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LOS ALAMOS NATIONAL LABORATORY
SOFTWARE QUALITY ASSURANCE PLAN
FOR THE
YUCCA MOUNTAIN PROJECT

Effective Date: ____________________

G. Cort Preparer	Date
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LOS ALAMOS NATIONAL LABORATORY SOFTWARE QUALITY ASSURANCE PLAN FOR THE YUCCA MOUNTAIN PROJECT

1.0 PURPOSE

This Software Quality Assurance Plan (SQAP) establishes a comprehensive, life-cycle based program of quality assurance that shall be applied to all Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP) software and computational data employed to support licensing. This plan shall be based upon a policy of design control exercised throughout the software-development life-cycle. It shall emphasize a high level of technical documentation and independent assessment of all software and computational data products.

2.0 REFERENCES

The standards specified in ANSI/IEEE Std 730-1984, *IEEE Standard for Software Quality Assurance Plans* were used as a resource in specifying the format and information content of this document.

All documents referenced by this SQAP and its implementing quality administrative procedures (QP) are cited in Appendix B.

Appendix C contains a glossary of terms used throughout this SQAP and its implementing QPs.

A list of acronyms used throughout this SQAP and its implementing QPs is provided in Appendix D.

3.0 ORGANIZATION

The organizational structure of the Software Quality Assurance (SQA) effort is shown schematically in Figure 1 and is described in detail below.

3.1 Technical Software Management Group

The Technical Software Management Group shall be responsible for management of all LANL YMP software and computational data that is used to support licensing. These responsibilities shall include

- Administration, interpretation and enforcement of the SQAP and its implementing procedures
- Oversight of the LANL YMP Certification Environment
- Provision of Software Configuration Management (SCM) support for software development and maintenance tasks
- Maintenance of an archive of certified software and computational data for use within the LANL YMP
- Distribution of sanctioned LANL YMP software and computational data to external participants
- Make recommendations to the Technical Project Officer (TPO) regarding software management and issues.

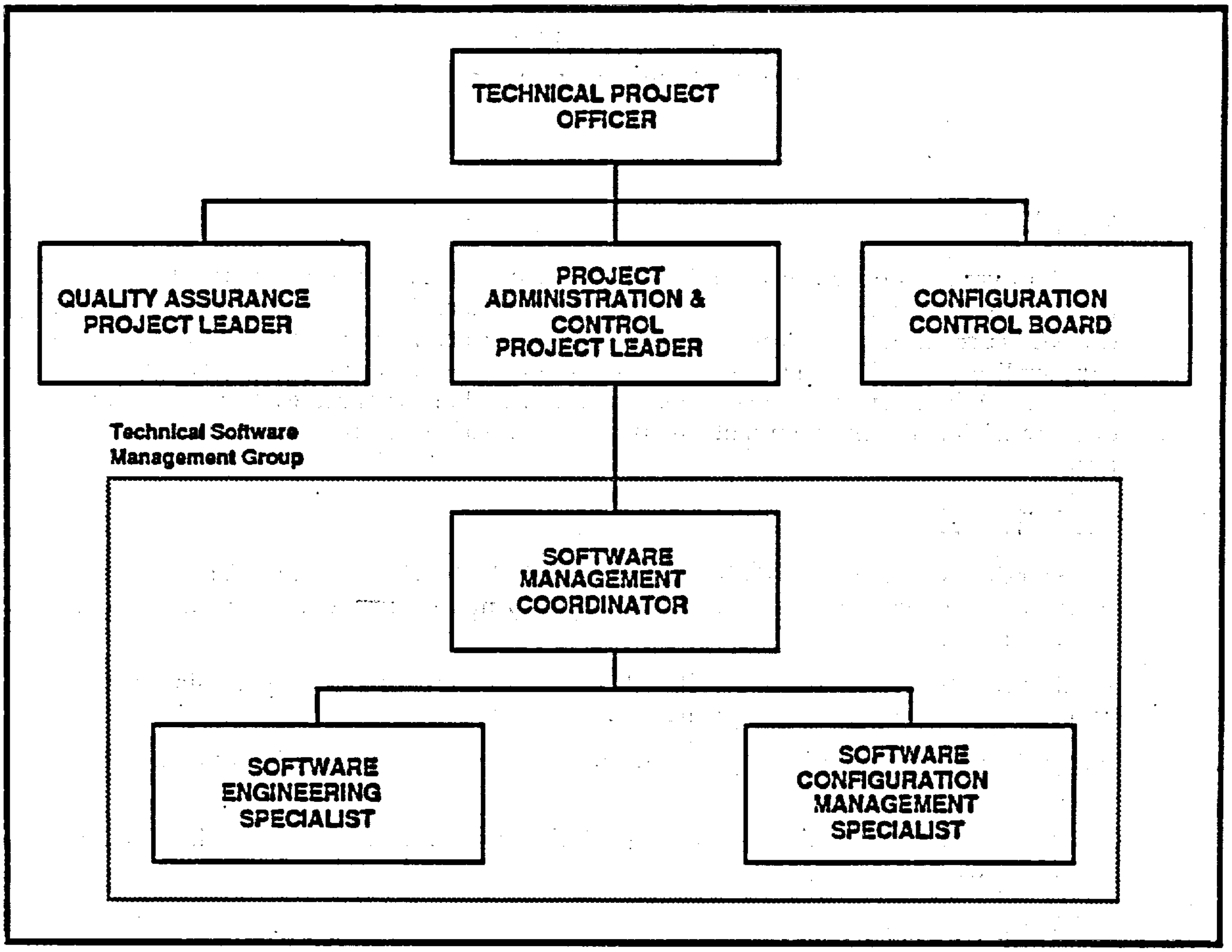

Figure 1. Organizational Structure

The Software Management Coordinator shall be responsible for providing overall technical management of the Technical Software Management Group. The Software Management Coordinator shall report to the Project Administration and Control Project Leader, from which the authority to conduct the software management program is derived.

3.1.1 Software Configuration Management (SCM) Organization

The SCM Organization shall be responsible for all SCM tasks including

- Configuration Identification;
- Configuration Control;
- Configuration Auditing;
- Configuration Status Accounting.

The Software Management Coordinator shall delegate authority to the Software Configuration Management Specialist (Software Configuration Manager) to conduct the business of the SCM Organization according the provisions of TWS-QAS-QP-03.20, *Software Configuration Management*.

3.1.2 Software Engineering Organization

The Software Engineering Organization shall be responsible for the development of software tools to support the implementation of the software quality assurance program.

The Software Management Coordinator shall delegate authority to Software Engineering Specialists to conduct the business of the Software Engineering Organization.

3.2 Configuration Control Board (CCB)

The CCB shall report administratively to the Technical Project Officer (TPO). The CCB shall have the following responsibilities:

- Evaluate and assess the technical merit and organizational impact of all proposed changes to LANL software and computational baselines
- Authorize all software development activities that are within the scope of this SQAP
- Specify the life-cycle phases, baselines, baseline components, and formal reviews that are associated with a software-development task
- Provide the forum for all formal reviews of software or computational data baselines
- Approve or disapprove all software and computational data baselines submitted for review
- Evaluate requests for variances to the provisions of the SQAP;
- Make recommendations to the TPO regarding software management and issues.

The organization and operation of the CCB are described in detail in TWS-QAS-QP-03.20, *Software Configuration Management*.

3.3 Quality Assurance Organization

The Quality Assurance Organization shall be responsible for all verification activities to assess compliance of the LANL YMP with the provisions of this SQAP and its implementing procedures. The Quality Assurance Project Leader shall allocate the necessary resources to conduct the necessary surveys and audits to accomplish this goal.

3.4 User and Development Organizations

The organizations that develop and use the technical software and computational data that are managed under the provisions of this SQAP shall be organizationally independent from the Technical Software Management Group. The members of these organizations report through Principal Investigators, Technical Coordinators, and Project Leaders to the TPO.

4.0 Documentation

4.1 Documentation Philosophy

The LANL YMP documentation policies shall ensure comprehensive and appropriate technical documentation for all software and computational data. Documentation of software and computational data shall be based upon the principle of baseline management and shall emphasize identification, assessment, and control of specific software and documentation components (baselines) at well defined points in the life cycle. Intermediate stages of development shall remain solely within the jurisdiction of the development organization.

A series of distinct, time-ordered baselines shall compose the complete record of development of any software system. This development record shall be supplemented by a collection of standard forms that document the significant SQA events (reviews, audits, certification) that control the software's progress through the life cycle. In combination these baselines and forms shall establish the SQA legacy of the software development process and shall compose the sole auditable information produced during the development or formal assessment of any software or computational data.

4.2 Documentation Classes

Two classes of documentation shall be produced: baselines and supplemental documentation. A baseline shall be a collection of source code modules and supporting information that compose a software application or computational data set at a well defined stage of development (often the conclusion of a life-cycle phase or subphase). Supplemental documentation shall consist of a series of standard forms that are completed to document significant events that occur as a baseline progresses through the life cycle.

4.3 Baselines and Baseline Documentation

Baselines shall compose the sole, certifiable information products of the development process. Specific baselines shall be associated with each life-cycle phase, and each baseline shall comprise a well-defined collection of components. The format and information content of each baseline component shall be standardized.

4.3.1 Baseline Classifications

Two classes of baselines shall be supported: software baselines and computational data baselines. Software baselines shall be further subdivided into computer-program baselines and reuse-component baselines.

4.3.1.1 Computer Program Baselines

A computer-program baseline shall encapsulate one or more functionally related computer programs and any associated documentation, computational data, or support software.

4.3.1.2 Reuse-Component Baselines

A reuse-component baseline shall encapsulate one or more functionally related subprograms (subroutines, functions, or procedures) as well as any associated documentation, computational data, or support software. Reuse-component baselines furnish a vehicle for sharing certified subprograms among LANL YMP software applications.

4.3.1.3 Computational Data Baselines

LANL YMP data that is generated or used by a certified computer program baseline and is intended for use to support licensing shall be organized into a computational-data baseline. The baseline shall be composed of one or more functionally related data sets (interface tables) as well as any associated documentation and support software.

4.3.2 Software Development Baselines

Any baseline that is associated with a requirements, design, or implementation life-cycle phase shall be a development baseline. Each development baseline shall be prepared by one or more members of the appropriate software development organization. The following development baselines shall be supported by this SQAP.

4.3.2.1 Requirements Baseline

A requirements baseline shall document the functional and performance requirements of an application and shall describe external interfaces and design constraints. A requirements baseline shall also specify validation criteria that must be satisfied by any models or methods employed by the application.

4.3.2.2 Preliminary-Design Baseline

A preliminary-design baseline shall document the functional design of the software at the program or reuse-component level. It shall:

- Identify the top-level modules and state their purpose;
- Identify all major algorithms;
- Specify top level data structures;
- Describe all external interfaces including data bases, interface tables, messages, displays, and metafiles
- Allocate major requirements or groups of requirements to specific top-level modules.

4.3.2.3 Verification and Validation (V &V) Plan Baseline

A V&V plan baseline shall provide preliminary documentation of the strategy for verifying and validating the application.

4.3.2.4 Detailed-Design Baseline

A detailed-design baseline shall document the comprehensive design of the software's algorithms, data structures, and interfaces at the module level.

4.3.2.5 V&V Procedures Baseline

A V&V procedures baseline shall provide documentation of the V&V plan at an advanced stage of development and shall establish that the V&V procedures are an accurate implementation thereof.

4.3.2.6 Implementation Baseline

An implementation baseline shall encapsulate the results of the following processes:

- Translation of the software design into source code;
- Completion of the final version of the V&V plan;

- Generation of the V&V procedures (test drivers) from the V&V plan;
- Generation and interpretation of the test results
- Creation of documentation for users of the application.

4.3.3 Other Baselines

4.3.3.1 Operational Baseline

An operational baseline shall consist of the application's object- or executable code and all documentation necessary to utilize the application.

4.3.3.2 Computational-Data Baseline

A computational-data baseline shall consist of the data generated by a certified software application, all information necessary to recreate the data (or references thereto), and descriptive documentation. All computational data that is incorporated into a computational-data baseline shall be in interface-table format (see Section 5.4, below).

4.3.4 Baseline Organization

4.3.4.1 Modules

The fundamental unit of information present in a LANL YMP baseline shall be the module. A module shall be a file that contains a single source-code routine, an interface table, or an independent, high-level, text document.

4.3.4.2 Products

Within a baseline, functionally related modules shall be grouped into larger scale associations called products. The products that are associated with software baselines shall be computer programs and reuse components (independent subprograms that may be incorporated into any LANL YMP software). Within a computational-data baseline, functionally related interface tables shall be grouped into distinct products.

4.3.4.3 Applications

An application shall comprise all of the modules and products that are associated with a suite of functionally related computer programs, reuse components, or interface tables. Individual baselines establish the time-ordered progression of development of the application software.

4.3.5 Hierarchical Development Documentation

Baselines shall be constructed in a hierarchical fashion that incorporates the most detailed development documentation into a documentation prolog within each source-code module. The most detailed development information shall be incorporated into the prologs of the lowest-level modules. More general information shall be placed into the prologs of higher-level routines. Source-code module-documentation shall be supplemented with independent text documents that contain high-level information that is inappropriate for individual source-code modules or that provides instruction to users of the software.

4.3.6 Baseline Evolution

Baseline evolution is the process of producing a baseline by refining one or more previous baselines. Software development is the process of baseline evolution within the framework of the software life-cycle.

As a development task proceeds through the life cycle, existing documentation components shall be refined and new high-level and source-code-based documentation components shall be developed. During the Implementation Phase, code shall be incorporated into individual source-code modules, and appropriate documentation components shall be completed. In this manner, subsequent baselines shall incorporate and elaborate upon all of the information contained in their predecessors.

4.3.7 Baseline Components

LANL YMP baselines shall consist of three fundamental components: source-code modules, high-level documents, and interface tables. Source-code modules shall contain information (and associated in-line documentation) that can be compiled (or interpreted) into binary form for subsequent execution on a computer system. High-level documents shall encapsulate information that cannot be associated with a single module of source code. Interface tables shall encapsulate computational data. To provide a concise summary of the baseline's components, a file list shall be generated for each baseline.

4.3.7.1 Source-Code Modules

A source-code module shall be the fundamental unit of controllable information associated with a computer program or reuse component. Source-code modules shall be of two types: primary modules and support modules.

Primary modules shall compose the routines of the programs or reuse components that implement an application. Support modules shall compose the routines that implement an application's V&V support programs.

The LANL YMP baseline-documentation effort shall place as much technical documentation as is practical within the standard documentation prolog located within each source-code module.

The source-code documentation-prolog is constructed from a block of comment statements. Consequently, it is programming-language-specific. The prolog for a particular programming language shall be described in a software standards document, which specifies coding and documentation standards for the subject language.

4.3.7.2 High-Level Documents

Information that is not included in the documentation prolog of the source-code modules shall be organized into high-level documents. High-level documents shall contain information that is global to a collection of modules or that is difficult to represent within the structured format of the prolog.

High-level documents shall be created using a word processing system that is acceptable to the Software Management Coordinator. All information (text and graphics) associated with a baseline document shall be rendered in computer-readable and electronically storable form.

High-level documents conform to the format and information-content standards specified in Appendixes C - M of TWS-QAS-QP-03.19, *Documentation of Software and Computational Data*.

4.3.7.3 Interface Tables

Interface tables shall be used to encapsulate all certified data that is associated with a computational-data baseline. Refer to Section 5.4.1 and Appendix A for additional information on interface tables.

4.3.7.4 The File List

The file list shall provide a concise summary of the components that are present in a baseline. The file list shall be implemented as one or more text files. The SCM Organization shall provide a standards document that describes the use, content, and format of a file list.

4.3.8 Coding Standards

The goal of software development is to transform design information into reliable, useful, maintainable code. Standards imposed upon this process can significantly improve the overall quality of an implementation. Therefore, coding standards that address issues of modularity, intermodule interfaces, control structures, naming conventions, and any other topics that are appropriate to the implementation programming-language shall be applied to all software-development tasks.

Prior to the start of coding in a particular programming language, a software standards document that specifies the coding standards for the language shall be developed. Upon approval of the software standards document by the CCB, coding may commence.

The Technical Software Management Group shall assist the technical community in the development of coding standards for the programming languages of interest. This assistance shall be provided on a best effort basis.

4.3.9 Relationship to the Software Life-Cycle

Each baseline shall be associated with only one life-cycle phase.

Before authorizing work on any development task, the CCB shall specify which baselines, and which specific components of each baseline, shall be produced at each stage of the life cycle. In this manner, the CCB shall customize the documentation effort to the overall size, complexity, development heritage, and intended use of the proposed software system.

The CCB shall have the authority to configure each baseline by omitting particular components from the baseline's complement. This may be done if the associated information can be adequately represented at a lower level of the documentation hierarchy. In this manner, information can be repackaged to reduce the overall number of documents while retaining a high information content.

Baselines or baseline components should be eliminated from the life cycle only if the information that they would otherwise contain can be adequately represented at a lower level in the documentation hierarchy. Hence, elimination of documentation components shall never eliminate information, but merely permits it to be repackaged in a manner that is more appropriate for the development task.

4.3.10 Relationship to Reviews and Audits

A proposed baseline is certified by the SCM Organization following formal review and resolution of all review issues to the satisfaction of the Change Control Authority. Only a proposed baseline may be the subject of any formal review or configuration audit.

4.4 Supplemental Documentation

Significant events (such as problem reports, baseline submissions, reviews, configuration audits, or variances) that occur throughout the life cycle shall be documented on standard forms provided by the SCM Organization. After completion and authentication, these forms shall become Project QA records and shall provide the sole documentary evidence of these events. See TWS-QAS-QP-03.19, *Documentation of Software and Computational Data*, for additional information on Supplemental Documentation Forms.

5.0 STANDARDS, PRACTICES, AND CONVENTIONS

5.1 Purpose

The following sections specify the software life-cycle that mediates all development activities and specify how baselines are verified and validated within the life-cycle framework. Special requirements for creating, managing, and using computational data are also described.

5.2 Software Life-Cycle

The software life-cycle shall provide a framework within which specific software or documentation components (baselines) can be developed and certified by formal reviews and configuration audits. The CCB shall guarantee a suitable level of design control by specifying an appropriate sequence of development phases and attendant baselines, and by establishing a schedule of reviews that is adequate to assess each baseline. Figure 2 provides a summary of the phases and baselines supported by this SQAP and its implementing QPs.

5.2.1 Life-Cycle Phases

The life-cycle phases that shall be supported by this SQAP and its implementing QPs are: Requirements, Design, Implementation, and Operation. The product of each life-cycle phase that is specified for a software-development task shall be one or more baselines.

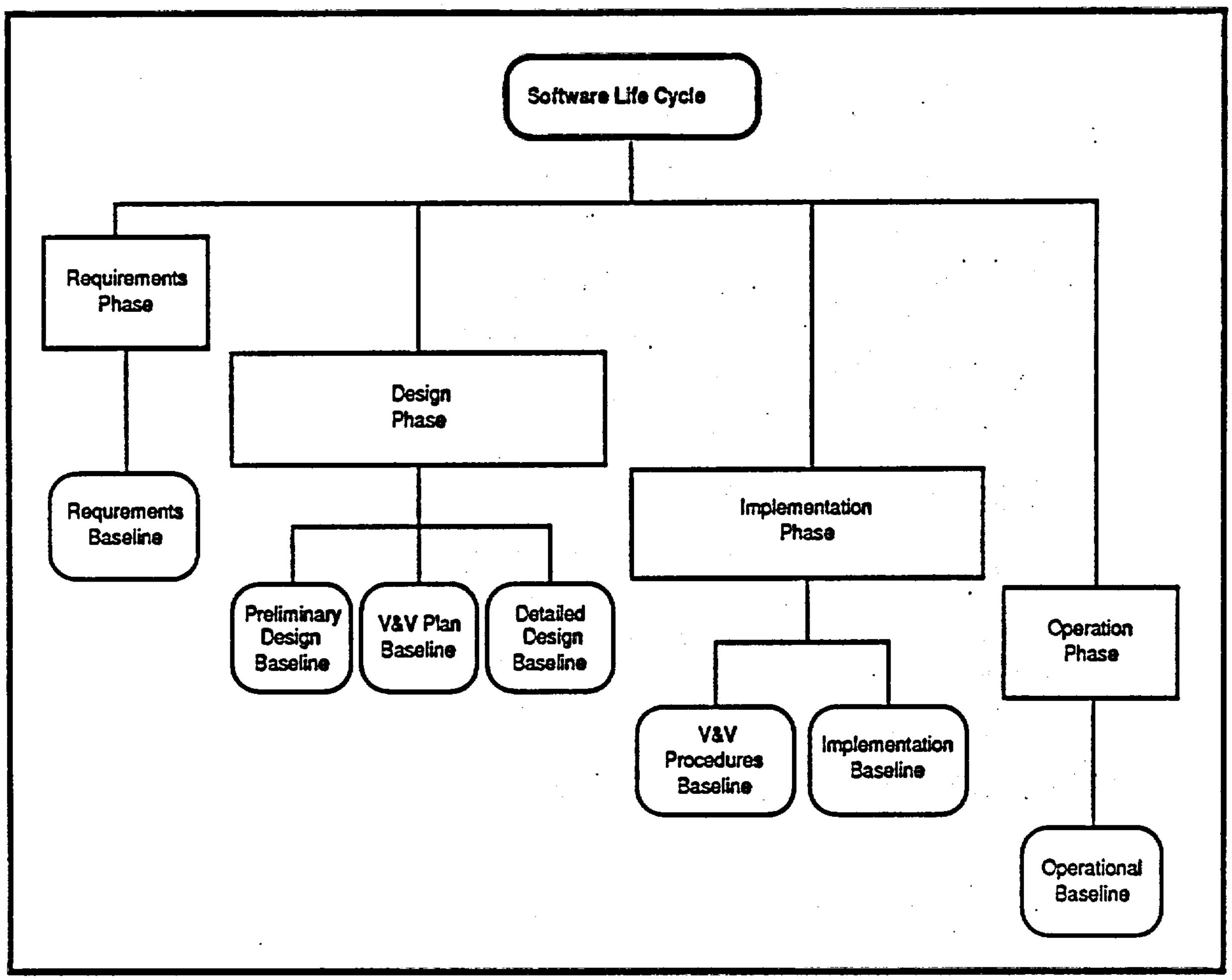

Figure 2. Life-Cycle Phases and Baselines.

