at scales of 10 µm.	Liu et al. 2004; Fredrickson et al. 2004
X-ray absorption spectroscopy	Determination of element coordination structure, nearest neighbors, and bond distances in contaminated sediment.	Catalano et al. 2004; Catalano et al. 2006 Basic experimental synchrotron measurements are modeled with FEFF, FEFFIT, and IFEFFIT (see below) to

Method/		
Instrument	Analyses/Calculations	Procedures
Synchrotron diffraction	Identification of mineral structures in sediment thin sections.	extract molecular information. Catalano et al. 2004. Mineral structures are derived by application of the FIT2D
Cryogenic laser induced fluorescence spectroscopy (CLIFS)	Vibronic spectra of U(VI) in water and solids to establish molecular and mineralogic environment.	software (see below). Wang et al. 2004 (for aqueous solutions); Wang et al. 2005a (for solids). Data analysis with IGOR and Globals programs (see below).
Batch kinetic desorption experiments	Sediments are bathed in electrolyte of known composition and the time-variant release of contaminants and other solid associated ions are monitored by aqueous phase analyses.	Procedures vary as per element and its concentration. Examples include Liu et al. 2003 (Cs137); Liu et al. 2004 (U); McKinley et al. 2005 (Sr90). Kinetic rate laws and rate constants are calculated from the data using microscopic, diffusion-based transport models (See below). Steady state values can be used to establish thermodynamic parameters, such as the solubility product of a precipitated contaminant phase (e.g. Ilton et al. 2006).
Batch adsorption experiments	Sediments are bathed in electrolyte of known composition that has been spiked with a contaminant of interest. The adsorption of the contaminant is monitored as a function of pH, ionic strength, or ion composition.	Example procedures are equilibrium - Turner et al. 1996 (U) and Zachara et al. 2002 (Cs); kinetic - Liu et al. 2003 (Cs), Liu et al. 2004 (U), and McKinley et al. 2006 (Sr). Experimental results are fitted with various geochemical models (MINTEQ; Geochemists Workbench; GMIN; or FITEQL see below) to identify suites of adsorption reactions (ion exchange or surface complexation).
Column experiments	Sediment (<2 mm or < 4 mm) is packed into a cylindrical plastic, glass, or stainless steel column. Electrolyte with or without a contaminant tracer is applied to the column to study the release (from contaminated sediment) or sorption/retardation (for uncontaminated sediments) of key contaminants of concern.	Qafoku et al. 2005. The data is in the form of chemical concentration as a function of leaching volume of fluid and must be modeled with commercial and research codes to yield useable information. CXTFIT is used to fit physical transport parameters such as dispersivity, while other models are linked with a solver of the advective-dispersion equation to describe 1-dimensional reactive transport. The reactive transport models include a commercial one (the Geochemists Workbench) and others assembled by the research team including the Distributed Rate Model (DRM) and the Dual Continuum Model (DCM). These are described below.
MINTEQA2 Version 4	Commercial software used to calculate aqueous speciation, precipitation/dissolution, and adsorption/desorption equilibria for low- to intermediate-strength solutions.	Code published by Allison et al. 1991 and 1998 linked to a thermodynamic data base of our own synthesis (see below).

Method/		
Instrument	Analyses/Calculations	Procedures
Geochemists	Commercial software to calculate geochemical	Geochemists Workbench Release 6.
Workbench	equilibria, reaction network modeling, and reactive	from Craig Bethke, Hydrogeology
	transport.	Program, University of Illinois
CXTFIT	Commercial software for fitting column effluent data.	Toride et al. 1999
FITEQL (V	Commercial software used to calculate equilibrium	Herbelin and Westall 1999
4.0)	constants and their statistics for aqueous, surface, and	
	precipitated phases from batch experimental data.	
GMIN	An equilibrium geochemical model used to calculate	Felmy 1995
	aqueous speciation, precipitation/ dissolution, and	
	adsorption desorption equilibria for high ionic	
	strength solutions. Maintained by PNNL.	
Spectral Fitting	Commercial software used to fit fluorescence	Beechem et al. 1991
Software	emission spectra on U(VI) derived from CLIFS	
	analyses. The fitting allows determination of the	
	precise spectral wavelengths and deconvolutes	
	spectral signatures resulting from multiple	
Phase	fundamental species.	Matariala Data Ing. Livarmana CA
Identification	Commercial software used to manipulate powder diffraction files are for comparison with reference	Materials Data Inc. Livermore, CA; ICDD 2003
for Powder	spectra in for mineral identification.	ICDD 2003
Diffraction	spectra in for innicial identification.	
(JADE+, V 5)		
Reactive	The Dual Continuum Model (DCM) is used to model	Lichtner et al. 2000; Lichtner et al. 2001
Transport	the reactive transport of contaminants in one-dimen-	, , , , , , , , , , , , , , , , , , , ,
Modeling	sional laboratory columns and in multidimensional	
	field simulations. Model is a reaction-based simulator	
	and requires significant parameterization using batch	
	and column data and physical measurements of	
	sediment characteristics. Maintained by LANL.	
Empirical	The distributed rate model (DRM) is used to	Culver et al. 1997
Kinetic	empirically describe complex kinetic	
Modeling	desorption/dissolution phenomena in sediment that is	
	controlled by chemical kinetics or diffuse mass	
	transport. The basic model describes kinetic	
	phenomena using a statistical distribution of first	
Surface	order rate constants. Maintained at PNNL. The surface complexation model (SCM) is used to	Davis et al. 2004
Complexation	describe the surface chemical reactions of U(VI) that	Davis Ct al. 2004
Model	are responsible for its adsorption to vadose zone and	
Wiodei	aquifer sediments. Maintained by USGS.	
Thermodynami	A large thermodynamic database that is constantly	The database relies on the following and
c Data Base	updated based on literature advances. The database	many other sources: Grenthe et al. 1992
	describes stability constants for aqueous complexes	(U); Guillaumount et al. 2003 (U); Rard
	and solubility products for precipitated phases	1999 (Tc)
	relevant to S&T research and issues. This database is	
	used in almost every S&T geochemical study. There	
	are hundreds of entries in the database for a variety of	
	contaminants that are used in MINTEQA@;	
	Geochemists Workbench, and all of the reactive	
	transport codes. Maintained at PNNL.	

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