5.2.1.1 Requirements Phase

During the Requirements Phase the developer shall specify the functional and performance requirements that will be met by the completed software and shall specify any associated design constraints, attributes and external interfaces.

5.2.1.2 Design Phase

During the Design Phase, the developer shall produce a software design based upon the requirements. The design shall specify the overall structure of the software (control and data flow) and, in the final stages, shall be sufficiently detailed to represent algorithms, control logic and data structures. During this phase verification and validation issues may first be addressed, possibly resulting in formal testing documents.

5.2.1.3 Implementation Phase

During the Implementation Phase the developer shall translate the formal design into a programming language and shall complete all remaining verification and validation tasks.

5.2.1.4 Operation Phase

During the Operation Phase, the sanctioned software-product shall be released to the user community. During this phase, formal change proposals or problem reports are submitted to initiate adaptive, perfective, or corrective maintenance of the software. Change proposals or problem reports that are submitted against the software during this phase shall, if approved, result in the reinitiation of one or more of the preceding phases for change incorporation.

5.2.1.5 Life-Cycle Customization

For software tasks of low to moderate complexity, the Requirements and/or Design Phases may be eliminated from the overall life cycle provided that the information that would otherwise be generated during any eliminated phase is developed and reviewed during the next formal life-cycle phase that is present. In this manner, the overhead associated with traversing the life cycle for less complex development tasks shall be minimized without sacrificing information content and degree of design control. The criteria for determining which life-cycle phases may be eliminated are presented in Section 5.2.2.

5.2.2 Life-Cycle Specification

Before authorizing work on a development task, the CCB shall specify and document a life cycle that is commensurate with the expected size, complexity, scope of development, and intended use of the proposed software. The minimum components of the software life-cycle shall be determined by the software class of the subject application.

Based upon the software class, the CCB shall identify the life-cycle phases that will be traversed to complete the development task. The CCB shall also identify the baselines that will be produced during each phase as well as the documentation components that will be included in each baseline. The CCB shall define the reviews that will be held to evaluate the various baselines and shall establish a tentative review schedule.

The CCB shall document the resulting life-cycle configuration, and a copy of this documentation shall be provided to the development organization to direct the development effort.

5.2.2.1 Software Class

Software class is a designation that is used to describe the size, complexity, intended use, and organizational role of a software application. The following software class designations are supported:

5.2.2.1.1 Administrative Data Base Application (ADB). An administrative data base application is software that implements a data base for the management of nontechnical information.

5.2.2.1.2 Auxiliary Software (AUX). Auxiliary software is software that is relatively complex but does not contain a mathematical or numerical model of a physical process or configuration.

5.2.2.1.3 Component-Model Software (CMS). Component-model software is software that implements a well-established, general numerical or mathematical model of a process, configuration, or condition that may be incorporated into a subsequent physical model.

5.2.2.1.4 Electronic Calculation (EC). Electronic calculation software is software that is relatively non-complex and for which the results can be verified in the same manner as a manual calculation.

5.2.2.1.5 Manifest Product Software (MP). Manifest product software is software that can be readily examined for correctness without reference to the design or implementation of the software.

5.2.2.1.6 Mathematical Support Software (MSS). Mathematical support software is software that implements a common mathematical function or procedure.

5.2.2.1.7 Real-time Software (RTS). Real-time software is software that is used to perform real-time data acquisition or to control instrumentation.

5.2.2.1.8 Scientific and Engineering Software (SES). Scientific and engineering software is software that contains a mathematical or numerical model of a physical process or configuration.

5.2.2.1.9 Software Invocations (SI). A software invocation is software that contains a command sequence to start or control the operation of a program or small command file.

5.2.2.1.10 Software-Support Tools (SST). Software-support tools are software that are used to support the development, assessment for certification, or management of LANL YMP software.

5.2.2.1.11 Technical Data Base Application (TDB). A technical data base application is a software application that is used to store, access, file, and/or manage collections of technical data.

5.2.2.2 Minimum Life-Cycle Requirements

The CCB shall specify the life-cycle phases that must be traversed to complete a software task. As a minimum, the CCB shall require those phases specified in Table 1 for the corresponding software class. The CCB may specify additional phases for the life cycle defined for a particular development task. For the least complex software (ADB, EC, MP, SI), the CCB shall specify at least an Implementation Phase. For moderately complex software (AUX, CMS, MSS, SST), the CCB

shall require both a Design Phase and an Implementation Phase. For the most complex applications (RTS, SES, TDB), the CCB shall specify all three phases (Requirements, Design, and Implementation).

	Requirements	Design	Implementation
ADB			•
AUX		•	•
CMS		•	•
EC			•
MP			•
MSS		•	•
RTS	•	•	•
SES	•	•	•
SI			•
SST		•	•
TDB	•	•	•

Table 1. Minimum Life-Cycle Requirements.

5.2.2.2.1 Requirements Phase Issues. As specified in Table 1, a formal requirements phase is not required for the lower complexity software classes. However, the developer shall be responsible for performing the appropriate requirements analysis and documenting the results during the earliest phase (Design or Implementation) of the specified life cycle. The elimination of the Requirements Phase for these software classes merely reflects the fact that the requirements are expected to be simple enough to be identified and documented during a later phase.

5.2.2.2.2 Design Phase Issues. For the least complex software classes, neither the Requirements nor the Design phase is required for the formal life-cycle. In this event, the developer shall be responsible for developing and documenting (during the Implementation Phase) all information that would otherwise have been produced during the eliminated phases. As above, elimination of the Design Phase merely reflects the fact that for these software classes, the design is expected to be simple enough to be identified and documented within the Implementation Phase.

5.2.2.3 Minimum Documentation Requirements

The minimum documentation components that shall be produced during the development of a software application are specified in terms of the subject software class in Table 2. However, the CCB may specify additional documentation components for a particular development task.

	MMS	SDD	SRS	TR	UM	VDD	VVP	VVR
ADB		2	3		4	•		•
AUX		2	3	•	•	•	•	•
CMS	1	2	3	•	•	•	•	•
EC		2	3		4	•		•
MP		2	3		4	•		•
MSS		2	3	•	•	•	•	•
RTS		•	•	•	•	•	•	•
SES	•	•	•	•	•	•	•	•
SI		2	3		4	•		•
SST		2	3	•	•	•	•	•
TDB		•	•	•	•	•	•	•

[1] The MMS may be omitted if the model can be cited in the echnical literature. This citation shall be made in the References section of the source-code documentation-prolog of the top-level routine(s).

[2] The SDD may be omitted only if (a) the application consists of only one product, and (b) none of the items listed in Section 4.1.4 of the SDD are components of the subject software. The information that would otherwise be present in the other SDD sections shall be addressed in the source-code documentation-prolog of the top level routine.

[3] The SRS may be omitted only if the requirements for the corresponding products can be adequately stated in a single paragraph. In such cases, the single-paragraph statement of requirements shall be placed in the Purpose section of the source-code documentation-template of the top level routine.

[4] The UM may be eliminated if adequate instructions for the user can be embedded in the executable code as prompts, menus, and/or help facilities.

Table 2. Minimum Documentation Requirements.

5.2.2.3.1 Allocation of Documentation Components to Life-Cycle Phases. Table 3 specifies the life-cycle phase in which each documentation component is required to be developed. The CCB shall employ this information in conjunction with Tables 1 and 2 to determine the life-cycle phase during which a required documentation component must be developed. Furthermore, if the CCB specifies additional documentation components in excess of those required by Table 2, the CCB shall utilize Table 3 to determine the life-cycle phase in which the additional components will be developed.

5.2.2.3.2 Baseline Composition. At the discretion of the CCB, the documentation components allocated to a particular life-cycle phase may be further divided into discrete baselines (collections of documents) to be produced during the same phase. If baselines are specified, the CCB shall document the composition of each.

	MMS	SAD	SCL	SDD	SRS	TR	UM	VDD	VVP	VVR
Requirements					•					
Design	•			•					1	
Implementation	2					•	•	3	•	•
Operation		•	•					4		

[1]The VVP is generally produced during the Implementation Phase. However, the CCB may require that the V&V Plan portion of the VVP be produced during the Design Phase.

[2]The MMS is generally produced during the Design Phase. However, if the Design Phase has been omitted from the life cycle by the CCB, the MMS may be produced during the Implementation Phase.

[3]The developer shall produce Sections 1 - 3 of the VDD for delivery with the Implementation Baseline.

[4]The SCM Organization shall complete Section 4 of the VDD for inclusion with a release to the U. S. Nuclear Regulatory Commission upon official request for such a release.

Table 3. Allocation of Documentation Components.

5.2.2.4 Maintenance Activities

For maintenance activities the software life-cycle shall be specified based upon which documentation components of the subject application are impacted by the enhancement or repair task. Table 3 shall be used to determine the minimum life-cycle phases that are included in the life cycle for the maintenance task.

5.2.3 Characteristics of the Life Cycle

5.2.3.1 Software Development

All software development activities shall be performed from within the formal software life-cycle. Included among these activities are development of new software, software maintenance, and conversion of acquired or existing software to conform to the provisions of this SQAP and its implementing QPs. Software development activities shall be performed during one or more of the Requirements, Design, or Implementation life-cycle phases.

5.2.3.2 Software Use

The use of sanctioned LANL YMP software to perform technical calculations in support of licensing activities shall be performed during the Operational phase of the life cycle. Identification, submission, and certification of any resulting computational-data baselines shall also be performed during this phase.

5.2.3.3 Life-Cycle Configuration

A specific life-cycle configuration shall be identified for every software development or maintenance activity by the CCB in accordance with the provisions of Section 5.2.2. The configuration shall specify the life-cycle phases to be traversed, the baselines to be produced during each phase, the software and documentation components that comprise each baseline, and the reviews that must be performed throughout the life-cycle process.

5.2.3.4 Life-Cycle Execution

A software development activity shall be performed by executing the life-cycle phases specified by the CCB sequentially beginning with the Requirements Phase (if specified), proceeding through the Design Phase (if specified), and concluding with the Implementation Phase. The sequence in which these phases are executed shall not deviate from this order, although provisions shall be made for revisiting an earlier life-cycle phase to incorporate changes to the requirements or design developed during the current phase (see Section 5.2.4.5).

5.2.4 Life-Cycle Overview

5.2.4.1 Requirements-Phase Activities

During this phase, the developer shall compile the Requirements Baseline (see Section 4.3.2.1 and TWS-QAS-QP-03.19 *Documentation of Software and Computational Data*). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data*) and shall submit the baseline to all reviews required by the CCB (see Section 6.0 and TWS-QAS-QP-03.17 *Reviews of Software and Computational Data*).

The SCM Organization shall audit the Requirements Baseline prior to scheduling and initiating a formal review by the CCB. The developer shall resolve issues identified by the audit process. SCM auditing activities and issue resolution shall be performed in accordance with Section 7.4 and TWS-QAS-QP-03.20 *Software Configuration Management*.

The CCB shall perform all formal reviews specified for the Requirements Baseline. The developer shall resolve all issues identified by each formal review. Reviews and issue resolution shall be performed in accordance with Section 6.0 and TWS-QAS-QP-03.17 *Reviews of Software and Computational Data*.

At the conclusion of any Requirements-Phase in-process review and after all associated review-issues have been resolved, the SCM Organization shall transfer a copy of the approved baseline to the CPL. After the completion of the Software Requirements Review and after all associated review-issues have been resolved, the SCM shall certify the Requirements Baseline in accordance with the provisions of Section 7.2.5 and TWS-QAS-QP-03.20 *Software Configuration Management*.

5.2.4.2 Design-Phase Activities

During this phase, the developer shall compile all of the baselines that are specified for the Design Phase by the CCB (see Section 4.3.2 and TWS-QAS-QP-03.19 *Documentation of Software and Computational Data*). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data*) and shall submit the baseline(s) to all reviews required by the CCB.

The SCM Organization shall audit Design-Phase baseline(s) prior to scheduling and initiating a formal review by the CCB. The developer shall resolve issues identified by the audit process. SCM auditing activities and issue resolution shall be performed in accordance with Section 7.4 and TWS-QAS-QP-03.20 *Software Configuration Management*.

The CCB shall perform all formal reviews specified for the Design-Phase baseline(s). The developer shall resolve all issues identified by each formal review. Reviews and issue resolution shall be performed in accordance with Section 6.0 and TWS-QAS-QP-03.17 *Reviews of Software and Computational Data*.

If Design-Phase activities result in changes to the software requirements, design, or V&V activities, affected documents from previous life-cycle phases shall be updated. These updates shall be performed according to the provisions of Section 5.2.4.5.

At the conclusion of any Design-Phase in-process review and after all associated review-issues have been resolved, the SCM Organization shall transfer a copy of the approved baseline to the CPL. After the completion of the Critical Design Review and after all associated review-issues have been resolved, the SCM shall certify the Design-Phase baselines in accordance with the provisions of Section 7.2.5 and TWS-QAS-QP-03.20 *Software Configuration Management*.

5.2.4.3 Implementation-Phase Activities

During this phase the developer shall compile all of the baselines that are specified for the Implementation Phase by the CCB (see Section 4.3.2 and TWS-QAS-QP-03.19 *Documentation of Software and Computational Data*). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data*) and shall submit the baseline(s) to all reviews required by the CCB.

The SCM Organization shall audit each Implementation-Phase baseline prior to scheduling and initiating a formal review by the CCB. The developer shall resolve issues identified by the audit process. SCM auditing activities and issue resolution shall be performed in accordance with Section 7.4 and TWS-QAS-QP-03.20 *Software Configuration Management*.

The CCB shall perform all formal reviews specified for the Implementation-Phase baselines. The developer shall resolve all issues identified by each formal review. Reviews and issue resolution shall be performed in accordance with Section 6.0 and TWS-QAS-QP-03.17 *Reviews of Software and Computational Data*.

If Implementation-Phase activities result in changes to the software requirements, design, or V&V activities, affected documents from previous life-cycle phases shall be updated to accommodate the changes. These updates shall be performed according to the provisions of Section 5.2.4.5.

At the conclusion of any Implementation-Phase in-process review and after all associated review-issues have been resolved, the SCM Organization shall transfer a copy of the approved baseline to the CPL. After the completion of the Software Acceptance Review and after all associated review-issues have been resolved, the SCM Organization shall certify and sanction the Implementation baseline. (see Section 7.2.5 and TWS-QAS-QP-03.20 *Software Configuration Management*.)

5.2.4.4 Operational-Phase Activities

During this phase the SCM Organization shall distribute copies of the sanctioned application to LANL YMP or external users who make a formal request for the software. Users shall employ the software in technical calculations.

Also during the Operational Phase, formal requests to enhance or repair the software shall be submitted to the SCM Organization. Discrepancies that are discovered during software use shall also be formally reported to the SCM Organization.

5.2.4.5 Design Iteration

During life-cycle execution, information may be developed that results in changes to software requirements, design, or V&V strategy that were developed and documented in an earlier life-cycle phase. In this event, it shall be necessary to modify or update the affected documentation components to reflect the new information. The mechanism that permits earlier phases to be revisited for this purpose is termed design iteration and shall comply with the following requirements:

- If the baseline-closure review for the prior phase has not yet been completed, the developer shall update the appropriate components of the associated baseline(s). These updates shall be assessed at the baseline-closure review for the baseline(s).
- If the baseline-closure review has been held, the developer shall submit a formal request to the CCB to reopen the phase. If the request is approved, the CCB shall reopen the phase and provide the developer with a copy of the appropriate components of each previously certified baseline that requires update. The update process shall proceed within that life-cycle phase according to the provisions of Section 5.2.4.1 or 5.2.4.2, as appropriate.

5.2.4.6 Rapid Prototyping

Rapid prototyping shall permit tasks (e.g. coding) to be performed outside of the scope of the normal software life-cycle if the work is necessary to develop information that is required at the current stage of development. The software quality assurance program shall ensure that prototype information is properly engineered before being incorporated into a baseline.

5.2.5 Relationship of the Life-Cycle Model to Software Heritage

The software heritage is a designation that specifies the previous development history of a software application. Two heritage designations are supported: acquired software and development software. Within the acquired software category, three subclasses are defined: system software (SS), acquired commercial software (ACS), and acquired noncommercial software (ANS). Within the development software category, two subclasses are defined: new development software (NDS) and pre-existing development software (PDS).

5.2.5.1 Development Software

Development software encompasses all software that is developed by LANL YMP members, contractors, or subcontractors.

5.2.5.1.1 New Development Software. New development software is development software that is produced subsequent to the adoption of this SQAP and its implementing QPs.

All new development software shall comply with the requirements specified in this SQAP, its implementing QPs, and the standards documents relevant to the programming languages in which the modules are implemented. The developer shall adhere to the life cycle specified by the CCB.

5.2.5.1.2 Pre-existing Development Software. Pre-existing development software is development software that was placed into service prior to the adoption of this SQAP and its implementing QPs.

For pre-existing development software, the CCB shall specify a life cycle that is adequate to establish and/or develop life-cycle documentation to the degree possible and to qualify the software for use. The CCB shall specify the required life-cycle phases and associated documentation components according to the requirements for the subject software class. All documentation components and reviews required by this SQAP for new development software of the same software class shall be obtained or developed for pre-existing development software during the appropriate life-cycle phase or, if this is not possible, the reasons shall be documented and maintained with the software. The CCB shall specify one or more of the following strategies to establish this documentation.

- Obtain Documentation from Software Custodian. All available documentation for the software shall be obtained from the software's custodian. At each stage of the life cycle, the appropriate documentation shall be assessed to determine the degree to which it satisfies the minimum documentation requirements specified in Table 2 for new development software of the same class. Supplied documentation shall be compared against the descriptions of LANL YMP standard documentation elements as described in Appendixes C - M of TWS-QAS-QP-03.20 *Documentation of Software and Computational Data*. In performing this assessment, issues of documentation packaging and format shall not be considered. The degree to which the existing documentation satisfies these criteria shall be the sole determining factor. In the event that it is not possible to produce a satisfactory suite of documentation in this manner, the reasons shall be documented, maintained with the software, and distributed to the users of the software.

- Reverse Engineering. If the documentation obtained from the custodian is insufficient or inadequate to satisfy the requirements specified on the LCS for the development task, and if adequate local expertise and resources are available to mount a reverse-engineering effort, the CCB may specify such an effort to develop the specified documentation components. The goal of the reverse-engineering effort shall be to produce adequate documentation with minimal changes to primary source-code modules. The reverse-engineering effort shall proceed through the specified software life-cycle in an orderly fashion, and shall produce the necessary documentation components to the specifications of Appendixes C - M of TWS-QAS-QP-03.19 *Documentation of Software and Computational Data* during the appropriate life-cycle phases thereof. If it is not possible to complete the required documentation suite with the reverse engineering effort, the reason shall be documented, maintained with the computer software and distributed to the users of the software.
- Re-engineering. If features of the software or application environment preclude mounting a reverse-engineering effort, and if adequate local expertise and resources are available for re-engineering, the CCB may specify that the application be completely redeveloped. An application that is being re-engineered shall be reclassified as new development software and treated accordingly.
- Qualification. Regardless of the life-cycle approach employed, the CCB shall ensure that adequate verification and validation is performed on the software to demonstrate that the software satisfies its requirements and provides acceptable results for specific applications. If sufficient information is unavailable from the custodian to demonstrate the veracity of the software, the CCB shall ensure that verification and validation are performed at a level commensurate with the software class of the application. If the software requirements cannot be extracted from the application, it shall be satisfactory to substitute a compendium of requirements that specify the intended domain of use and to perform verification and validation activities against this subset. This approach may be substituted for a formal life-cycle if insufficient documentation is available from the custodian to certify the application, and if insufficient local expertise or resources are available to support a reverse-engineering or re-engineering effort.

5.2.5.1.3 Modifications to Development Software. Whenever development software enters the change processing cycle for enhancement or repair, the affected modules shall be subject to a formal, software-development life-cycle as specified by the CCB. Affected modules shall conform to the LANL YMP documentation standards specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data* and the standards documents relevant to the programming languages in which the application is implemented.

5.2.5.2 Acquired Software

Acquired software encompasses all software that is not originally developed by a LANL YMP member, contractor, or subcontractor. Acquired software is divided into three categories: system software (SS), acquired commercial software (ACS), and acquired noncommercial software (ANS). The degree of development control, documentation, and qualification required for any particular acquired software application is determined by its associated category as described below.

5.2.5.2.1 System Software. System software is acquired software that is closely associated with a commercially marketed computer system and is supplied by a commercial or noncommercial entity for distribution to a large installed user-base (at least 1000 users). System software includes operating systems and operating system utilities, compilers and interpreters, standard libraries, software drivers, and interface software for peripheral devices. In particular, all software for which documentation may be obtained from the Los Alamos Computing Information Center shall be considered system software.

System software that is employed in support of YMP quality-affecting applications shall be explicitly identified in the documentation that describes the associated application. No other documentation, development controls, software configuration management, qualification, or version control is required for system software.

5.2.5.2.2 Acquired Commercial Software. Acquired commercial software is acquired software that is general purpose in nature and is supplied to a large installed user base by a commercial or noncommercial entity outside of the YMP. Examples of acquired commercial software include word processors, spreadsheets, data base management systems, communications packages, graphics packages, etc. Note specifically that LANL YMP applications developed using such software are not considered acquired software. Such applications shall be classified as new or pre-existing development software.

To be classified as acquired commercial software, a software package must satisfy the following criteria:

- The software package must be general purpose in nature and produced for a diverse audience;
- There must be a large installed user base (at least 100) users for the package;
- A formal users guide must be furnished for the code by the supplier;
- A formal mechanism must exist for notifying the supplier of discrepancies;
- A formal mechanism must exist for obtaining user support during regular business hours;

- The supplier must distinctly identify each release of the software and must provide a formal mechanism for distributing new releases.

Acquired commercial software that is employed in support of YMP quality-affecting activities shall be explicitly identified in the documentation of the associated software application. Furthermore, this documentation must demonstrate that the above six criteria are satisfied by the software package. No other documentation, development controls, software configuration management, qualification, or version control is required for acquired commercial software.

5.2.5.2.3 Acquired Noncommercial Software. Acquired noncommercial software is all acquired software that is not classified as system software or acquired commercial software.

Acquired noncommercial software that is obtained from a YMP participant external to LANL, and that has been qualified under the participant's YMP-approved software quality assurance plan, shall be exempt from all of the software development and qualification provisions of this SQAP. It shall be incumbent upon said external participant to perform all software control, tracking, and maintenance operations for the subject software.

For such software, the SCM Organization shall ensure that an approved software application is obtained from the external participant and shall install the baseline in the Certification Environment. The SCM Organization shall execute any installation tests distributed with the software and shall compare the results to certified values provided by the external participant. The SCM Organization shall report discrepancies to the external participant, and it shall be incumbent upon the external participant to resolve any such issues. After successful installation in the Certification Environment, the SCM Organization shall employ the installed software to qualify technical calculations performed with the software by LANL YMP members.

For acquired noncommercial software that is not qualified under a YMP-approved software quality assurance plan, the CCB shall specify a life cycle that is adequate to establish and/or develop life-cycle documentation to the degree possible and to qualify the software for use. The CCB shall specify the required life-cycle phases and associated documentation components according to the requirements for the associated software class. All documentation components and reviews required by this SQAP for new development software of the same software class shall be obtained or developed for acquired noncommercial software during the appropriate life-cycle phase or, if this is not possible, the reasons shall be documented and maintained with the software. One of the strategies described in Section 5.2.5.1.2 shall be used to produce the appropriate documentation and to qualify the subject software.

5.2.5.2.4 Modifications to Acquired Software. Whenever acquired software enters the change-processing cycle for enhancement or repair, the affected modules shall be subject to a formal, software-development life-cycle as specified by the CCB and shall be treated in every respect as new development software. Affected modules shall conform to the LANL YMP documentation standards specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data* and the standards documents relevant to the programming languages in which the application is implemented.

5.3 Verification and Validation

Verification and validation shall be performed on all software prior to its use in performing technical calculations or, if this is not possible, a written justification shall be prepared and maintained with the software, and the software shall be identified and controlled accordingly. In all cases, verification and validation of any software application shall be completed prior to submittal of a license application to the extent that the software is used to support the license application.

The purpose of the LANL YMP formal verification and validation (V&V) activities is to provide a comprehensive, independent, and traceable V&V process for all software and data developed or used to support licensing. This goal is achieved through an aggressive program of formal testing, evaluation, and independent assessment.

5.3.1 Verification of Software

A program of software verification shall demonstrate that the requirements specified for the software are accurately and completely reflected in the emerging software system and shall demonstrate that the performance and operation of the system is consistent with these requirements. This program shall achieve these goals by establishing the traceability of each requirement through the design and into the software implementation and/or by instituting a formal program of testing to demonstrate correct operation of the system.

5.3.1.1 Requirements Traceability

The V&V effort shall demonstrate traceability of the software requirements into subsequent software baselines throughout all phases of the life cycle.

5.3.1.1.1 Requirements Phase. The requirements shall be specified in a manner that allows them to be easily identified and tracked through life-cycle phases. The requirements specification shall clearly state and uniquely identify each software requirement.

5.3.1.1.2 Design Phase. The documents produced during the design phase shall demonstrate traceability of the software requirements. Each software module shall address at least one requirement, and each requirement specified in the Software Requirements Specification shall be implemented in one or more software modules.

5.3.1.1.3 Implementation Phase. The verification effort shall demonstrate that the source code is an accurate rendition of the design by comparing the source code to the pseudocode.

5.3.1.2 Formal Testing

The goal of a program of formal testing shall be to demonstrate the correct operation of software.

5.3.1.2.1 Completeness and Sufficiency. The tester shall ensure that the formal testing is adequate to demonstrate correct operation of the software and is appropriate to the intended use, complexity, and development heritage of the software under test. The tester shall ensure accurate correspondence between test cases and the current requirements and design documentation. In particular, if requirements and/or design information are changed owing to design iteration during the development life-cycle, the developer shall ensure that tests cases are modified appropriately to reflect the new requirements or design information.

The following issues shall be considered for the formal testing effort.

- To the extent that it is practical, the testing effort shall demonstrate that all requirements are correctly implemented.
- The testing effort should exercise all user interfaces, special exit paths, error handling, and recovery procedures. Boundary data values shall be provided to exercise the software at processing interfaces or control transition-points. In general, the program of testing should exercise the software to the maximum degree practical.
- The testing effort shall be appropriate to the intended use, complexity, and development heritage of the software. Small codes generally require a less extensive program of testing than do larger systems. Verification of scientific and engineering software requires a greater commitment to formal testing than does a manifest product application. Electronic calculation software may require no formal testing at all. Finally, the development heritage of a software product may significantly influence the level of testing required. This is particularly true of acquired noncommercial software, for which there is usually no local development expertise. Such software can generally only be verified through a thorough program of formal testing.

The CCB, through the mechanism of formal reviews, shall be the judge of the adequacy of the testing effort.

5.3.1.2.2 Test Classes. Test cases shall be produced in the following classes as appropriate:

- Verification tests shall be designed to demonstrate the correct operation of the software with respect to the documented software requirements. Verification tests shall constitute the chief means for verifying software applications. Verification tests shall be clearly identified in the test plan and test procedures.
- Validation tests shall be employed to demonstrate the veracity of a mathematical or numerical model. Validation tests shall be employed as appropriate within the overall validation strategy. Validation tests shall be clearly identified in the test plan and test procedures.
- Regression tests shall represent a subset of the overall test suite. Regression tests shall be employed to test a new software version without executing the entire test suite. Regression tests shall be clearly identified in the test plan and test procedures.

- Acceptance tests shall be employed to demonstrate the correct operation of the software after installation on another computer system and shall provide a suitable benchmark or sample problem to demonstrate successful installation. Suitable acceptance tests shall be provided for every software application by enhancing existing verification tests. Acceptance tests shall be clearly identified in the test plan and test procedures.

5.3.1.2.3 Operation-Based Verification. For analytical or data-acquisition instrumentation it is often simpler (and more effective) to verify correct operation of the instrumentation system than to verify the software component independently. For example, running a suite of standard samples through an analytical instrument provides significantly more authoritative evidence of correct operation than can be gleaned from a traditional program of software verification. This approach verifies the software based upon demonstrably correct operation of the overall system.

An operation-based verification program should be constructed around the following guidelines.

- Standards shall be chosen over a sufficiently wide range to verify correct operation of the instrumentation system in the domain in which it is intended to be used.
- Each standard shall be traceable to a YMP-sanctioned source.
- Records shall exist to certify that the instrumentation is properly calibrated.

5.3.2 Model Validation

Much of the software developed for the LANL YMP incorporates mathematical models. All mathematical models embodied in such software shall be subject to validation to ensure that they accurately represent physical reality within the domain of application. The validation strategy for each model shall be described in detail in the software documentation. If specific sets of verified, traceable data are used for comparison in the validation process, these data sets shall be identified and justification for their use shall be documented.

The CCB, through the mechanism of formal baseline reviews, shall be the judge of the adequacy of the proposed validation strategies.

5.3.3 Verification of Computational Data

5.3.3.1 Verification of Derived Data

Derived data shall be verified by establishing that software and computational data from which the derived data are generated are certified and appropriate.

The verification effort shall demonstrate that the data was produced by certified YMP software. Furthermore, it shall establish that any input information employed by the generating software is directly traceable to a LANL computational-data baseline. (Exception: program control information is not subject to this traceability restriction). This requirement is typically met if all noncontrol data-sources are Universal Interface Tables (see TWS-QAS-QP-03.18, *Creation, Management, and Use of Computational Data*). In cases where interface tables cannot be used as input, the individual or organization producing the computational data shall propose an alternative verification strategy for consideration by the CCB through the mechanism of an SCM variance (see Section 7.2.11).

To establish the appropriateness of the generating software and its input, the development organization must document, to the extent possible, that the generating software is employed in a manner that is consistent with (1) its domain of applicability and (2) any assumptions or limitations that are implicit to its design. This shall require a determination that the software is appropriate for application to the problem and evidence that all control input is within reasonable bounds. A similar determination shall be made to establish that any approved data that is provided as input is employed in a manner that is consistent with the domain in which it is verified.

5.3.3.2 Verification of Primary Data

Primary data shall be verified by establishing the pedigree of the data set under consideration, with particular attention to the source of the data. Because the original source of a primary data set may not be in interface-table format, verification of primary data shall also consist of establishing that the interface table in which it is contained is an accurate representation of the original data source. Furthermore, if the primary data set qualifies as existing data under the provisions of NUREG-1298, it shall be qualified in accordance with this regulation prior to submission for verification. In cases where interface tables cannot be used as input, the individual or organization producing the computational data shall propose an alternative verification strategy for consideration by the CCB through the mechanism of an SCM variance (see Section 7.2.11).

5.3.4 Validation of Computational Data

Validation of computational data shall

- Define the domain in which the data is to be validated;
- Establish an adequate level of confidence in the veracity of the data within that domain.

5.3.5 LANL YMP Certification Environment

The Technical Software Management Group shall provide an independent hardware setting and software context in which software and computational data can be independently assessed. This environment shall be physically and administratively isolated from the development environment and shall provide the computers and software necessary to independently authenticate the program of V&V that has been applied to a baseline by the development organization.

The certification environment shall provide an independent domain in which SCM personnel can authenticate much of the V&V work performed by the developer. These authentication operations shall be performed as part of the Physical Configuration Audit and the Functional Configuration Audit.

5.3.5.1 Configuration

The certification environment shall be composed primarily of computer systems under the physical and administrative control of the Technical Software Management Group. These systems shall include standard VAX/VMS and Unix platforms as well as a collection of microcomputer resources. Supercomputer support shall be established through the resources of the Los Alamos Central Computing Facility.

The certification environment shall maintain independent software resources that provide support for many common libraries, compilers, and applications.

5.3.5.2 Access Control

The certification environment shall be maintained by, and access shall be restricted to, Technical Software Management Group personnel. Submission of baselines from the development organization to the certification environment shall be mediated by the SCM Organization. After admission to the certification environment, changes to a baseline shall be strictly controlled and shall require the concurrence and active intervention of the SCM Organization.

5.3.5.3 Operation

The V&V authentication operations that are performed within the certification environment shall include:

- *Verification of Requirements Traceability:* The requirements-traceability activities described in Section 5.3.1.1 shall be repeated within the certification environment.
- *Regeneration of Applications:* Whenever a baseline is submitted for review, any associated software products (primary or support) shall be rebuilt (recompiled and/or relinked) within the certification environment, thereby guaranteeing that any certified components of the software are included into these products. This process can be expected to identify discrepancies that might otherwise be introduced as a result of local dependencies in the developer environment.
- *Re-creation of Supporting Data:* Support data that is required for the execution of the V&V program shall be regenerated from the rebuilt support software.
- *Re-creation of Derived Data (for Computational Data Baselines):* The output interface tables of a proposed computational-data baseline shall be recreated. The certification environment ensures that only certified applications and input data are used to regenerate these interface tables.
- *Execution of the V&V Procedures:* The V&V procedures shall be executed to reproduce the test results. The rebuilt primary and support software shall be employed in this effort, thereby

guaranteeing independence of the results from the original developer environment.

5.3.5.4 Exceptions

Special circumstances may arise in which all or part of the certification environment's intended role cannot be supported. Issues of cost, compatibility, or resource availability may contribute to such situations.

The CCB shall be the judge of whether a situation exists in which the role of the certification environment in V&V authentication must be restricted or eliminated. In such cases, an alternative authentication strategy shall be identified and shall require the approval of the CCB in the form of an SCM variance (see Section 7.2.11, for additional information on SCM variances).

Examples of specific circumstances in which the certification environment is inappropriate to regenerate test results or computational data are listed below:

- *Real-time Systems:* The certification environment generally will not support the special hardware and software configurations unique to analytical instrumentation, telemetry, data acquisition, or other real-time systems. Consequently, an alternative strategy shall be identified for verification of such software.
- *Duplication of Experimental Data:* The certification environment is not intended as a setting in which experiments are independently reproduced, even if computer-controlled analytical-instruments or data-acquisition systems were employed in the experiments. Rather, the data should be treated as primary data for verification purposes (Reference Section 5.3.3.2).
- *Excessive Cost:* If, in the judgement of the TPO, the cost of reproducing a computational data set within the certification environment is prohibitively large, an alternative strategy for authenticating the data shall be formulated. One possibility is to arrange to have the initial version of the computational data set produced within the certification environment or under SCM supervision, thereby eliminating the need for regeneration.

5.3.6 V&V Tools

In the course of doing business, the SCM Organization will develop a suite of software tools that facilitate many V&V operations, particularly in the area of software verification. A partial list of such tools is provided in Section 7.5.4.

The Technical Software Management Group shall implement V&V tools on a best-effort basis. All V&V tools shall be developed in accordance with the provisions of this SQAP and its implementing procedures. These tools need not be present to implement this SQAP. To facilitate V&V activities, the SCM Organization shall share any such certified tools with the development organizations.

5.3.7 Documenting the V&V Process

5.3.7.1 Documentation

The developer shall produce three levels of V&V documentation: a formal V&V plan, V&V procedures, test results, and a V&V report. These documents shall provide the complete formal record of all V&V activities performed on the software.

The V&V plan shall document the strategy to be employed in verifying and validating the software. The purpose of the V&V plan shall be to specify a level of V&V that is adequate to assure that the software performs its intended functions and that no functions are degrading the overall system. The V&V plan shall provide detailed specifications of all tests to be performed and shall describe any other non-testing V&V activities (such as analysis, inspection, or demonstration) in sufficient detail to provide objective criteria to evaluate the results upon completion.

The V&V procedures shall be a translation of the formal testing portions of the V&V plan into programmed instructions that are suitable for execution on the target computer system. Through the vehicle of the V&V procedures, the tests specified in the V&V plan are executed and their results recorded for later inspection.

The test results shall document the execution history of the V&V procedures. As such, they comprise the output of the V&V procedures and may be compared against test criteria specified in the V&V plan to determine whether the test was passed or failed.

The V&V report shall provide a summary of the results of all of the V&V activities that have been performed on the software. Therein, the results of the formal testing shall be analyzed and conclusions shall be reported regarding the acceptability of the software. Other (nontesting) V&V activities shall be analyzed and the results interpreted within the context of the qualification criteria specified in the V&V plan.

5.3.7.2 Documentation Maintenance

The developer shall ensure that all V&V documentation is maintained current with the latest versions of the software requirements and design. In particular, if design iteration results in changes to requirements or design, all affected V&V documentation shall be updated or modified to accommodate those changes during the appropriate life-cycle phase.

5.4 Management of Computational Data

All computational data within the scope of this SQAP shall be subject to the following data-management requirements. Policies for creating, using, and managing computational data are presented in detail in TWS-QAS-QP-03.18, *Creation, Management, and Use of Computational Data.*

5.4.1 Interface Tables

Interface tables shall provide a mechanism for encapsulating computational data. Each interface table shall be partitioned into two sections. The abstract partition shall contain information that identifies the interface table and specifies the heritage and certification status of the data contained in the data partition. The data partition shall contain the actual computational data, divided into data elements. Appendix A provides additional information regarding the architecture and taxonomy of LANL YMP interface-tables.

Data shall be read from and written to interface tables using a suite of standard tools that is provided by the Technical Software Management Group. These tools permit a program to interact with interface tables independent of their internal architecture.

The Technical Software Management Group also shall supply a standard tool that records sufficient information in each output interface-table to

- identify each input interface table;
- identify the associated computational baseline (if any);
- identify the generating software (and any associated sanctioned baseline).

In this manner, each output interface-table automatically incorporates the information necessary to trace its heritage to a primary data source.

All locally developed LANL YMP computer programs shall use interface tables for data input and output operations. (Exception: intermediate information that is not retained by the computer program may be read from and written to scratch files that are not in interface-table format. Prior to the conclusion of program execution, all scratch files created during the run shall be deleted). In special cases other exceptions to this policy may be granted by the CCB in accordance with the policies and procedures that govern SCM variances (see Section 7.2.11). In particular, acquired software generally will not produce interface tables. In such cases, the user shall ensure that all data to be employed in support of a license application is transcribed into interface tables and the release id of the generating software recorded in the abstract partition prior to incorporating the data into a computational-data baseline.

5.4.2 Computational Data Baselines

Computational data baselines shall provide the mechanism for bundling selected, functionally related data-sets into a package for certification. All computational data baselines shall be in interface-table format. Computational data baselines shall undergo formal verification and validation (See TWS-QAS-QP-03.22, *Verification and Validation of Software and Computational Data*) and shall be assessed according to the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data*. The components of a computational-data baseline are described in TWS-QAS-QP-03.19, *Documentation of Software and Computational Data.*

The appropriate principal investigator, technical coordinator, or project leader shall provide guidance to individual researchers as to which data should be incorporated into a computational-data baseline. A computational-data baseline should contain all numerical data necessary to trace a derived numerical result from experiments or modeling studies back to its origins (the experiment number, journal article, laboratory notebook, etc.).

A computational-data baseline should encompass all of the relevant data interface-tables for a specific study (e.g. a set of experiments rather than a single experiment, or a set of computer simulations examining a certain phenomenon rather than a single computer run). A complete suite of summary interface tables shall be included in the baseline.

5.4.3 The LANL YMP Computational Data Archive

The Technical Software Management Group shall maintain an archive of certified LANL YMP data. The data archive shall contain the output interface-tables (and the accompanying Data Set Description documents) for all certified computational data baselines. The Technical Software Management Group shall maintain a catalog of the interface tables that reside in the archive and shall make the catalog available to users. Only data resident in the LANL YMP Computational Data Archive shall be eligible for transfer to the Site and Engineering Properties Data Base (SEPDB) or Reference Information Base (RIB).

6.0 REVIEWS

Formal reviews shall be performed to assess the technical content of each proposed baseline and to ensure compliance with the provisions of this SQAP at each stage of the life cycle. Reviews shall be performed under the auspices of the CCB. Formal reviews shall provide an independent environment for the assessment of each product, identification of discrepancies or other review issues, and specification of the means and timetable by which review issues are resolved.

The SCM Organization shall identify the appropriate reviewers, schedule a formal review, and distribute the review materials. Adequate time shall be provided for the reviewers to evaluate the materials prior to the review.

During a formal review, the CCB shall assess issues raised by reviewers and decide which issues have merit. Issues with merit shall be documented and an issue resolution plan and schedule shall be developed.

Upon resolution of the review issues and approval by the CCB, the baseline shall be certified by the SCM Organization.

Procedures for performing baseline reviews are established in TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

6.1 In-Process Reviews

An in-process review shall be a formal review of a baseline at an intermediate stage of development. An in-process review shall provide the mechanism to evaluate and certify a baseline at a stage of development other than the end of a life-cycle phase.

An in-process review shall not initiate closure of the baseline being reviewed. After completion of an in-process review, the corresponding life-cycle phase shall remain open.

6.1.1 In-Process Review of the Requirements Baseline

An in-process review of the Requirements Baseline shall assess the purpose and scope of the software to be developed or modified, and shall assure that the requirements specified to-date for the software task are complete, verifiable, consistent, and specified in sufficient detail to complete the software design.

In preparation for an in-process review of a requirements baseline, reviewers shall analyze and evaluate the requirements and document informally the problems identified. Issues to be considered during the review shall include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*
- *Clarity of Presentation.* All requirements should be clearly stated in language understandable to the user community in general.
- *Technical Feasibility.* Each requirement shall be within the capabilities of current technology or technology projected to be attainable during the development period.
- *Absence of Design Information.* The requirements specification should be free of design information.
- *Editorial Issues.* The requirements specification should be free of spelling and grammatical errors. Reviewers should make note of any rewording or rephrasing suggestions.

6.1.2 In-Process Review of the Preliminary-Design Baseline

An in-process review of a preliminary-design baseline shall evaluate the basic design approach prior to proceeding with the detailed design effort.

In preparation for the review, reviewers shall analyze and evaluate the preliminary design and document informally the problems identified. Issues to be considered during the review shall include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*
- *Design Approach.* The preliminary design shall incorporate and satisfy all major requirements specified for the software. In particular, major requirements or groups of requirements shall be assigned to specific top-level modules.
- *Top-Level Descriptions.* The preliminary design shall identify all top-level modules and their functions. It shall specify all top-level data structures and all major algorithms.
- *External Interfaces.* The preliminary design should describe all external interfaces including data bases, interface tables, messages, prompts, displays, and metafiles.

6.1.3 In-Process Review of the Verification and Validation (V&V) Plan

An in-process review of the V&V plan shall evaluate the preliminary strategy for verifying and validating the application.

In preparation for the review, reviewers shall analyze and evaluate the V&V planning documents and document informally any problems identified. Issues to be considered during the review shall include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*

- *Test Identification.* The scope of each test shall be identified, i.e, verification test, validation test, regression test, or acceptance test. A given test may fall into more than one of these categories.
- *Test Objectives and Test Inputs.* The objectives of each test shall be clearly stated and all test inputs shall be delineated.
- *Success Criteria.* Success criteria or expected outputs shall be defined for each step in each test procedure. They shall be consistent with the objectives of the test.
- *Test Completeness.* All significant aspects of the software design should be exercised.

6.1.4 In-Process Review of the Detailed-Design Baseline

An in-process review of the detailed design shall examine the comprehensive design of the software's algorithms, data structures, and interfaces at the module level.

In preparation for the review, reviewers shall analyze and evaluate the detailed design documents and record informally any problems identified. Issues to be considered during the review shal! include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*
- *Design Approach.* The detailed design shall incorporate and satisfy all requirements specified for the software.

6.1.5 In-Process Review of V&V Procedures

An in-process review of the V&V Procedures shall assure thorough testing of the software product and shall assure that the V&V Procedures accomplish the intent of the V&V Plan.

In preparation for the review, reviewers shall analyze and evaluate the V&V documents and record informally any problems identified. Issues to be considered during the review shall include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*
- *Test Procedures/Plan Compatibility.* The test procedures shall be consistent with the Test Plan and shall cover all required test areas.
- *Test Identification.* The scope of each test shall be identified, i.e., verification test, validation test, regression test, or acceptance test. A given test may fall into more than one of these categories.
- *Test Objectives and Test Inputs.* The objectives of each test shall be clearly stated and all test inputs shall be delineated.
- *Success Criteria.* Success criteria or expected outputs shall be defined for each test case. They shall be consistent with the objectives of the test.
- *Test Completeness.* All significant aspects of the software design should be exercised.
- *Test Sufficiency.* There should not be areas of overtesting or undertesting.
- *Hardware and Software Configuration.* The hardware and software configurations necessary to conduct the tests shall be adequately defined.

6.1.6 In-Process Review of the Implementation Baseline

An in-process review of an implementation baseline shall assess the implemented design (the code), verify that the implementation agrees with the design, and assess the verification and validation of the software.

In preparation for the review, reviewers shall analyze and evaluate the implementation-baseline documents and record informally the problems identified. Issues to be considered during the review shall include, but are not limited to:

- *Format and Content.* All documents shall adhere to the format and content specified in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*
- *Standards Compliance.* Listings of the source code shall be examined for compliance with any applicable standards documents.
- *Test Procedures/Plan Compatibility.* The test procedures shall be consistent with the test plan and shall cover all required test areas.
- *Test Sufficiency.* There should not be areas of overtesting or undertesting.

6.1.7 In-Process Review of a Computational-Data Baseline

An in-process review of a computational-data baseline shall verify the data source (whether it is primary data or derived data) and shall ensure that the data is valid.

In preparation for the review, reviewers shall analyze and evaluate the data-baseline documents and record informally any issues identified. Issues to be considered during the review shall include, but are not limited to:

- *Primary Data Source.* If the data is primary data, how was it collected, what organization collected the data, what are the credentials of the organization, and for what purpose was the data collected?
- *Derived Data Source.* If the data is derived data (results from a computer program), is the program certified by the LANL YMP Software Quality Assurance Program? If the program used other data to produce the derived data, was that data certified by the LANL YMP Software Quality Assurance program?
- *Intended Use.* If the data is derived data, was the input (if any) to the program within the bounds of the intended use of the program? If not, is there sufficient justification for exceeding the intended limits?

For additional information on the certification of computational data, refer to TWS-QAS-QP-3.22, *Verification and Validation of Software and Computational Data.*

6.2 Baseline-Closure Reviews

A baseline-closure review shall assess the suitability of a proposed baseline for certification and closure. Whenever a software baseline is closed, the corresponding life-cycle phase shall also be closed.

A baseline-closure review of software shall occur only at the end of a software-life-cycle phase. Reviews of computational data shall not be part of any software life-cycle.

When all review issues arising from a baseline-closure review have been resolved, the proposed baseline shall be certified and closed, placed under formal configuration control, and, in the case of a software-development baseline, the corresponding life-cycle phase shall be closed.

A closed baseline shall be subject to the formal change-control policies and procedures specified in TWS-QAS-QP-3.20, *Software Configuration Management*. Modification of a closed baseline shall require a formal change-processing cycle initiated by a Software Change Request or Software Incident Report.

6.2.1 The Software Requirements Review (SRR)

The Software Requirements Review shall be the baseline-closure review for a requirements baseline.

In addition to the requirements for an in-process review of the Requirements Baseline as stated in 6.1.1, the Software Requirements Review shall serve as the forum for the formal closure of the Requirements Baseline and the Requirements life-cycle phase.

The review issues that shall be addressed at the Software Requirements Review are the same as those addressed at the in-process review of a requirements baseline (refer to Section 6.1.1).

6.2.1.1 Life-Cycle Phase

The Software Requirements Review shall take place at the end of the Requirements Phase of the life cycle. The Software Requirements Review shall be completed, and all review issues shall be resolved to the satisfaction of the Change Control Authority, prior to closure of the Requirements life-cycle phase.

6.2.1.2 Baseline and Requirements Phase Closure

When a requirements baseline has been approved by the CCB and certified by the SCM Organization, it shall placed under formal configuration control and the Requirements Phase of the life cycle shall be closed; no further changes shall be made to the certified baseline except through formal change-processing procedures.

6.2.2 The Critical Design Review (CDR)

The Critical Design Review shall be the baseline-closure review for all baselines developed during the Design Phase.

The Critical Design Review shall adhere to the review requirements specified in Sections 6.1.2, 6.1.3, and 6.1.4 in evaluating the Design-Phase baselines. The Critical Design Review shall also serve as the forum for the formal closure of the Design-Phase baselines and for the Design Phase of the life cycle.

The review issues addressed at a Critical Design Review shall be the same as those specified in Sections 6.1.2, 6.1.3, and 6.1.4).

6.2.2.1 Life-Cycle Phase

The Critical Design Review shall take place at the end of the Design Phase of the life cycle. The CDR shall be completed, and all review issues shall be resolved to the satisfaction of the Change Control Authority, prior to closure of the Design Phase of the life cycle.

6.2.2.2 Baseline and Design-Phase Closure

When a detailed-design baseline has been approved by the CCB and certified by the SCM Organization, it shall be placed under formal configuration control and the Design Phase of the life cycle shall be closed; no further changes shall be made to the certified baseline except through formal change processing procedures.

6.2.3 The Software Acceptance Review (SAR)

The Software Acceptance Review shall be the baseline-closure review for all baselines developed during the Implementation Phase.

The Software Acceptance Review shall adhere to the review requirements of Sections 6.1.5 and 6.1.6 in evaluating the Implementation-Phase baselines. The Software Acceptance Review shall also serve as the forum for the formal closure of all Implementation-Phase baselines and the Implementation Phase of the life cycle.

The review issues addressed at a Software Acceptance Review shall be the same as those addressed in Sections 6.1.5 and 6.1.6).

6.2.3.1 Life-Cycle Phase

The Software Acceptance Review shall take place at the end of the Implementation Phase of the life cycle. The Software Acceptance Review shall be completed, and all review issues shall be resolved to the satisfaction of the Change Control Authority, prior to closure of the Implementation Phase.

6.2.3.2 Baseline and Implementation Phase Closure

When an implementation baseline has been approved by the CCB and certified by the SCM Organization, it shall be placed under formal configuration control and the Implementation Phase of the life cycle shall be closed; no further changes shall be made to the certified baseline except through formal change processing procedures.

6.2.4 Data Verification and Validation Review (DVR)

The Data Verification and Validation Review is the baseline-closure review for a computational-data baseline.

In addition to the requirements for an in-process review of a computational-data baseline as stated in 6.1.7, the Data Verification and Validation Review shall serve as the forum for the formal certification of data (primary or derived) to be used to support licensing.

The review issues addressed at a Data Verification and Validation Review shall be the same as those addressed at an in-process review of a computational-data baseline (refer to Section 6.1.7).

6.2.4.1 Baseline Closure

When a computational-data baseline has been approved by the CCB and certified by the SCM Organization, it shall be placed under formal configuration control; no further changes shall be made to the certified baseline except through formal change processing procedures.

6.3 Authorization for Formal Reviews

6.3.1 Software Reviews

All formal reviews of software baselines shall be authorized and documented by the CCB.

All authorized reviews for a software-development or data-production task shall be performed.

If at some point subsequent to review authorization, the CCB or the development organization determines a need for additional reviews, such reviews may be authorized by the CCB.

6.3.2 Reviews of Computational Data Baselines

Reviews of computational data shall be initiated by the custodian of the subject data. When it is determined that computational data is in need of certification, the data shall be compiled into a proposed computational-data baseline and submitted to the SCM Organization.

6.4 Reviewer Qualification and Identification

Permanent and rotating CCB members shall participate in all formal reviews, but they are not necessarily expected to be technical experts. If additional technical expertise is needed, the SCM Organization shall identify temporary CCB members to participate in the formal review. The developer, if not already a permanent or rotating CCB member, shall be made a temporary CCB member. Refer to TWS-QAS-QP-3.20, *Software Configuration Management*, for further details regarding CCB membership.

7.0 SOFTWARE CONFIGURATION MANAGEMENT

LANL YMP Software Configuration Management activities shall be predicated upon the principle of baseline management. As such, the purview of the SCM effort shall be restricted to the software and computational data baselines defined in TWS-QAS-QP-03.19, *Documentation of Software and Computational Data*. The scope of the SCM effort shall be restricted to specifying, managing, evaluating, and certifying the baselines that are the products of the development cycle.

7.1 Configuration Identification

An effective program of Configuration Identification shall be specified to

- Identify the software, documentation, and computational-data elements that are to be placed under configuration management
- Specify the criteria for organizing the elements into baselines
- Derive a methodology for unambiguously and uniquely labeling modules and releases

- Define a hierarchical framework for cataloging all baselines
- Specify a secure repository that implements the cataloging strategy.

7.1.1 Baselines

7.1.1.1 Definition

The following baselines shall be supported for LANL YMP software and computational data:

- Requirements Baseline
- Preliminary Design Baseline
- V&V Plan Baseline
- Detailed Design Baseline
- V&V Procedures Baseline
- Implementation Baseline
- Operational Baseline
- Computational Data Baseline

Baselines shall be identified and organized according to the criteria of Section 7.0 of TWS-QAS-QP-03.19 *Documentation of Software and Computational Data* as modified by the life-cycle-configuration process specified in Section 5.2 and detailed in TWS-QAS-QP-03.21 *Software Life Cycle,* Section 6.3.3.

7.1.2 Labeling of Modules

Every module that is maintained under Software Configuration Management shall be identified primarily by the name of the file that encapsulates it. The name of the product (if any) with which it is associated and the name of the corresponding application shall be used to distinguish the module from similarly named modules in other applications or products.

Distinct versions of each primary source-code-module or high-level documentation-module shall be identified by the number of the Baseline Submission Summary that accompanied its transfer into the Software Configuration Management domain.

7.1.3 Labeling of Releases

Each distinct release of a sanctioned software or computational-data baseline shall be identified by a unique release label.

7.1.3.1 Release Labels

A release label shall be a unique alphanumeric identifier that establishes the development context of the subject application and characterizes the application's major and minor functional levels. The structure of the release label shall be

application-aa-vv-rr

where

- **application**-is the name of the subject application.
- **aa**-is a serial numeric identifier that specifies the major release level of the application.

- vv-is a serial numeric identifier that specifies the major functional level (version number) of the release.
- rr-is a serial numeric identifier that specifies the minor functional level (revision number) of the release.

7.1.4 The Computer Program Library (CPL)

The repository for all certified baselines shall be the CPL. The Software Configuration Manager shall specify the architecture and organization of the CPL to

- Reflect the hierarchical organization of applications
- Provide a mechanism to record the chronological relationships between modules
- Provide the capability to identify changes between versions of a module and to track changes throughout the module hierarchy
- Supply a mechanism for identifying the change-processing status of all modules
- Incorporate a mechanism to associate the components of each distinct baseline
- Specify the means to distinguish specific releases of each application

7.2 Configuration Control

The Configuration Control effort shall establish organizational and administrative controls on changes to all baselines. This shall be accomplished by

- Specifying and implementing procedures for proposing, assessing, and incorporating, changes to baselines and establishing an organizational body to administer the process
- Enforcing CPL and certification environment access controls
- Administering the release of information from the CPL
- Certifying and sanctioning baselines
- Controlling code, data, and the acquisition thereof.

7.2.1 Configuration Control Board (CCB)

7.2.1.1 Role

The CCB shall make all decisions regarding the definition, evolution, assessment, and certification of software and computational data baselines.

7.2.1.2 Authority

The CCB shall have the authority to require changes in practices, procedures, or products that do not meet the requirements of this SQAP or any of its implementing procedures.

The CCB shall be vested with the authority to approve, table, or reject any proposed change to any certified baseline. Furthermore, the CCB shall have the authority to table the implementation of any approved change.

The CCB shall have the authority to approve, table, or reject any proposed baseline. CCB approval shall be required prior to certifying or sanctioning any baseline.

Within the LANL YMP, only the TPO (or designee) shall have the authority to overrule a decision of the CCB.

The TPO shall be empowered to designate one individual to act on his behalf on the CCB. This designation shall be documented in the minutes of the CCB meeting at which the designation is made. Within the scope and context of this SQAP, any authority or responsibility attributed to the TPO shall be assumed by the designee. The designee shall not further delegate this authority. Voting members of the CCB shall retain the right to appeal any decision made by the TPO's designee directly to the TPO.

7.2.1.3 Membership

On the authority of the TPO, the Software Configuration Manager shall appoint the members of the CCB and shall notify each of the corresponding term of service.

7.2.1.3.1 Permanent Members. The TPO and the Software Configuration Manager shall be permanent members of the CCB and shall cochair all CCB meetings. At the discretion of the TPO, additional permanent members shall be appointed from the ranks of the LANL YMP.

Permanent members shall be granted the right to participate in any vote of the CCB.

7.2.1.3.2 Rotating Members. The remaining voting members of the CCB shall be selected from the ranks of the LANL YMP. The term of service of a rotating member shall be specified at the time of selection.

Rotating members shall be granted the right to participate in any vote of the CCB.

7.2.1.3.3 Temporary Members. Temporary CCB members shall be employed to provide additional technical support for the CCB decision-making process. The term of service of a temporary member shall be specified at the time of selection.

If the originator of any request pending before the CCB is not already a permanent or rotating member, that person shall be specified as a temporary member for the meeting in which the request is considered.

Temporary CCB members shall be nonvoting participants.

7.2.1.3.4 Observer Members. The Software Configuration Manager may designate any number of observer CCB members. Observer members shall serve in a nonvoting capacity. The Software Configuration Manage may terminate the service of an observer member at any time.

7.2.1.4 Operation

7.2.1.4.1 Meetings. Meetings of the CCB shall be scheduled by the Software Configuration Manager on an as-needed basis.

The presence of at least 50% of the voting members (of which at least one must be a permanent member) establishes a quorum. A quorum shall be established prior to conducting any business at a meeting of the CCB.

7.2.1.4.2 Voting. Except as specified in Section 7.2.1.4.3, decisions of the CCB shall be made by majority vote of the permanent and rotating members.

7.2.1.4.3 Unilateral Actions. The TPO shall be empowered to overrule any decision of the CCB, countermand any CCB directive, and impose an alternative decision, directive, or action.

7.2.1.4.4 CCB Meeting Records. The business, decisions, and actions of every meeting of the CCB shall be recorded in a set of Minutes. Meeting minutes shall be presented at the following meeting for formal acceptance by the CCB.

7.2.2 Change Control Authority

The CCB shall be empowered to delegate (to the Software Configuration Manager or any collection of voting CCB members) the authority to evaluate, authorize, or reject any proposed request for change that is expected to result in only minor modifications to the associated baseline(s). The Change Control Authority shall be empowered to perform all of the operations and make all of the decisions otherwise reserved for the CCB, subject to the following conditions:

- The Change Control Authority may not approve requests for substantive changes (i.e. modifications that are expected to result in a change in the major release level) to the subject baseline. See Section 7.1.3.1 for additional information on releases;
- Any decision made by the Change Control Authority may be formally appealed to the full CCB or to the TPO.

7.2.3 Computer Program Library Control

All certified baselines are maintained within the CPL.

7.2.3.1 Access Control

Access to the CPL shall be restricted to SCM personnel conducting the legitimate business of the SCM Organization. Browsing of the CPL by other individuals shall be expressly prohibited.

Modules shall be removed from the CPL only as part of a documented release. Appropriate authorizations shall be obtained from the CCB and/or the SCM Organization before a release may proceed. (See Section 7.2.4 for additional information on Releases).

7.2.3.2 Change-Processing Status

The change-processing status shall specify the relationship of a module to the last certified version of its associated application. The change-processing status of every module shall be uniquely and unambiguously defined at every stage of the software life-cycle. The change-processing status of a module shall determine the development, SQA, and SCM activities in which the module may participate.

7.2.3.2.1 Certified Status. The change-processing status of a module is said to be CERTIFIED if it is part of a certified baseline, is stored in the CPL, and is not a component of an open engineering-release. Certified modules represent stable modules that are not in the process of change.

7.2.3.2.2 Modified Status. The change-processing status of a module is said to be MODIFIED if it is part of a certified baseline, is stored in the CPL, and is a component of an open engineering-release. Modified modules represent previously certified modules that are undergoing enhancement or repair.

7.2.3.2.3 New Status. The change-processing status of a newly developed module is said to be NEW until the associated baseline is certified. New modules represent modules that have never previously been under SCM control.

7.2.4 Releases

Releases shall be performed in support of the modification or enhancement of certified baselines, to disseminate certified software and computational data to the user community, and to make prerelease versions of applications available to the user community. Releases shall be authorized by the CCB and administered by the Software Configuration Manager.

In order to protect the integrity of certified components, the Configuration Control effort shall restrict the scope of all releases to the maximum extent that is practical.

7.2.4.1 Engineering Release

An engineering release shall transfer custody of selected modules from the SCM Organization to a developer for the purpose of modification.

An engineering release shall be termed open while the released modules are undergoing modification and during the subsequent formal audits and reviews. An engineering release shall be termed closed when the corresponding implementation baseline is certified.

Multiple, concurrent engineering-releases of any baseline or baseline component shall not be permitted. An application that is the subject of an engineering release shall be released to only one developer for the purpose of resolving only one CCB-authorized development task. To protect the integrity of certified baseline components, no engineering release shall include a module that is already in the MODIFIED change-processing status.

Only those modules that are expected to undergo change during the subsequent development cycle shall be released in an engineering release. All other modules shall remain in the CPL. (Exception:

program modules that do not require change shall be released in binary-code form, if possible).

7.2.4.2 Assessment Release

An assessment release shall be performed for the purpose of providing read-only copies of selected modules to the development organization, usually for assessment of the impact of a problem report or enhancement request. Alternatively, an assessment release shall be made to the SCM, SQA, or QA organizations to support any legitimate activity of the requesting organization. An assessment release shall be implicitly authorized when the CCB assigns a problem report or enhancement request for analysis. The preferred release format of assessment-release information shall be hard-copy.

7.2.4.3 Release of a Sanctioned Baseline

This release shall be performed to make the primary products of a sanctioned baseline available to the user community. It shall follow sanctioning of the application's implementation baseline.

Releases of sanctioned software-baselines shall be in binary-code format. (Exception: Applications written in interpreted programming languages shall be released as source code.) Computational data baselines shall be in interface-table format.

7.2.4.4 Probation Release

A probation release shall be performed to make an uncertified version of a baseline available to the user community. A probation release is generally performed to provide temporary, emergency bug fixes or to permit selected users access to uncertified software or data in support of a rapid prototyping effort.

The contents of a probation release shall be similar to those of a sanctioned release with the exception that the implementation baseline for the subject application is not yet sanctioned. Consequently, data generated by the applications of a probation release shall not be certifiable.

7.2.5 Baseline Certification and Baseline Sanctioning

The SCM Organization shall implement procedures to certify a baseline that has completed its baseline closure review and has been approved by the CCB. The certification process shall formally establish the approved baseline and shall effect its transfer into the CPL.

The SCM Organization shall implement procedures to sanction a certified implementation or computational-data baseline. Sanctioning shall result in the formal closure of the development life-cycle for the subject application. Sanctioning shall also include notification of the availability of the application to registered users and to the National Energy Software Center. Completion and documentation of the sanctioning process constitutes a formal approval to use the sanctioned baseline.

7.2.6 Baseline Admission

Information shall be admitted into the CPL only as a consequence of the baseline-certification process. In order to protect the integrity of certified modules that already reside within the CPL, the following restrictions shall be placed upon the baseline-admission process:

- For any module submitted with a change-processing status of CERTIFIED or MODIFIED, a corresponding predecessor module must already exist in the CPL, and the predecessor module must have the same change-processing status.
- For any module submitted with a change-processing status of NEW, there must be no predecessor module in the CPL.

7.2.7 Interface Control

Upon receipt of an approved formal request for sanctioned software or computational data, the SCM Organization shall distribute a copy to the requestor. Only sanctioned baselines shall be disseminated. The SCM Organization shall not perform any distribution that results in copyright infringement or any other violation of proprietary rights in the subject software or data.

7.2.8 Control of System Software and Acquired Commercial Software

Because the LANL YMP has no direct control over changes made by commercial software publishers to their products, the configuration control policies and procedures specified in the preceding sections shall not apply to system software or acquired commercial software.

7.2.9 Control of Data

Only certified computational data baselines shall be controlled by the SCM Organization. Computational data baselines shall be subject to all of the configuration control requirements specified in this SQAP.

7.2.10 Supplier Control

7.2.10.1 Acquired Noncommercial Software

Acquired noncommercial software shall be subject to all of the configuration control requirements specified in this SQAP.

7.2.10.2 Subcontracted Software

Subcontracted software shall be subject to all of the configuration control requirements specified in this SQAP.

7.2.11 Variances

The CCB shall be empowered to grant variances to specific provisions of this SQAP and its implementing procedures in special cases for which the subject provisions are ineffective, inappropriate, or require an excessive expenditure of resources to accomplish.

7.2.11.1 Documentation

For each variance authorization, the CCB shall provide documentation that includes

- A citation specifying the document name and paragraph number of the provision against which the variance is issued
- The specific justification for granting the variance
- Any constraints or conditions that restrict the application of the variance.

7.2.11.2 Limitations

Under no circumstances may the CCB issue a variance that contravenes any provision of *QARD Quality Assurance Requirements Document for the Radioactive Nuclear Waste Management Program.*

7.3 Configuration Status Accounting

7.3.1 CSA Records Identification and Collection

CSA records shall comprise all certified baselines, all supplemental-documentation forms, and all formal CSA reports.

A closed CSA record shall be a supplemental-documentation form that contains all required origination/approval signatures, a certified baseline, or an issued CSA report. A closed CSA record documents a baseline or event that has been completed.

An open CSA record shall be a supplemental-documentation form that contains some but not all of the required origination/approval signatures. An open CSA record documents an action that is in progress or that has been tabled.

A baseline shall enter the CSA domain when it is certified.

A formal CSA report shall enter the CSA domain when it is generated by the CSA effort.

A supplemental-documentation form shall enter the CSA domain when it is closed.

7.3.2 CSA Records Storage

7.3.2.1 The CSA Data Base

A summary of the latest version of every supplemental-documentation form received by the SCM Organization (except Standard Continuation Forms) shall be maintained in a secure electronic data base called the CSA data base. Summary information shall include at a minimum:

- The identifying number of the form;
- The name of the originator and origination date;
- A brief title.

7.3.2.2 The CSA Active File

The CSA active file shall be a temporary repository for paper copies of all closed supplemental documentation forms prior to their transfer to the LANL YMP Records Processing Center (RPC). The CSA active file shall be administered, updated, and maintained by the CSA effort of the SCM Organization.

7.3.2.3 Interface with the RPC

To comply with the requirements of TWS-QAS-QP-17.3, *Procedure for LANL YMP Records Management*, all closed CSA records shall be submitted to the RPC in a timely fashion. The CSA effort of the SCM Organization shall have responsibility for transmitting CSA records to the RPC.

7.3.3 Records Retention

Records in the CSA Active File shall be retained until such time as they are transmitted to the RPC, at which time they shall be purged from the file.

Records in the LANL YMP Records Management System shall be subject to the retention requirements specified in TWS-QAS-QP-17.3, *Procedure for LANL YMP Records Management*.

Subsequent to their submittal to the RPC, records in the CSA Data Base may be purged at the discretion of the Software Configuration Manager.

Records (baselines) in the CPL shall be maintained for the duration of the project, or until they have been transferred to the RPC, at the discretion of the Software Configuration Manager.

7.3.4 Reports

The CSA effort shall generate formal reports to support reviews and configuration audits and to keep project management apprised of the status of the software effort. CSA reports shall be of three types: periodic, on-demand, and ad hoc.

7.3.4.1 Periodic Reports

Periodic reports shall be generated at regular intervals and shall be distributed to a specific group of individuals and organizations. A principal investigator, project leader, the CCB, or a representative of the SCM Organization shall be authorized to request a new periodic report.

The Software Configuration Manager shall be empowered to accept, reject, or table a request for a new periodic report. The Software Configuration Manager's decision regarding the disposition of the request may be appealed to the CCB. The Software Configuration Manager (with the concurrence of the CCB) shall be authorized to discontinue generation of a periodic report.

7.3.4.2 On-Demand Reports

On-demand reports shall be generated and distributed at the specific request of a principal investigator, project leader, the CCB, or a representative of the SCM Organization, for distribution to a list of individuals and organizations specified when the request is made.

The Software Configuration Manager shall be authorized to accept, reject, or table the request. The Software Configuration Manager's decision regarding the disposition of the request may be appealed to the CCB.

7.3.4.3 Ad Hoc Reports

An ad hoc report shall be a custom CSA report that is generated at the request of a principal investigator, project leader, the CCB, or a representative of the SCM Organization, for distribution to a list of individuals and organizations specified when the request is made. An ad hoc report provides information that cannot be obtained from any existing periodic or on-demand report.

The Software Configuration Manager shall be authorized to accept, reject, or table the request for generation of an ad hoc report. The Software Configuration Manager's decision regarding the disposition of the request may be appealed to the CCB.

7.3.5 Change Tracking

The CSA effort shall maintain sufficient information in the Computer Program Library to identify differences between successive versions of a certified software application and to recreate any previously certified version. Furthermore, the CSA effort shall maintain a record of the complete development history of every certified software application in the associated suite of supplemental-documentation forms as cataloged in the CSA Database.

Through the mechanism of formal CSA reports, the CSA effort shall provide the capability to identify the current configuration of any certified software baseline and to track changes throughout the system of certified software. To accomplish this objective, the following minimum suite of CSA reports shall be established by the Software Configuration Manager:

- A summary listing of the current approved configuration showing all certified modules and their interrelationships.
- A summary listing of the status of proposed changes to the approved configuration. This report shall contain the identifying number and brief title for each formal change proposal or problem report and the current status of the proposed change. References to related Deficiency Reports (see TWS-QAS-QP-15.2 *Deficiency Reporting*) shall be provided.
- A brief chronology of versions of each sanctioned software application including a summary of the changes that produced each new version.
- A summary listing of the users to whom sanctioned software or data have been distributed for use in technical calculations.

7.4 Configuration Auditing

To identify issues that may undermine the success of a subsequent formal review, the Configuration Auditing effort of the SCM Organization shall assess all proposed baselines prior to their entry into the formal review process. Issues shall be formally documented and the SCM Organization shall withhold the proposed baseline from the formal review process until all issues are resolved to its satisfaction.

7.4.1 Functional Configuration Audit

The SCM Organization shall perform a functional configuration audit on every proposed baseline submitted for formal review. A functional configuration audit shall examine whether the development of the subject baseline has been satisfactorily completed and whether the component modules have achieved the functional characteristics specified in their technical documentation. In particular, it will identify major errors or omissions regarding requirements traceability between requirements and design baselines and between design and implementation baselines.

7.4.2 Physical Configuration Audit

The SCM Organization shall perform a physical configuration audit on every proposed baseline submitted for formal review. A physical configuration audit shall examine whether any required components are missing from the proposed baseline. As such, the physical configuration audit focuses upon determining whether any modules that should be part of the baseline are missing from the submission.

7.5 SCM Tools

7.5.1 Configuration-Identification Tools

7.5.1.1 Label Generator

This tool shall validate existing configuration-labels and shall generate new release or module labels for modified applications and modules. The tool shall also generate the appropriate CPL partition for new applications, products and modules.

7.5.1.2 Baseline Templates

A suite of electronic word processor templates for all baseline components shall be developed and maintained by the SCM Organization.

7.5.2 Configuration-Control Tools

7.5.2.1 CPL-Management System

This vendor-supplied environment shall provide an automated SCM system that can be customized to accommodate the requirements of this SCM plan. This tool will

- Automatically perform and verify all releases of applications from the CPL
- Automatically perform all software submission operations
- Automatically perform and verify baseline updates.

7.5.2.2 Interface Table Utilities

These reuse components shall provide a standard means by which interface tables may be read and written.

7.5.2.3 Certification Status Utility

This reuse component shall provide the means for every LANL YMP program to verify its own certification status as well as the certification status of all input interface-tables.

7.5.3 Configuration-Status-Accounting Tools

7.5.3.1 CSA Report Generators

These tools shall provide automatic generation of periodic or on-demand CSA reports from information contained in the CSA data base and the CPL.

7.5.4 Configuration-Auditing/Review Tools

7.5.4.1 Verification Matrix Generator

This tool shall generate a verification matrix for each of the following situations

- Requirements implementation
- Test coverage

7.5.4.2 Design Comparator

The design comparator tool shall compare the detailed design (as embodied in module pseudocode) of a module to the corresponding source code and shall identify discrepancies between the two.

7.5.4.3 Document Comparator

The document comparator shall be employed to compare any two text-based documents and identify differences with change bars.

7.5.4.4 Review-Packet Generator

The review packet generator tool shall compile the information necessary to support a review or audit into a standard distribution package.

7.5.4.5 Application-Structure-Chart Generator

The structure-chart generator shall generate a hierarchical representation of the module calling structure of an application. Two representations of the calling structure shall be supported:

- Tree representation
- Maintenance representation - a table that indicates, for each module, those modules that call the module and those modules that are called by the module.

7.5.4.6 Data Heritage Generator

The data heritage generator shall generate a graph structure that indicates the heritage (i.e. the generating software, input interface-tables, and the certification status of each) of any interface table.

7.5.4.7 Data Comparator

This tool shall provide a means to compare different computational-data sets and flag discrepancies that exceed a specified tolerance.

7.5.5 Tool Implementation

All SCM tools shall be developed in accordance with the provisions of this SQAP and its implementing procedures. Tools shall be developed on a best effort basis and need not be present to implement this SCM plan.

8.0 PROBLEM REPORTING AND CORRECTIVE ACTION

The LANL YMP shall provide a formal mechanism for reporting problems that are discovered in a certified baseline, requesting changes or enhancements to a certified baseline, or initiating a new software-development effort. Formal documentation shall be provided for each of the above events. A mechanism shall be specified whereby conditions adverse to quality and significant conditions adverse to quality can be addressed within the context of the deficiency reporting system as described in TWS-QAS-QP-15.2, *Deficiency Reporting*.

Procedures shall be implemented for evaluating a proposed change, determining the impact of the change on previous calculations or existing software, defining the appropriate level of development effort, authorizing subsequent work, and assessing the results at regular intervals. The CCB shall be the focus of these activities.

9.0 TOOLS, TECHNIQUES, AND METHODOLOGIES

All tools, techniques and methodologies used to implement this SQAP are described in TWS-QAS-QP-03.17 through TWS-QAS-QP-03.22, inclusive.

10.0 CODE CONTROL

Requirements for code control are described below. TWS-QAS-QP-03.20, *Software Configuration Management*, details the implementation of these requirements.

All certified code shall be maintained within a secure database (the CPL) under the administrative control of the SCM Organization. Access to the CPL shall be restricted to SCM personnel conducting the business of the CCB or SCM Organization.

Prior to performing any modification to a baseline, authorization shall be obtained from the CCB by the development organization. Any associated engineering release of code from the CPL shall reference this authorization.

An engineering release of source code from the CPL shall be restricted to only those modules that require modification. Additional code necessary for creating executable modules shall be released in binary format.

11.0 MEDIA CONTROL

Steps shall be taken to protect all technical and administrative information that is resident on computer-readable media. These steps shall include

- Protection of primary media from damage, loss, and misuse;
- Implementation of a strategy for recovery from catastrophic failures of the primary media. A documented program of backups shall be sufficient to satisfy this requirement.

The person or organization with primary administrative responsibility for a computer system shall demonstrate compliance with the above criteria.

12.0 SUPPLIER CONTROL

The requirements for supplier control are specified in Sections 7.2.8, 7.2.9, and 7.2.10. TWS-QAS-QP-03.20, *Software Configuration Management*, and TWS-QAS-QP-03.21, *Software Life-Cycle*, detail the implementation of these requirements.

13.0 RECORDS COLLECTION, MAINTENANCE, AND RETENTION

Records collection, retention and maintenance shall be the responsibility of the SCM Configuration Status Accounting (CSA) effort. TWS-QAS-QP-03.20, *Software Configuration Management*, details the policies and procedures for records management. Whenever these procedures require an interface with the RPC, the policies of TWS-QAS-QP-17.3, *Procedure for LANL YMP Records Management*, shall be followed.

APPENDIX A. INTERFACE TABLES

1.0 INTRODUCTION

An interface table is a standard text-file that is used for file input and output by LANL YMP software. Interface tables are read and written using standard subprograms that permit a software application to access the encapsulated data without any specific knowledge of the internal architecture of the interface table. This promotes a high level of reusability and simplifies management of the data.

LANL YMP data-management policies support two types of interface table. Data interface-tables are used as the source and destination of all computational data used and produced by a computer program. Configuration interface-tables are employed to identify the data interface-tables that are used by a computer program.

2.0 INTERFACE TABLE ARCHITECTURE

Interface tables are divided into two partitions. The abstract partition contains information that characterizes the heritage and certification status of the data contained in the data partition.

2.1 Abstract Partition

The abstract partition of an interface table contains information that identifies the interface table, characterizes the certification status of its constituent data, and provides extensive data-heritage information. The abstract partition establishes the data heritage by recording the name and associated release label (if any) of the generating software as well as the names and associated release labels of all input data-interface-tables. For primary data, source databases, experiment numbers, TWS-number and page numbers of the laboratory notebook, or the journal article reference from which the data were obtained are also provided in the data heritage. If the generating software or any of the input data-interface-tables are uncertified, this condition is reflected in the abstract partition. For universal interface-tables (see Section 4.1 of this Appendix), the release label of the corresponding computational-data baseline establishes the certification status of the interface table.

2.2 Data Partition

The data partition of an interface table contains the information that is to be provided to, or the results from the execution of, a computer program. The data partition is divided into data elements. Each data element contains header information that provides the name and characteristics the data element. The header is followed by lines containing the data values.

An interface table may contain any number of uniquely named data elements. Data elements may be organized into the data partition in any order.

3.0 CLASSES OF INTERFACE TABLES

3.1 Configuration Interface-Table

A configuration interface-table is an interface table that specifies the name and identification of each data interface-table used for input or output by a computer program. This permits the user to specify the interface tables that will be used for a particular program execution at run-time. Only one configuration interface-table is associated with a computer program.

3.2 Data Interface Tables

A data interface-table is an interface table that contains the computational data that is read or written by a LANL YMP computer program. There is no practical limit to the number of data interface-tables that may be associated with a computer program.

Although a data interface-table may contain an unlimited number of data elements, the software developer is advised to segregate a computer program's input information into at least two distinct types of data interface-table: a control interface-table and any number of processing interface-tables.

3.2.1 Control Interface-Tables

A control interface-table is an input data interface-table that contains any information necessary to configure a computer program for a run. It encapsulates the control information required to specify program options, set convergence criteria, establish maximum iteration counts, set timeouts, etc. Only one control interface-table may be defined for a computer program, and all control information should be placed into it. Information that is provided in a control interface-table is not transformed by the computer program that reads it.

3.2.2 Processing Interface-Tables

A processing interface-table is an input data-interface-table that contains the data that is to be transformed (processed) by the computer program. Any number of processing interface-tables may be associated with a computer program.

3.3 Summary Interface-Tables

A summary interface-table is an output data-interface-table that contains information that characterizes a particular execution of a certified software application. Included in this information is the name of the computer program, the release label of the associated application, starting and ending date/time for the run, names of all input interface tables, and names of all output interface tables. A standard, certified LANL YMP reuse component generates the summary interface-table automatically for each execution of the associated computer program.

4.0 Scope of Interface Tables

4.1 Universal Scope

The scope of a data interface-table that has been approved by the CCB and certified by the SCM Organization is universal. Universal interface-tables are always part of a computational-data baseline. Universal interface-tables are placed in the LANL YMP Computational Data Archive for use by LANL YMP members. A universal interface-table may contain primary or derived data.

4.2 Local Scope

The scope of an uncertified data-interface-table that is employed within the user's computing environment is local. A control interface-table is always local. Processing interface-tables may be local or universal, depending upon their certification status. An output interface table is local until it is incorporated into a proposed computational-data baseline, approved by the CCB, and certified by the SCM Organization.

In performing a study that employs computer software, the investigator may make numerous changes to input interface-tables, and only a small subset of the output interface-tables generated will be suitable for incorporation into a computational-data baseline. Local interface tables allow this sort of scientific inquiry to proceed in an unfettered manner.

The contents and use of local interface-tables are not controlled. The data elements in a local interface-table may be changed at the discretion of the user.

5.0 DATA MANAGEMENT SOFTWARE

Standard reuse-components are provided to LANL YMP software developers to provide uniform mechanisms for interface-table processing. This software is developed and maintained by the Technical Software Management Group.

5.1 Data-Configuration-Setup Software

The data-configuration-setup software is executed at the beginning of all software to identify the names of all input and output interface-tables and to write certification and data-heritage information into the abstract partition of each output interface-table. This subprogram opens the configuration interface-table for the program and reads the names of the input and output interface tables. It then writes the required certification and data-heritage information to all output interface-tables.

5.2 Interface-Table Reader

This certified LANL YMP reuse-component is a standard subprogram that is employed by all software to read data from an interface table. It requires the following minimum information as input: 1) the file specification of the interface table to read, 2) the name of the data element of interest, and 3) the destination of the information within the program. The interface-table reader then locates the requested information in the specified interface table and transfers it into the program.

5.3 Interface-Table Writer

This certified LANL YMP reuse component is a standard subprogram that is employed by all software to write data to a data interface-table. When provided with information similar to that required for the interface-table reader, it writes the requested information to the destination interface-table.

APPENDIX B. REFERENCES

ANSI/IEEE Std 730-1984, *IEEE Standard for Software Quality Assurance Plans,* June 1984.

ANSI/IEEE Std 828-1983, *IEEE Standard for Software Configuration Management Plans,* June 1983.

ANSI/IEEE Std 829-1983, *IEEE Standard for Software Test Documentation,* August 1983.

ANSI/IEEE Std 830-1984, *IEEE Guide To Software Requirements Specifications,* July 1984.

ANSI/IEEE Std 1042-1987, *IEEE Guide To Software Configuration Management,* September 1987.

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

NN1-1990-0334 *Software Supporting Scientific Investigations/Licensing*

NUREG-0856 *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management,* June 1983.

NUREG-1298 *Qualification of Existing Data for High-Level Nuclear Waste Repositories,* February 1988.

QARD Quality Assurance Requirements Document for the Civilian Radioactive Waste Management Program, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

Software Configuration Management: An Investment in Product Integrity. Edward H. Bersoff, Vilas D. Henderson, and Stanley G. Siegel, Prentice-Hall, Inc., 1980.

The Software Development Project, Planning and Management, Phillip Bruce and Sam M. Pederson, John Wiley and Sons, 1982.

TWS-QAS-QP-03.2 *Procedure for Preparation and Technical and Policy Review of Technical Information Products.*

TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

TWS-QAS-QP-03.18 *Creation, Management, and Use of Computational Data.*

TWS-QAS-QP-03.19 *Documentation of Software and Computational Data.*

TWS-QAS-QP-03.20 *Software Configuration Management.*

TWS-QAS-QP-03.21 *Software Life-Cycle.*

TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data.*

TWS-QAS-QP-15.2 *Deficiency Reporting*

TWS-QAS-QP-17.3 *Procedure for LANL YMP Records Management.*

APPENDIX C. DEFINITIONS

abstract partition. The abstract partition is a section of an interface table that contains information that identifies the interface table, characterizes the certification status of the data encapsulated in it, and provides extensive data heritage information.

acquired commercial software (ACS). Acquired commercial software is acquired software that is general purpose in nature and is supplied to a large installed user base by a commercial or noncommercial entity outside of the YMP.

acquired noncommercial software (ANS). Acquired noncommercial software is all acquired software that is not classified as system software or acquired commercial software.

acquired software. Acquired software encompasses all software that is not originally developed by a LANL YMP member, contractor, or subcontractor.

ad hoc report. An ad hoc report is a custom CSA report that is generated at the request of a principal investigator, project leader, the CCB, or a representative of the SCM Organization for distribution to a list of individuals and organizations specified when the request is made.

administrative data base application (ADB). An administrative data base application is software that implements a data base for the management of nontechnical information.

application. An application is composed of all of the modules and products that are associated with a suite of functionally-related computer programs, reuse components, or interface tables.

auxiliary software (AUX). Auxiliary software is software that is relatively complex but does not contain a mathematical or numerical model of a physical process or configuration.

baseline. A baseline is an ordered collection of software, documentation, and/or computational data that represents a reference point or plateau in the development of a software application or computational-data set.

baseline certification. Baseline certification is the process of placing an approved baseline under configuration control. The certification process is documented on a Baseline Certification Notice form.

Baseline Certification Notice. A Baseline Certification Notice is a supplemental-documentation form that is issued by the SCM Organization after an approved baseline has been placed under configuration management.

baseline-closure review. A baseline-closure review is a formal review the purpose of which is to assess the suitability of a proposed baseline for closure and, in the case of a software development baseline, subsequent closure of the corresponding life-cycle phase. The baseline closure reviews are:

- **Software Requirements Review (SRR)**
- **Critical Design Review (CDR)**
- **Software Acceptance Review (SAR)**
- **Data Verification and Validation Review (DVR)**

baseline evolution. Baseline evolution is the process of deriving a subsequent baseline through elaboration or refinement of the current baseline.

baseline sanctioning. The baseline sanctioning is the process that encompasses the performance of a technical and policy review of the certified implementation baseline, issuance of an Engineering Change Notice, and notification of the National Energy Software Center.

Baseline Submission Summary. The Baseline Submission Summary is a supplemental-documentation form that is completed by the developer to submit a proposed baseline into the formal audit and review process.

CCB Meeting Announcement. The CCB Meeting Announcement is a supplemental-documentation form that is issued by the SCM Organization to announce the time, date, and location of a meeting of the CCB and to disseminate the meeting agenda.

CCB Meeting Minutes. The CCB Meeting Minutes is a supplemental-documentation form that is completed by the permanent or rotating CCB member who is charged with recording the minutes of the meeting.

CCB Participation Notice. The CCB Participation Notice is a supplemental-documentation form that is issued by the SCM Organization to announce the selection of an individual for service on the CCB.

certification. See **baseline certification.**

certification environment. The LANL YMP Certification Environment is an independent hardware setting and software context in which software and computational data can be independently assessed. It is physically and administratively isolated from the development environment and provides the computers and software necessary to independently authenticate the V&V program that has been applied to a baseline.

change control authority. The change control authority is a person or group of persons, authorized by the CCB to act in its stead on issues of change control including evaluation of baselines and verification that review issues have been resolved.

change processing. Change processing is the formal process of proposing, assessing, implementing, and certifying changes to the LANL YMP software system.

change-processing status. The change-processing status is a designation that specifies the relationship of a module to the last certified version of its associated application. The following change-processing statuses are supported:

- **Certified status,**
- **Modified status,**
- **New status.**

component-model software (CMS). Component-model software is software that implements a well-established, general numerical or mathematical model that may be incorporated into a subsequent physical model.

computational data. Computational data is any information that is used as input to, or is generated as output from, a computer program.

computational-data baseline. A computational-data baseline is a baseline that encapsulates certified LANL YMP data and any associated documentation and support software. It consists of the data generated by a certified software-application, any information necessary to recreate that data, and descriptive documentation.

computer program baseline. A computer program baseline is a baseline that encapsulates one or more computer programs and any associated documentation, computational data, or support software.

computer program library (CPL). The CPL is an electronic data base that is the secure repository for all certified baselines.

configuration audit. A configuration audit is an assessment that is performed to identify and initiate correction of major deficiencies that would otherwise undermine the effectiveness of a subsequent formal review.

configuration auditing. Configuration auditing is the process of independently assessing the physical and functional attributes of a baseline to identify deficiencies that would otherwise threaten the integrity and effectiveness of a subsequent review.

configuration control. Configuration control is the orchestration of the processes by which the software portion of a system can achieve and maintain visibility throughout its passage through the system life-cycle. It provides the documentation, procedures, and an organizational body to control the system implementation and any changes to it.

configuration control board (CCB). The CCB is the organizational body that assesses all requests for changes to the certified baselines of the LANL YMP software system. It has authority to approve or reject any proposed change or the implementation of any previously approved change.

configuration identification. Configuration identification is the SCM discipline that defines the entities to be controlled by the SCM process, derives unique identifying labels for each entity, and specifies a hierarchical organization within which they can be cataloged.

configuration interface-table. A configuration interface-table is an interface table that specifies the name and identification of each data interface table used for input or output by an application.

configuration status accounting. Configuration status accounting is the means by which the outputs of the configuration identification, control, and auditing functions are recorded, stored in a data base, and reported upon.

control interface-table. A control interface-table is an input data interface table that contains any input information necessary to configure the computer program for the run. It specifies the control information required to specify program options, set convergence criteria, establish maximum iteration counts, set timeouts, etc.

CPL Transmittal Request. The CPL Transmittal Request is a supplemental-documentation form is used to document the transfer of modules between the requestor and the CPL.

Critical Design Review (CDR). The Critical Design Review is the baseline-closure review for a detailed-design baseline. It signals the end of the Design Phase of the software life-cycle. When the Critical Design Review has been conducted and all issues arising from the review have been resolved, the Design Phase is closed.

CSA active file. The CSA active file is a temporary repository for paper copies of all supplemental documentation forms prior to their transfer to the LANL YMP Records Processing Center.

CSA data base. The CSA data base is an electronic data base in which all supplemental documentation forms are stored.

CSA Information Request. The CSA Information Request is a supplemental-documentation form is used to request generation and distribution of a CSA report.

CSA report. A CSA report is the formal mechanism for communicating information maintained by the SCM Organization (especially information that is resident on supplemental documentation forms) to authorized Project personnel. A CSA report is generated by the CSA function to support reviews and audits, establish documentary evidence of traceability, and to keep Project management apprised of the status of the software effort. CSA reports are of three types: periodic, on-demand, and ad hoc.

custodian. The individual or group who has responsibility for an existing development software application prior to its certification.

data archive. The LANL YMP data archive is a central repository in which all certified data interface tables are stored for use by all LANL YMP Project members.

data interface table. A data interface table is an interface table that contains the data read or written by a LANL YMP software application. All computational data should be read from and written to data interface tables.

data partition. The data partition is the section of an interface table that contains the information that is to be provided to, or is the result of, an execution of a computer program.

Data Set Description. The Data Set Description is a user documentation component that describes the interface tables associated with a computational-data baseline.

Data Verification and Validation Review (DVR). The Data Verification and Validation Review is the baseline-closure review for a computational-data baseline.

derived data. Derived data is any computational data that are output by a computer program into interface-table format.

detailed-design baseline. The detailed-design baseline is a formal baseline that is produced during the Design Phase of the software life-cycle. Its purpose is to document the comprehensive design of the software's algorithms, data structures, and interfaces at the module level.

development baseline. A development baseline is any baseline that is associated with the Requirements, Design, or Implementation life-cycle phase is a development baseline.

development documentation. Development documentation is formal documentation that encompasses all information that describes or characterizes the evolution of a particular software or computational data product as it progresses through the life cycle. The primary audience for development documentation is the software developer, analyst, or maintenance programmer.

developer. See **development organization.**

development software (DS). Development software is software that is developed under the auspices of the LANL YMP.

development organization. The development organization (developer) is the person or persons responsible for producing the baselines at each phase of the development life-cycle.

electronic calculation (EC). Electronic calculation software is software that is relatively non-complex and for which the results can be verified in the same manner as a manual calculation.

Engineering Change Directive. The Engineering Change Directive is a supplemental-documentation form that is issued by the CCB to authorize work on a software task.

Engineering Change Notice. The Engineering Change Notice is a supplemental-documentation form that is issued by the SCM Organization to notify potential users of the availability of a sanctioned software application. It formally closes the software-development task initiated by the Engineering Change Directive.

evidential documentation. Evidential documentation is information that is employed in the licensing arena to document the veracity of a particular software or computational-data baseline. Evidential documentation components are specified in NUREG-0856 and may include development documentation and user's documentation components.

file list. A file list consists of one or more text module that provide a concise summary of the components of a baseline.

functional configuration audit. A functional configuration audit is a formal configuration audit performed by the SCM Organization to ensure that the development of the subject baseline has been satisfactorily completed and that the component modules have achieved the functional characteristics specified in their technical documentation.

implementation baseline. The implementation baseline is a formal baseline that is produced during the Implementation Phase of the software life-cycle. Its purpose is to provide documentation of the following processes:

- Translation of the software design into source code;
- Completion of the final version of the V&V plan;
- Generation of the V&V procedures from the V&V plan;
- Generation and interpretation of the Test Results;
- Creation of documentation for users of the application.

in-process review. An in-process review is a formal review of a baseline at an intermediate stage of development. In-process reviews provide the mechanism to evaluate and certify a baseline at stages of development other than the end of a life cycle. In-process reviews are conducted in the same manner as the corresponding baseline closure reviews. The in-process reviews are:

- In-Process Review of the Requirements Baseline.
- In-Process Review of the Preliminary-Design Baseline.
- In-Process Review of the Verification and Validation Plan.
- In-Process Review of the Detailed-Design Baseline.
- In-Process Review of the Verification and Validation Procedures.
- In Process Review of the Implementation Baseline.
- In Process Review of a Computational-Data Baseline.

interface table. An interface table is a standard text file that is used with all software developed for the LANL YMP for all file input and output. An interface table is divided into two partitions. The abstract partition contains information that characterizes the heritage and certification status of the data contained in the data partition.

interface table reader. The interface table reader is a certified LANL YMP reuse-component that is employed to read data from an interface table.

interface table writer. The interface table writer is a certified LANL YMP reuse-component that is employed to write data to a data interface table.

LANL YMP certification environment. See **certification environment.**

LANL YMP data archive. See **data archive.**

Life Cycle Specification. The Life Cycle Specification is a supplemental-documentation form that is issued by the CCB to configure the life cycle for a software-development task. It specifies the required life-cycle phases, baselines, baseline components and reviews.

local interface table. A local interface table is an uncertified data interface table that is employed within the user's local computing environment.

manifest product software (MP). Manifest product software is software that can be readily examined for correctness without reference to the design or implementation of the software.

mathematical support software (MSS). Mathematical support software is software that implements a common mathematical function or procedure.

model validation. Model validation is a process that is performed to ensure that the subject model is an accurate representation of physical reality within the domain of application.

Models and Methods Summary. The Models and Methods Summary is a document that is provided to apprise potential users of the details of the mathematical models and numerical methods employed by the software and to comply with the requirements of Section B of NUREG-0856. As such, the Models and Methods Summary has a role as user documentation and evidential documentation.

module. A module is a computer-readable and electronically storable file that is the fundamental unit of information that is uniquely labeled and managed by the SCM Organization.

module label. The module label is a unique identifier that is applied to every certified module. It associates the module name and a module sequence number with the names of the associated application and product.

module sequence number. The module sequence number is a serial numeric identifier that specifies the major functional revision (enhancement) level, minor functional revision (update) level, and the number of documentation modifications since the last functional change to the module.

new development software (NDS). New development software is development software that is developed subsequent to acceptance of this SQAP and its implementing procedures.

observer CCB member. An observer CCB member is a nonvoting member appointed by the TPO to observe the operation of the CCB.

on-demand report. An on-demand report is a standard CSA report that is generated at the specific request of a principal investigator, project leader, the CCB, or a representative of the SCM Organization for distribution to a list of individuals and organizations specified when the request is made.

operational baseline. The operational baseline is a formal baseline that consists of an application's object- or executable code and all documentation required to utilize the application.

operation-based verification. Operation-based verification is a program of software verification that relies on the use of standard samples to verify correct operation of an instrumentation system and from which correct operation of the software subsystem can be inferred.

periodic report. A periodic report is a standard CSA report that is generated at regular intervals and distributed to a specific group of individuals and organizations.

permanent CCB member. A permanent CCB member is a voting member of the CCB appointed by the TPO for an unlimited term of service.

physical configuration audit. A physical configuration audit is a formal configuration audit performed by the SCM Organization to verify that the proposed baseline is complete and that its component modules accurately conform to their technical documentation.

pre-existing development software (PDS). Pre-existing development software is development software that was developed prior to acceptance of this SQAP and its implementing procedures.

preliminary-design baseline. The preliminary-design baseline is a formal baseline that is produced during the Design Phase of the software life-cycle. Its purpose is to document the functional design of the software at the product level.

primary data. Primary data is computational data that is not the output of a computer program or is not initially in interface-table format. Possible sources of primary data are notebooks, reports, or any software that does not produce interface tables (e.g. data acquisition systems).

primary product. A primary product is a product that implements one or more major requirements of a baseline.

processing interface table. A processing interface table is an input data-interface-table that contains the data that is to be transformed (processed) by the computer program.

product. A product is a collection of functionally related modules such as a computer program, reuse component, or computational data interface tables.

proposed baseline. A proposed baseline is a body of information that is submitted into the formal audit/review process.

pseudocode. Pseudocode is a standard, block structured program design language for describing procedural algorithms.

real-time software (RTS). Real-time software is software that is used to perform real-time data acquisition or to control instrumentation.

registered user. A registered user of a sanctioned application or computational data baseline is any individual for whom an approved Software/Data Dissemination Request is on file with the SCM Organization.

release. A release is a formal transfer of information from the SCM Organization to a user, a developer, or some other authorized entity. Four categories of release are supported: engineering release, assessment release, sanctioned release, and probation release.

release label. A release label is an alphanumeric identifier that uniquely identifies each formal release of a certified software or computational-data baseline.

requirements baseline. The requirements baseline is a formal baseline that is produced during the Requirements Phase of the software life-cycle. The purpose of the requirements baseline is to document the functional and performance requirements of the application and to describe external interfaces and design constraints.

reuse-component baseline. A reuse-component baseline is a formal baseline that encapsulates one or more functionally related subprograms (subroutines, functions, or procedures) as well as any associated documentation, computational data, or support software.

review. A review is a formal assessment activity that is performed to identify deficiencies that preclude the certification of a baseline or hinder the ongoing development task. Review business is conducted at a formal CCB meeting that includes representatives of the major Project disciplines including Project management, the development organization, and the SCM Organization.

Review/Audit Item Disposition. The Review/Audit Item Description is a supplemental-documentation form that is issued to document discrepancies or other issues that are identified during a formal audit or review.

Review/Audit Report & Recommendations. The Review/Audit Report & Recommendations is a supplemental-documentation form that is used to document the conclusions and recommendations of the reviewers (auditors) upon concluding a formal review (configuration audit).

Reviewer Qualifications Summary. The Reviewer Qualifications Summary is a supplemental-documentation form that is used to document the qualifications of a reviewer who is not a LANL YMP member.

review packet. A review packet is a compendium of all of the technical information required to assess a baseline at a particular stage of the life cycle.

rotating CCB member. A rotating CCB member is a voting member of the CCB appointed by the TPO for a limited term of service.

sanctioning. See **baseline sanctioning.**

scientific and engineering software (SES). Scientific and engineering software is software that contains a mathematical or numerical model of a physical process or configuration.

SCM Variance Authorization. The SCM Variance Authorization is a supplemental-documentation form that is issued by the CCB to authorize an exemption from the provisions of the LANL software quality assurance program.

Software Acceptance Review (SAR). The Software Acceptance Review is the baseline-closure review for the Implementation Baseline. It signals the end of the Implementation Phase of the software life-cycle. When the Software Acceptance Review has been conducted and all issues arising from the review have been resolved, the Implementation Phase is closed.

Software Assessment and Support Document. The Software Assessment and Support Document is evidential documentation that is provided to comply with the requirements of Section D of NUREG0856. It describes all work that was performed to ensure the functional adequacy and integrity of the software application.

Software Change Request. The Software Change Request is a supplemental-documentation form that is used to request an enhancement to a certified baseline or to request initiation of an entirely new development effort.

software class. Software class is a designation that is used to describe the size, complexity, intended use, and organizational role of a software application. The following software class designations are supported: Administrative Data Base Application (ADB), Auxiliary Software (AUX), Component-Model Software (CMS), Electronic Calculation (EC), Manifest Product Software (MP), Mathematical Support Software (MSS), Real-time Software (RTS), Scientific and Engineering Software (SES), Software Invocation (SI), Software-Support Tools (SST), and Technical Data Base Application (TDB).

software configuration management (SCM). Software configuration management is the discipline of identifying the configuration of a system at discrete points in time for the purposes of systematically controlling changes to this configuration and maintaining the integrity and traceability of this configuration throughout the life cycle.

software configuration management (SCM) organization. The SCM organization is the group that is responsible for the conduct of all SCM activities. It is administratively and technically responsible through the Software Configuration Manager to the Software Management Coordinator.

software configuration manager. The software configuration manager is responsible for the technical and administrative management of the SCM organization.

Software/Data Dissemination Request. The Software/Data Dissemination Request is a supplemental-documentation form that is used by a potential user to request transmittal of a copy of a LANL-YMP-sanctioned baseline.

Software/Data Review Notice. The Software/Data Review Notice is a supplemental-documentation form that is issued by the SCM Organization to announce the formal review of a software or computational-data baseline.

Software Design Document. The Software Design Document is a development document that describes the top-level design of a software application.

software heritage. The software heritage is a designation that specifies the previous development history of a software application. Two heritage designations are supported: acquired software and development software. Within the acquired software category, three subclasses are defined: system software (SS), acquired commercial software (ACS), and acquired noncommercial software (ANS). Within the development software category, two subclasses are defined: new development software (NDS) and pre-existing development software (PDS).

Software Incident Report. The Software Incident Report is a supplemental-documentation form that is used to report a discrepancy that has been discovered in a certified LANL YMP baseline.

software invocation (SI). A software invocation is software that contains a command sequence to start or control the operation of a program or small command file.

Software Requirements Review (SRR). The Software Requirements Review is the baseline-closure review for the Requirements Baseline. It signals the end of the Requirements Phase of the software life-cycle. When the Software Requirements Review has been conducted and all issues arising from the review have been resolved, the Requirements Phase is closed.

Software Requirements Specification. The Software Requirements Specification is a document that enumerates the functional and performance requirements of the application and describes external interfaces and design constraints.

software standards document. A document that specifies the coding and documentation standards that must be followed for a particular programming language.

software-support tools (SST). Software-support tools are software that are used to support the development, assessment for certification, or management of LANL YMP software.

source code documentation prolog. The source code documentation prolog is a programming-language-specific block of comment statements. It is included at the beginning of every source-code module and is the repository for most of the design documentation associated with the module.

Source Code Listings. The Source Code Listings document is an evidential documentation component that provides a compendium of listings of all of the source code that is delivered with the software application. The Source Code Listings document is provided to comply with the requirements of Section E(6) of NUREG-0856.

source-code module. A source-code module is the fundamental unit of controllable information associated with a computer program or reuse component.

Standard Continuation Form. The Standard Continuation Form is a supplemental-documentation form that is used to continue the text provided on any other supplemental-documentation form.

summary interface table. A summary interface table is an output data interface table that contains information that characterizes a particular execution of a certified software application. Included in this information is the name of the release label of the software application, software product name, starting and ending date/time for the run, names of all input files, and names of all output files. A summary interface table is generated automatically by a standard, certified LANL YMP reuse-component.

supplemental documentation forms. Supplemental documentation forms are standard forms that are used to document all significant events that occur within the scope of the LANL YMP software management effort.

support product. A support product is a product that is employed to aid in the development or testing of a primary product.

system software (SS). System software is acquired software that is closely associated with a commercially marketed computer system and is supplied by a commercial or noncommercial entity for distribution to a large installed user-base (at least 1000 users). System software includes operating systems and operating system utilities, compilers and interpreters, standard libraries, software drivers, and interface software for peripheral devices. In particular, all software for which documentation may be obtained from the Los Alamos Computing Information Center shall be considered system software.

technical contact. The technical contact for a software application is an individual familiar with the development, configuration, and operation of the software.

technical data base application (TDB). A technical data base application is a software application that is used to store, access, file, and manage collections of technical data.

temporary CCB member. A temporary CCB member is a nonvoting member of the CCB appointed to a restricted term of service by the TPO or Software Configuration Manager. Temporary members are employed to supplement the CCB's technical expertise in support of formal reviews.

Test Results. The Test Results document is development documentation that contains a record of the execution of the V&V procedures. As such it constitutes the primary record of the software testing activity.

universal interface table. A universal interface table is a data interface table that has been approved by the CCB and certified by SCM as part of a computational-data baseline.

users documentation. Users documentation is the information that a user of a particular application requires to successfully apply the application to the solution of a problem. Typical user's documentation modules are the User's Manual, Models and Methods Summary, and the Version Description Document. Users documentation is *never* incorporated into source code modules.

Users Manual. The Users Manual is a document that provides a user of a software application with information necessary to install and run the application. As such the Users Manual is one of the principal components of user documentation. The Users Manual is also evidential documentation that must be supplied to U. S. Nuclear Regulatory Commission to meet the requirements of Section C of NUREG-0856.

V&V Plan and Procedures. The V&V Plan and Procedures is development documentation that encapsulates the V&V plan and the V&V procedures.

V&V-plan baseline. The V&V-plan baseline is a formal baseline that is produced during the Design Phase of the software life-cycle. Its purpose is to provide preliminary documentation of the strategy for verifying and validating the application.

V&V-procedures baseline. The V&V-procedures baseline is a formal baseline that is produced during the Implementation Phase of the software life-cycle. Its purpose is to provide documentation of the V&V Plan at an advanced stage of development and to establish that the V&V Procedures are an accurate implementation thereof.

V&V Report The V&V Report is a document that presents a critical analysis of the Test Results with respect to the expected results specified in the V&V Plan. The V&V Report is development documentation.

validation. See **model validation** and **validation of computational data.**

validation of computational data. Validation of computational data is a process for establishing the domain in which a data set is to be used and achieving an adequate level of confidence in the veracity of the data within that domain. Validation of computational data requires a subjective analysis of the assumptions and limitations that apply to the data and an evaluation of its domain, applicability, and veracity.

verification. See **verification of computational data** and **verification of software.**

verification of computational data. Verification of computational data is a process for establishing that the information upon which a data set is based is appropriate.

verification of software. Verification of software is a process for demonstrating that (1) the requirements specified for the software are accurately and completely reflected in the emerging software system and (2) that the performance and operation of the system is correct and consistent with these requirements.

Version Description Document. The Version Description Document is a document that describes the content and capabilities of each delivered version of the system. As such, it is a primary users documentation component. The Version Description Document is also evidential documentation that shall be supplied to the U. S. Nuclear Regulatory Commission (upon request) to meet requirements specified in Section E of NUREG-0856.

APPENDIX D. ACRONYM GLOSSARY

ACS - Acquired Commercial Software
ADB - Administrative Data Base Application
ANS - Acquired Noncommercial Software
ANSI - American National Standards Institute
AUX - Auxiliary Software
BCN - Baseline Certification Notice
BSS - Baseline Submission Summary
CCB - Configuration Control Board
CDR - Critical Design Review
CFS - Common File System
CIC - Computing Information Center
CIR - CSA Information Request
CMA - CCB Meeting Announcement
CMM - CCB Meeting Minutes
CMS - Component-Model Software
CPL - Computer Program Library
CPN - CCB Participation Notice
CSA - Configuration Status Accounting
CTR - CPL Transmittal Request
DS - Development Software
DSD - Data Set Description
DVR - Data Verification and Validation Review
EC - Electronic Calculation
ECD - Engineering Change Directive
ECN - Engineering Change Notice
FCA - Functional Configuration Audit
ICN - Integrated Computing Network
IEEE - Institute of Electrical and Electronics Engineers
LANL - Los Alamos National Laboratory
LCS - Life Cycle Specification
MMS - Models and Methods Summary
MP - Manifest Product Software
MSS - Mathematical Support Software
NDS - New Development Software

NESC	-	National Energy Software Center
NNWSI	-	Nevada Nuclear Waste Storage Investigations
NRC	-	Nuclear Regulatory Commission
PCA	-	Physical Configuration Audit
PDL	-	Program Design Language
PDR	-	Preliminary Design Review
PDS	-	Pre-existing Development Software
QA	-	Quality Assurance
QAPL	-	Quality Assurance Project Leader
QP	-	Quality Administrative Procedure
RID	-	Review/Audit Item Description
RPC	-	Records Processing Center
RQS	-	Reviewer Qualifications Summary
RRR	-	Review/Audit Report and Recommendations
RTS	-	Real-Time Software
SAD	-	Software Assessment and Support Document
SAR	-	Software Acceptance Review
SDDR	-	Software/Data Dissemination Request
SCF	-	Standard Continuation Form
SCL	-	Source-Code Listings
SCM	-	Software Configuration Management
SCR	-	Software Change Request
SDD	-	Software Design Document
SES	-	Scientific and Engineering Software
SI	-	Software Innovations
SIR	-	Software Incident Report
SQA	-	Software Quality Assurance
SQAP	-	Software Quality Assurance Plan
SRN	-	Software Review Notice
SRR	-	Software Requirements Review
SRS	-	Software Requirements Specification
SS	-	System Software
SST	-	Software-Support Tools
SVA	-	SCM Variance Authorization
TDB	-	Technical Data Base application
TPO	-	Technical Project Officer
TR	-	Test Results
TWS	-	Terminal Waste Storage

UM	- Users Manual
VDD	- Version Description Document
VVP	- V&V Plan and Procedures
VVR	- V&V Report
V&V	- Verification and Validation
YMP	- Yucca Mountain Project

REVIEWS OF SOFTWARE AND COMPUTATIONAL DATA

Effective Date: ____________________

______________________________	____________________
D. R. Hines Preparer	Date
______________________________	____________________
S. L. Bolivar Quality Assurance Project Leader	Date
______________________________	____________________
R. J. Herbst Technical Project Officer	Date

REVIEWS OF SOFTWARE AND COMPUTATIONAL DATA

1.0 PURPOSE

This document describes procedures for all formal reviews of software and computational data that take place under the auspices of the Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP).

2.0 SCOPE

This procedure applies to LANL YMP software or computational data baselines that are used to support licensing. This procedure does not apply to unofficial internal reviews conducted by the development organization.

3.0 REFERENCES

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

QARD *Quality Assurance Requirements Document for the Civilian Radioactiv: Waste Management Program,* U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

The Software Development Project, Planning and Management. Phillip Bruce and Sam M. Pederson, John Wiley and Sons, 1982.

TWS-QAS-QP-03.19 *Documentation of Software and Computational Data.*

TWS-QAS-QP-03.20 *Software Configuration Management.*

4.0 DEFINITIONS

See LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project,* Appendixes C and D, respectively for a glossary of terms and list of acronyms used throughout this document.

5.0 RESPONSIBILITIES

5.1 Developer

The responsibilities of the development organization under this procedure are
- Prepare the software or data baseline
- Complete the File Transfer Block of the Baseline Submission Summary
- Submit the software or data baseline and the Baseline Submission Summary to the SCM Organization to initiate the formal audit/review process
- Resolve all issues that arise during any audits and reviews

5.2 Software Configuration Management (SCM) Organization

The responsibilities of the SCM Organization under this procedure are
- Conduct the SCM audits

- Maintain the proposed baseline in the LANL YMP Certification Environment while the baseline undergoes formal review
- Conduct any official business delegated to it by the CCB

5.3 Configuration Control Board (CCB)

The responsibilities of the CCB under this procedure are

- Provide the forum for all formal YMP baseline reviews
- Approve, approve conditionally, or reject any proposed baseline

6.0 PROCEDURE

The following sections describe the general procedures for any formal review of software or computational data. The overall procedure is summarized in the flowchart of Appendix A.

6.1 Procedure for the Developer

6.1.1 Baseline Preparation

Prepare the baseline (as described in TWS-QAS-QP-3.19, *Documentation of Software and Computational Data*), ensuring that all components specified for the baseline are present and complete.

6.1.2 Preparation of Baseline Submission Summary

Prepare the Baseline Submission Summary as follows:

- General Information. Fill in the date, title, LCS reference, and the originator's name, telephone number, organization, and mail stop.
- Baseline. Check the appropriate box to indicate the baseline to be reviewed.
- Review Type. Check the appropriate box to indicate review type, i.e., in-process review or baseline closure review.
- Development Effort. Give an estimate (in person-days) of time expended in the development effort to bring the proposed baseline to the point of submission.
- File Transmittal Block. Complete the File Transmittal Block. Completion of this section provides the SCM Organization with information necessary to transmit the proposed baseline to the Certification Environment. For additional information on completing the File Transmittal Block, refer to TWS-QAS-QP-03.20, *Software Configuration Management*, Section 6.2.9.1.1.
- Sign and date the form.

6.1.3 Submission of Proposed Baseline

Submit the Baseline Submission Summary to the SCM Organization. If network access is impractical or impossible, submit the proposed baseline on magnetic or optical media. Await the outcome of the SCM audits.

6.1.4 Resolution of SCM Audit Issues

Resolve any issues identified during the SCM audits and resume the process at Step 6.1.1 or proceed to Step 6.1.5 if no audit issues were identified.

6.1.5 Formal Review

Await notification of review time and place. Attend the formal review of the proposed baseline to provide technical support and defense of the baseline.

6.1.6 Resolution of Review Issues

If review issues were identified, resolve the issues specified on the Review/Audit Item Disposition forms and the Review/Audit Report and Recommendation form to the satisfaction of the Change Control Authority. Resume the process at an entry point specified by the Change Control Authority.

6.2 Procedure for the SCM Organization

6.2.1 Receipt of Proposed Baseline

Upon receipt of the Baseline Submission Summary from the developer, transfer the proposed baseline to the LANL YMP Certification Environment and log the Baseline Submission Summary into the Configuration Status Accounting (CSA) database.

6.2.2 SCM Audits

Perform the SCM audits (refer to TWS-QAS-QP-3.20, *Software Configuration Management*, for details of the SCM auditing procedure). Record audit issues on Review/Audit Item Disposition forms, and summarize the audits on a Review/Audit Report and Recommendations form. Refer to Sections 6.5.1 and 6.5.3 for the procedure for completing these forms.

If no audit issues are identified, in the "Disposition" section of the Baseline Submission Summary, check "Accepted", sign and date the form, and proceed to Step 6.2.3.

If audit issues are identified, perform the following actions and await resumption of the process at Step 6.2.1.

- In the "Disposition" section of the Baseline Submission Summary, check "Not Accepted", supply an explanation under "SCM/CCB Comments", and sign and date the form and return a copy to the submitter.
- Return copies of all Review/Audit Item Disposition forms and the Review/Audit Report and Recommendations form to the submitter for resolution.
- Remove the proposed baseline from the LANL YMP Certification Environment.

6.2.3 Identification of Review Participants

Identify any temporary CCB members that will participate in the formal review. For such members, initiate the CCB Participation Notice and the Reviewer Qualifications Summary according to the provisions of TWS-QAS-QP-3.20, *Software Configuration Management*.

Establish CCB membership for the developer. If the developer is not already a CCB member, issue the necessary CCB Participation Notice form to accomplish this.

Permanent and rotating CCB members are automatically qualified participants in all formal reviews.

6.2.4 Review Scheduling

Schedule the formal review and prepare a Software/Data Review Notice (to be distributed with the review packets) as follows:

- General Information. Fill in the date, BSS reference, name of the application, and the Software Review Notice identification number.
- Review Of. Check the appropriate box to indicate the baseline to be reviewed.
- Review Type. Check the appropriate box to indicate review type, i.e., in-process review or baseline-closure review.
- Review Date, Review Time, Review Location. Furnish the review date, time, and location.
- Participants. Supply the names of all review participants.
- Comments. Supply any additional comments as necessary to clarify or qualify the information already supplied.
- Sign and date the form.

6.2.5 Preparation and Distribution of Review Packets

Prepare one review packet for each review participant and distribute the packets and the Software Review Notice.

6.2.6 Baseline Review

Participate in the formal review of the proposed baseline through permanent and rotating CCB members.

6.2.7 Review Issues

If review issues are identified, deliver the completed Review/Audit Item Disposition and the Review/Audit Report and Recommendations form to the submitter for issue resolution. Await resumption of the process at Step 6.2.1.

6.3 Procedure for Reviewers

All persons that have received the Software/Data Review Notice and the review packet for a proposed baseline should participate in the CCB meeting at which the proposed baseline is reviewed.

6.3.1 Baseline Assessment

Upon receipt of the review packet for a proposed baseline, assess the proposed baseline prior to conduct of the formal review with respect to the issues specified in Sections 6.1 and 6.2 of *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

6.3.2 Documentation of Review Issues

During evaluation of the baseline prior to the review, annotate the review packet documents with issues to be discussed at the formal review.

6.3.3 Review Participation

Participate in the formal review, wherein the issues identified by each reviewer are presented and discussed.

6.4 Procedure for the CCB Chair

6.4.1 Review-Issue Documentation

At the beginning of the review, designate a permanent or rotating member of the CCB to record review issues on Review/Audit Item Disposition forms and to compose the Review/Audit Report and Recommendations form.

6.4.2 Review Moderator

Moderate the discussion of the reviewers as follows:

- Maintain emphasis on identification of problems. Discourage extended discussions of potential solutions.
- Ensure that the review progresses through the baseline documentation in an orderly fashion.
- Ensure that all items and issues identified by the reviewers are addressed during the meeting.

6.5 Procedure for the CCB

6.5.1 Assessment of Review Issues

Assess and discuss issues raised by the reviewers and decide which issues have merit. Document those issues that are judged to have merit on Review/ Audit Item Disposition forms. Prepare each form as follows:

- General Information. Fill in the date and the name of the application.
- Review/Audit. Indicate the baseline being reviewed and the review type (example: "In-process review of the Detailed Design Baseline").
- RRR Reference. Enter the number of the Review/Audit Report and Recommendation form that summarizes the collection of Review/Audit Item Disposition forms.
- Module. Enter the name of the module referenced by the form.
- Issuing Organization Write "CCB" (or "SCM" if the form is the result of an SCM audit).
- Number of Errors. Enter the number of errors identified by this form.
- Classification. Indicate the type of error or issue addressed by the form.
- Issue Description & Comments. Describe the issue(s) addressed by the form.

6.5.2 Identification of the Change Control Authority

If review issues requiring resolution are identified, determine the Change Control Authority for issue resolution. The Change Control Authority is the person or persons who verify that all review issues have in fact been resolved or addressed. One person shall be designated "leader" of the Change Control Authority. Possible Change Control Authority designations include:

- The Software Configuration Manager
- One or more members of the SCM Organization
- One or more permanent or rotating members of the CCB
- A combination of SCM personnel and CCB members
- The CCB itself. In this case a subsequent formal review of the same material is scheduled.

6.5.3 Review Report and Recommendation

Summarize the review. Prepare a Review/Audit Report and Recommendations form as follows:

- General information. Fill in the date and the name of the application.
- Review/Audit. Indicate the baseline being reviewed and the review type (example: "In-process review of the Detailed Design Baseline").
- SRN Reference. Enter the number of the Software/Data Review Notice that initiated the review.
- BSS Reference. Enter the number of the associated Baseline Submission Summary.
- Issued By. Write "CCB" (or "SCM" if the form is the result of an SCM audit).
- Resubmission Deadline. If resubmission of the proposed baseline is required, determine a date for resubmission and enter the date.
- Total RID's. Enter the total number of Review/Audit Item Disposition forms resulting from the review or audit.
- Change Control Authority. If resubmission of the proposed baseline is required, enter the name of the person identified as the leader in Section 6.5.2.
- Review Summary. Provide a summary of the review, highlighting the major points and issues.
- Recommendations. Determine whether the proposed baseline is to be approved, approved conditionally, or if a complete rework is necessary. Check the appropriate box to indicate the decision. If either of the latter options is chosen, provide an explanation in the Review Summary.
- Resubmission Scope. Determine the scope of resubmission of the proposed baseline. Check the appropriate box to indicate the decision.
- Sign and date the form.

7.0 QUALITY ASSURANCE DOCUMENTATION

Execution of this procedure results in no formal Project QA records or records packages. However, as described in TWS-QAS-QP-03.20, *Software Configuration Management*, after certification, the corresponding baselines and supplemental-documentation are incorporated into records packages by the SCM Organization. The supplemental documentation forms that are included into these records packages are listed in Section 9.0.

8.0 ACCEPTANCE CRITERIA

LANL YMP software and data baselines are considered to have met acceptance criteria when reviewed and approved by the CCB.

9.0 ATTACHMENTS

Exhibit 1: Baseline Submission Summary

Exhibit 2: Review/Audit Item Disposition

Exhibit 3: Review/Audit Report and Recommendations

Exhibit 4: Software/Data Review Notice

Appendix A: Flow Chart

BASELINE SUBMISSION SUMMARY

DATE	TITLE			BSS-
LCS REFERENCE	ORIGINATOR	TELEPHONE	ORGANIZATION	MAIL STOP

BASELINE

- ☐ REQUIREMENTS
- ☐ PRELIMINARY DESIGN
- ☐ V & V PLAN
- ☐ DETAILED DESIGN
- ☐ V & V PROCEDURES
- ☐ IMPLEMENTATION
- ☐ COMPUTATIONAL DATA

REVIEW TYPE

- ☐ IN-PROCESS
- ☐ BASELINE CLOSURE

DEVELOPMENT EFFORT (PERSON-DAYS) ________

FILE TRANSMITTAL BLOCK

CONTACT	PHONE	MAIL STOP
HARDWARE PLATFORM	OPERATING SYSTEM	
FILE FORMAT (ASCII, TAR, CPIO, VMS BACKUP, ETC.)		

METHOD OF DISTRIBUTION

☐ TAPE
TAPE TYPE ________
DENSITY ________
LABEL ________
FILE NAME ________

☐ DISK
DISK TYPE ________
DENSITY ________
FORMAT ________
FILE NAME ________

☐ NETWORK FILE TRANSFER
☐ CFS
☐ FTP NODE ________
☐ DECNET
FULL PATHNAME ________

SCM DISPOSITION	SCM/CCB COMMENTS
☐ ACCEPTED ☐ NOT ACCEPTED	SCF-

LOS ALAMOS
Yucca Mountain Project

________ ORIGINATOR (SUBMISSION) ________ DATE

________ SCM REPRESENTATIVE (DISPOSITION) ________ DATE

REVIEW/AUDIT ITEM DISPOSITION

DATE	APPLICATION NAME	REVIEW/AUDIT	RID-
RRR REFERENCE	MODULE	ISSUING ORGANIZATION	NUMBER OF ERRORS

CLASSIFICATION

- ☐ CODING STANDARDS
- ☐ REQUIREMENTS TRACEABILITY
- ☐ DATA REFERENCE
- ☐ CONTROL-FLOW
- ☐ INSUFFICIENT INFORMATION
- ☐ VERIFICATION
- ☐ DATA DECLARATION
- ☐ INTERFACE
- ☐ MISSING COMPONENT
- ☐ VALIDATION
- ☐ COMPUTATION
- ☐ INPUT/OUTPUT
- ☐ EDITORIAL
- ☐ MODELS & METHODS
- ☐ COMPARISON
- ☒ OTHER (EXPLAIN BELOW)

ISSUE DESCRIPTION & COMMENTS

SCF-

ISSUE RESOLUTION

SCF-

LOS ALAMOS
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DEVELOPER (RESOLVED) DATE

CHANGE CONTROL AUTHORITY (VERIFIED) DATE

REVIEW/AUDIT REPORT & RECOMMENDATIONS

DATE	APPLICATION NAME	REVIEW/AUDIT	RRR-

SRN REFERENCE	BSS REFERENCE	ISSUED BY	RESUBMISSION DEADLINE	TOTAL RID'S

CHANGE CONTROL AUTHORITY

REVIEW SUMMARY

SCF-

RECOMMENDATIONS	RESUBMISSION
☐ APPROVED	☐ NONE REQUIRED
☐ APPROVED CONDITIONALLY	☐ PARTIAL RESUBMISSION
☐ REWORK	☐ FULL RESUBMISSION

LOS ALAMOS
Yucca Mountain Project

SCM/CCB REPRESENTATIVE (ISSUED) DATE

CHANGE CONTROL AUTHORITY (CLOSED) DATE

SOFTWARE/DATA REVIEW NOTICE

DATE	BSS REFERENCE	APPLICATION NAME	SRN-

REVIEW OF

- ☐ REQUIREMENTS
- ☐ DETAILED DESIGN
- ☐ COMPUTATIONAL DATA
- ☐ PRELIMINARY DESIGN
- ☐ V & V PROCEDURES
- ☐ V & V PLAN
- ☐ IMPLEMENTATION

REVIEW TYPE

- ☐ IN-PROCESS
- ☐ BASELINE CLOSURE

REVIEW DATE	REVIEW TIME	REVIEW LOCATION

PARTICIPANTS

SCF-

COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

SCM REPRESENTATIVE

DATE

APPENDIX A
Flow Chart

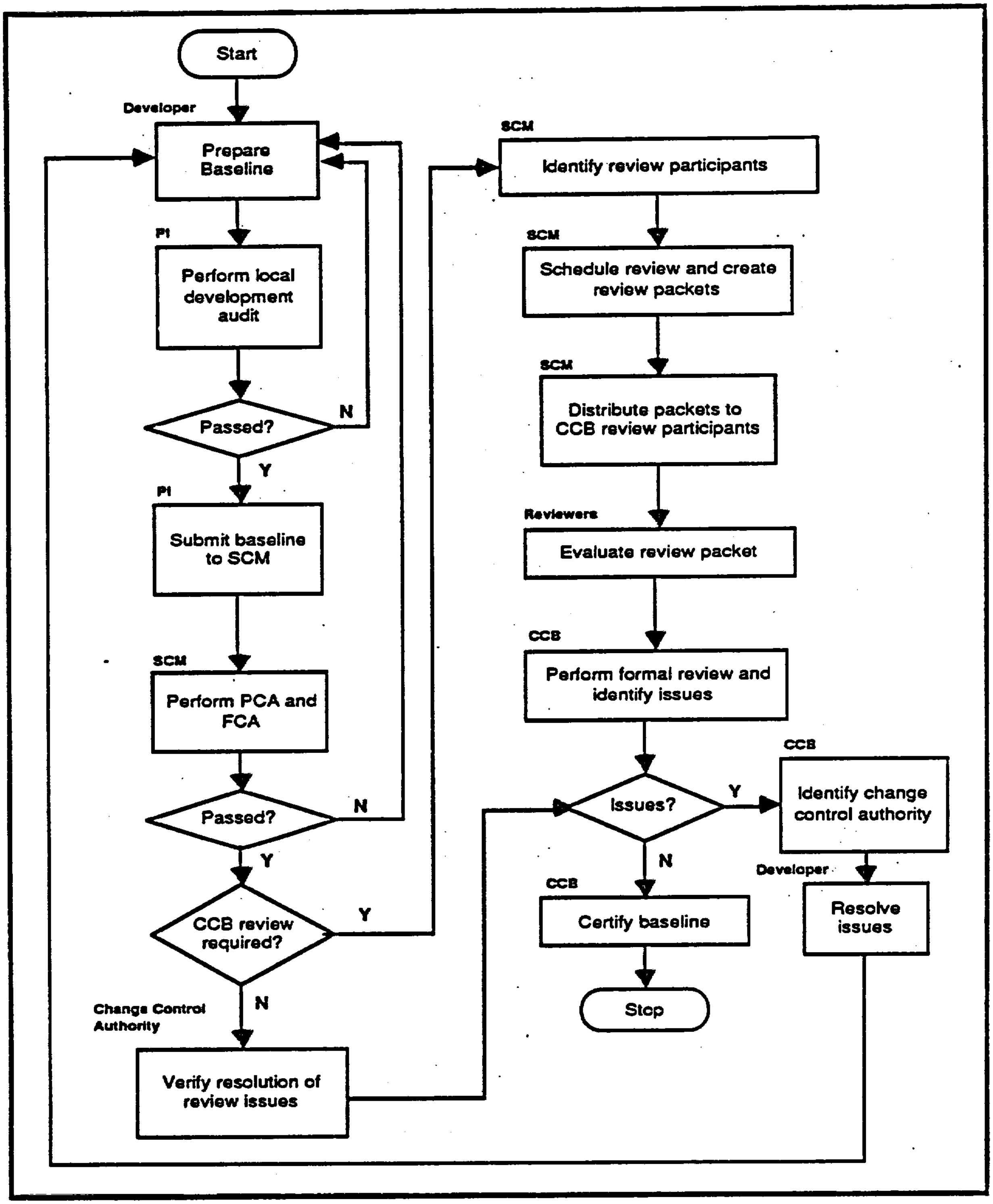

Figure 1. Review Process

CREATION, MANAGEMENT, AND USE OF COMPUTATIONAL DATA

Effective Date: ____________________

____
G. Cort
Preparer

____
Date

____
S. L. Bolivar
Quality Assurance Project Leader

____
Date

____
R. J. Herbst
Technical Project Officer

____
Date

CREATION, MANAGEMENT, AND USE OF COMPUTATIONAL DATA

1.0 PURPOSE

This quality administrative procedure (QP) establishes requirements to ensure quality in the formatting, heritage, maintenance, and dissemination of computational data for the portion of the Yucca Mountain Project (YMP) being conducted at Los Alamos National Laboratory (LANL).

2.0 SCOPE

This QP applies to data generated by or provided as input to computer programs used to support licensing and to all such data that is incorporated into computational data baselines.

3.0 REFERENCES

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

QARD *Quality Assurance Requirements Document for the Civilian Radioactive Waste Management Program*, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

TWS-QAS-QP-03.19 *Documentation of Software and Computational Data.*

TWS-QAS-QP-03.20 *Software Configuration Management.*

TWS-QAS-QP-03.21 *Software Life Cycle.*

TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data.*

4.0 DEFINITIONS

See LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project*, Appendixes C and D, respectively for a glossary of terms and list of acronyms used throughout this document.

5.0 RESPONSIBILITIES

Specific responsibilities of the Software Developer, Code User, and Software Configuration Management organization are outlined in Section 6.0. General responsibilities are listed below.

5.1 Software Developer

The Software Developer assumes responsibility for ensuring that the software for which he/she is responsible utilizes the standardized input/output (I/O) procedures specified by this QP.

5.2 Code User

The Code User assumes responsibility for ensuring that the required documentation procedures are adhered to both in the transfer of data from the data archive to the user's local computer system and in the submission of new data for certification and archiving in the data archive.

5.3 SCM Organization

The SCM Organization ensures that all data submitted for storage in the Computer Program Library (CPL) is checked for quality and is safely and securely stored and protected against loss or damage. The SCM Organization also administers the data archive.

6.0 PROCEDURE

6.1 Creation of Computational Data in Interface-Table Format

6.1.1 Procedure for the Software Developer

Incorporate the data-configuration-setup software, interface-table reader, and the interface-table writer reuse components into the software under development.

6.1.2 Procedure for the Code User

6.1.2.1 Primary Data

Primary data is computational data that is not the output of a computer program or is not initially in interface-table format. Possible sources of primary data are notebooks, reports, or any software that does not produce interface tables (e.g. data-acquisition systems).

Transcribe the primary data into an interface table. This may be done by interactively creating the interface table using a text editor or by processing the primary data with auxiliary software that creates the interface table.

6.1.2.2 Derived Data

Derived data is any computational data that is output by a computer program into interface-table format. Ensure that the interface table that is the destination for the derived data is accurately specified in the program's configuration interface table. Execute the program with all required input.

6.2 Computational Data Baselines

6.2.1 Procedure for the Producer of the Data

6.2.1.1 Preparation of Computational Data Baselines

Refer to TWS-QAS-QP-03.19, *Documentation of Software and Computational Data,* for directions regarding the preparation of computational data baselines.

6.2.1.2 Verification and Validation of Computational Data

Perform verification and validation of computational data in accordance with the provisions of TWS-QAS-QP-03.22, *Verification and Validation of Software and Computational Data.*

6.2.1.3 Submission of Computational Data Baselines.

Submit a computational data baseline for formal review and certification in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.2.2 Procedure for the CCB

6.2.2.1 Assessment of Computational Data Baselines

Refer to TWS-QAS-QP-03.17, *Reviews of Software and Computational Data,* for directions regarding the formal review of computational data baselines.

6.2.3 Procedure for the SCM Organization

6.2.3.1 Certification and Sanctioning of Computational Data Baselines

Certify and sanction a computational data baseline according to the provisions of TWS-QAS-QP-03.20, *Software Configuration Management.*

6.3 Management of Computational Data

6.3.1 Control of Computational Data Baselines

6.3.1.1 Procedure for the SCM Organization

Archive each certified computational data baseline in the CPL in accordance with the provisions of TWS-QAS-QP-03.20, *Software Configuration Management.*

6.3.2 Distribution of Certified Data

6.3.2.1 Procedure for the SCM Organization

Perform the following steps to make certified computational data available to users.

6.3.2.1.1 Update the Data Archive. Deposit the output interface-tables and the associated Data Set Description document of each certified computational data baseline in the LANL YMP Computational Data Archive.

6.3.2.1.2 Update the Data Archive Catalog. Place an entry in the data archive catalog for the certified computational data baseline. Ensure read-only access to the catalog for any user with network access to the host computer.

6.3.2.1.3 Interface with Users. Service requests for certified data made on Software/Data Dissemination Requests submitted by prospective users of the data. Refer to Section 6.2.9 of TWS-QAS-QP-03.20, *Software Configuration Management*, for additional information on processing Software/Data Dissemination Requests.

6.3.2.1.4 Interface with Project Databases. Provide copies of certified data-baselines to the Site and Engineering Properties Database and/or to the Reference Information Base as appropriate. However, do not transfer the contents of any certified data baseline that was generated by software for which unresolved V&V issues are outstanding. The interface tables of such data sets can be distinguished by an asterisk (*) as the last character in the release id of the generating software.

6.4 Use of Computational Data

6.4.1 Procedure for Prospective Users

6.4.1.1 Obtaining the Data

Obtain the data in accordance with the procedures of Section 6.2.9.1 of TWS-QAS-QP-03.20 *Software Configuration Management*.

6.4.1.2 Configuration Interface-Table

Modify the configuration interface-table of the computer program to which the certified data is to be supplied as input. Ensure that the appropriate entries in the configuration interface-table reference the subject certified interface-tables. Execute the computer program.

7.0 QUALITY ASSURANCE DOCUMENTATION

Execution of this procedure produces no formal Project QA records or records packages. However, after certification of the proposed computational data baseline, the attendant interface tables and documents (see TWS-QAS-QP-03.19, *Documentation of Software and Computational Data*, Section 7.7) are incorporated by the SCM Organization into the baseline's certified-baseline-records-package as described in Section 7.2.1 of TWS-QAS-QP-03.20, *Software Configuration Management*.

8.0 ACCEPTANCE CRITERIA

Acceptance criteria for computational data baselines are specified in TWS-QAS-QF-03:19, *Documentation of Software and Computational Data*, and TWS-QAS-QP-03.17, *Reviews of Software and Computational Data*.

9.0 ATTACHMENTS

N/A

DOCUMENTATION OF SOFTWARE AND COMPUTATIONAL DATA

Effective Date: ____________________

G. Cort **Preparer**	**Date**
S. L. Bolivar **Quality Assurance Project Leader**	**Date**
R. J. Herbst **Technical Project Officer**	**Date**

DOCUMENTATION OF SOFTWARE AND COMPUTATIONAL DATA

1.0 PURPOSE

This quality administrative procedure (QP) describes the procedures for documenting the process and products of all Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP) software- and computational-data-development activities. Furthermore, it provides detailed descriptions of the components of all LANL YMP software and computational-data baselines that are generated at each stage of the development process.

2.0 SCOPE

This procedure applies to all software- and computational-data baselines used to support licensing.

3.0 REFERENCES

ANSI/IEEE Std 829-1983, *IEEE Standard for Software Test Documentation,* August 1983.

ANSI/IEEE Std 830-1984, *IEEE Guide To Software Requirements Specifications,* July 1984.

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

NUREG-0856 *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management,* June 1983.

TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

TWS-QAS-QP-03.18 *Creation, Management, and Use of Computational Data.*

TWS-QAS-QP-03.20 *Software Configuration Management.*

TWS-QAS-QP-03.21 *Software Life Cycle.*

4.0 DEFINITIONS

See LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project,* Appendixes C and D, respectively, for a glossary of terms and list of acronyms used throughout this document.

5.0 RESPONSIBILITIES

5.1 Software Developer

Any individual or group of individuals who develop software for the LANL YMP are charged with the following documentation responsibilities as specified by the Configuration Control Board:

- Prepare a requirements baseline
- Prepare a preliminary design baseline
- Prepare a verification and validation (V&V) plan baseline
- Prepare a detailed design baseline
- Prepare a V&V procedures baseline

- Prepare the implementation baseline.

5.2 Software User

The responsibilities under this QP of the software user are as follows:

- Prepare computational data baselines.

5.3 Software Configuration Management (SCM) Organization

The responsibilities of the SCM organization under this QP are

- Prepare and distribute sanctioned software
- Distribute computational data baseline
- Furnish a unique identifying number for supplemental documentation forms.

5.4 Originator of Supplemental Documentation Form

The responsibilities under this QP of the originator of any supplemental documentation form are

- Prepare all supplemental documentation forms in accordance with the directions of Section 6.2.

6.0 PROCEDURE

6.1 Baseline Preparation

6.1.1 Requirements Baseline

6.1.1.1 Procedure for Developer

Prepare a proposed requirements baseline as follows:

6.1.1.1.1 Authorization. To determine whether work on a proposed requirements baseline is authorized, perform the following steps.

- Refer to the Life Cycle Specification for the development task to determine whether a requirements baseline is specified. If it is not specified, a requirements baseline is not developed. Proceed to Step 6.1.2.1.
- If a requirements baseline is specified, confirm that the Requirements Phase is open. Confirmation may be obtained from the Software Configuration Manager. If the Requirements Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle.

6.1.1.1.2 Preparation of Baseline Components. The components of a Requirements Baseline always consist of a file list and the Software Requirements Specification document. Prepare these modules as follows:

- Ensure that there is an entry for the Software Requirements Specification in the file list. If no file list exists, create the file list. Otherwise, update the existing file list.
- Prepare the Software Requirements Specification according to the provisions of Appendix H.

6.1.1.1.3 Submission of Proposed Requirements Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.2 Preliminary Design Baseline

6.1.2.1 Procedure for Developer

Prepare a proposed preliminary design baseline as follows:

6.1.2.1.1 Authorization. To determine whether work on a proposed preliminary design baseline is authorized, perform the following steps.

- Refer to the Life Cycle Specification for the development task to determine whether a preliminary design baseline is specified. If it is not specified, a preliminary design baseline is not developed. Proceed to Step 6.1.3.1.
- If a preliminary design baseline is specified, confirm that the Design Phase is open. Confirmation may be obtained from the Software Configuration Manager. If the Design Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle.

6.1.2.1.2 Preparation of Baseline Components. Prepare the modules that compose a proposed preliminary design baseline as follows:

- If the Life Cycle Specification for the development task specifies a Software Design Document as a baseline component, prepare the Software Design Document to comply with the provisions of Appendix G.
- Create primary source-code modules for the top-level and executive routines of each of the application's products. Include a source-code documentation-prolog in each. Appendix A describes the functional organization of the source-code documentation-prolog.
- Complete the following sections of the prolog for each top-level primary source-code module:
  - Purpose
  - Revision History
  - Functional Description
  - Assumptions and Limitations
  - Special Comments
  - Requirements Traceability
  - References
- Create a file list that summarizes the components of the proposed baseline.

6.1.2.1.3 Submission of Proposed Preliminary Design Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.3 V&V Plan Baseline

6.1.3.1 Procedure for Developer

Prepare a proposed V&V plan baseline as follows:

6.1.3.1.1 Authorization. To determine whether work on a proposed V&V plan baseline is authorized, perform the following steps.

- Refer to the Life Cycle Specification for the development task to determine whether a V&V plan baseline is specified. If it is not specified, a V&V plan baseline is not developed. Proceed to Step 6.1.4.1.
- If a V&V plan baseline is specified, confirm that the Design Phase is open. Confirmation may be obtained from the Software Configuration Manager. If the Design Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle.

6.1.3.1.2 Preparation of Baseline Components. Prepare the modules that compose a proposed V&V plan baseline as follows:

- Prepare the V&V plan portion of the V&V Plan and Procedures document. This document is described in detail in Appendix L. Prepare Sections 1.0 - 4.0 of the V&V Plan and Procedures as independent text-documents, as in-line documentation to the testing software, or as a combination of each as appropriate to the development task. Prepare the portions of the V&V Plan and Procedures that describe the program of formal testing (Sections 4.1ff) within the documentation prologs of the source-code modules that implement the testing software.
- Update the file list to include the components of this baseline.

6.1.3.1.3 Submission of Proposed V&V Plan Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.4 Detailed Design Baseline

6.1.4.1 Procedure for Developer

Prepare a proposed detailed design baseline as follows:

6.1.4.1.1 Authorization. To determine whether work on a proposed detailed design baseline is authorized, perform the following steps.

- Refer to the Life Cycle Specification for the development task to determine whether a detailed design baseline is specified. If it is not specified, a detailed design baseline is not developed. Proceed to Step 6.1.5.1.
- If a detailed design baseline is specified, confirm that the Design Phase is open. Confirmation may be obtained from the or from the Software Configuration Manager. If the Design Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle.

6.1.4.1.2 Preparation of Baseline Components. Prepare the modules that compose a proposed detailed design baseline as follows:

- If a Software Design Document is specified for the development, prepare it to comply with the provisions of Appendix G.
- If a Models and Methods Summary is specified for the development, prepare it to comply with the provisions of Appendix D.
- If a V&V Plan and Procedures document is specified, prepare it in accordance with the directions of Step 6.1.3.1.2, above.
- Identify each routine associated with the application, and ensure that a primary source-code module (with embedded documentation prolog) exists for each. Complete all sections of each documentation prolog. If these modules already exist (e.g. as a result of a prior preliminary design phase), update the existing prologs. Otherwise, create new modules and complete their prologs. In particular, ensure that the Pseudocode section of each documentation prolog is completed to comply with the LANL YMP pseudocode standards described in Appendix B.
- Update the file list for the baseline to include any modules generated for this baseline.

6.1.4.1.3 Submission of Proposed Detailed Design Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.5 V&V Procedures Baseline

6.1.5.1 Procedure for Developer

Prepare a proposed V&V procedures baseline as follows:

6.1.5.1.1 Authorization. To determine whether work on a proposed V&V procedures baseline is authorized, perform the following steps.

- Refer to the Life Cycle Specification for the development task to determine whether a V&V procedures baseline is specified. If it is not specified, a V&V procedures baseline is not developed. Proceed to Step 6.1.6.1.
- If a V&V procedures baseline is specified, confirm that the Implementation Phase is open. Confirmation may be obtained from the Software Configuration Manager. If the Implementation Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle.

6.1.5.1.2 Preparation of Baseline Components. Prepare the modules that compose a proposed V&V procedures baseline as follows:

- Prepare the V&V Plan and Procedures document, which is described in detail in Appendix L. If no V&V plan baseline exists, compose the V&V plan in accordance with the directions of Step 6.1.3.1.2. Otherwise, update the existing V&V Plan and Procedures to reflect any new features of the V&V program.
- Produce the V&V procedures by developing source code that implements the testing program described in Sections 4.1ff of the V&V Plan and Procedures.
- Develop all test software necessary to support the testing effort, and document this software using standard source-code

documentation-prologs. Ensure that the support modules generated for this baseline are included in the file list.

6.1.5.1.3 Submission of Proposed V&V Procedures Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.6 Implementation Baseline

6.1.6.1 Procedure for Developer

Prepare a proposed implementation baseline as follows:

6.1.6.1.1 Authorization. Confirm that the Implementation Phase is open. Confirmation may be obtained from the Software Configuration Manager. If the Implementation Phase is not open, submit a Software Change Request or Software Incident Report to initiate a formal change processing cycle, and repeat the process.

6.1.6.1.2 Preparation of Baseline Components. Prepare the modules that compose a proposed implementation baseline as follows:

- Complete all primary source-code modules by developing code that corresponds to the pseudocode specified in the associated documentation prolog.
- If the V&V Plan and Procedures is specified for the development task, complete this document and any associated support modules as directed in Step 6.1.5.1.2.
- If the Test Results document is specified for the development task, generate it and incorporate it into the baseline. The Test Results document is described in Appendix I.
- If the Users Manual is specified for the development task, create it to comply with the provisions of Appendix J.
- If the Models and Methods Summary is specified for the development task, create it to comply with the provisions of Appendix D.
- If the Version Description Document is specified for the development task, complete Section 3.1, Release Notes. Do not complete any other sections of the Version Description Document.
- If the V&V Report is specified for the development task, create it to comply with the standards of Appendix M.

6.1.6.1.3 Submission of Proposed Implementation Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.7 Operational Baseline

6.1.7.1 Procedure for the SCM Organization

Prepare an operational baseline as follows:

6.1.7.1.1 Authorization. If a Baseline Certification Notice exists for an implementation baseline, proceed to Step 6.1.7.1.2 to generate a corresponding operational baseline.

6.1.7.1.2 Generation of an Operational Baseline. Generate an operational baseline as follows:

- Create binary code for the application's primary products. If the application is implemented in a Fourth Generation Language or other interpreted language, skip this step.

6.1.8 Computational Data Baseline

6.1.8.1 Procedure for Developer

Prepare a proposed computational data baseline as follows:

6.1.8.1.1 Preparation of Baseline Components. Prepare the modules that compose a proposed computational data baseline as follows:

- Produce all primary interface tables in accordance with the directions of TWS-QAS-QP-03.18, *Creation, Management, and Use of Computational Data.*
- Produce any testing and support modules necessary to verify and validate the computational data including V&V Plan and Procedures and Test Results. At a minimum, include a V&V Report for every proposed computational data baseline.
- Prepare the Data Set Description document for a proposed computational data baseline to comply with the provisions of Appendix C.
- Ensure that each interfaces table, software module, or high-level document associated with the computational data baseline is included in the baseline's file list.

6.1.8.1.2 Submission of Proposed Computational Data Baseline. Submit the proposed baseline for formal audit and review as specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.2 Preparation of Supplemental Documentation Forms

LANL YMP supplemental documentation consists of a suite of standard forms that are used to document all significant events that occur within the scope of the LANL YMP software-management effort. Table 1 contains summary descriptive information for each of these forms as well as a reference to the document (TWS-QAS-QP-0x.xx) in which the form is described.

6.2.1 General Instructions

6.2.1.1 Procedure for Preparer

Because the LANL YMP supplemental documentation forms share many common features, the following general procedures are executed by the preparer of any form. Specific instructions on the preparation and processing of particular forms are provided in the documents referenced in Table 1.

6.2.1.1.1 Obtaining the Form. Obtain a copy of the subject form from the SCM Organization.

6.2.1.1.2 Form Identification. The upper-right field of each Supplemental documentation form specifies a unique identifying number for the form. This field is reserved for the use of the SCM Organization.

6.2.1.1.3 General Information. Complete the general information specified in the fields located at the top of the form. This information includes date; name, address, organization, and phone for the preparer; and title or subject of the request.

6.2.1.1.4 Specific Information. Complete the form-specific information that composes the remainder of the form. See the QP referenced in Table 1 for detailed instructions.

6.2.1.1.5 References. Reference fields are provided to allow the preparer to identify a predecessor form that provides background information pertinent to the current request. Reference fields are generally located in the upper-left corner of the form, positioned below the Date field. The type of form that may be referenced through the reference field is specified in the field title.

6.2.1.1.6 Continuations. Special reference fields are provided in the lower-right corner of each narrative-text field of a form. These continuation fields specify the Standard Continuation Form upon which text from the narrative field is continued. If a narrative field is too small to hold all of the text that is intended for it, reference a Standard Continuation Form in the continuation field and complete the text on the corresponding Standard Continuation Form.

6.2.1.1.7 Signature. Sign the form in the block provided in the lower right.

6.2.1.2 Procedure for the SCM Organization

6.2.1.2.1 Assigning the Form Identifier. Assign a unique, serial numeric identifier to the form, and record the identifier in the field in the upper-right corner of the form.

6.2.2 Standard Continuation Form

6.2.2.1 Procedure for Preparer

The following sections provide instructions for completing the Standard Continuation Form.

6.2.2.1.1 Reference. In this field, specify the reference number of the form that is being continued.

6.2.2.1.2 Section of Form Continued. Specify the title of the section being continued. For example, "Review Summary" for the corresponding field of a Review/Audit Report & Recommendations.

6.2.2.1.3 Comments. Continue the text from the original form here.

7.0 QUALITY ASSURANCE DOCUMENTATION

Execution of this procedure produces no formal Project records or records packages. Rather, (as described in TWS-QAS-QP-03.20, *Software Configuration Management*) after certification by the SCM Organization, each baseline is incorporated into a certified-baseline records-package. The following sections describe the baseline components that are

Form	Title	Ref. x.xx	Originator	Links	Additional Signature(s)
BCN	Baseline Certification Notice	3.20	SCM	LCS	
BSS	Baseline Submission Summary	3.17	Developer	LCS	SCM
CIR	CSA Information Request	3.20	Manager		SCM/CCB
CMA	CCB Meeting Announcement	3.20	CCB		
CMM	CCB Meeting Minutes	3.20	CCB	CMA	
CPN	CCB Participation Notice	3.20	SCM	RQS	
CTR	CPL Transmittal Request	3.21	Developer SCM	SCR,SIR ECD	SCM
ECD	Engineering Change Directive	3.21	CCB	SCRs,SIRs	
ECN	Engineering Change Notice	3.20	CCB	BCN,ECD	
LCS	Life Cycle Specification	3.21	CCB	ECD	
RID	Review/Audit Item Disposition	3.17	CCB/SCM	RRR	Developer
RQS	Reviewer Qualifications Summary	3.20	Reviewer		SCM
RRR	Review/Audit Report and Recommendations	3.17	CCB/SCM	BSS SRN	
SCF	Standard Continuation Form	3.19	N/A		N/A
SCR	Software Change Request	3.21	Developer CCB/SCM		SCM CCB Analyst
SDDR	Software/Data Dissemination Request	3.20	External Participant		SCM
SIR	Software Incident Report	3.21	Developer CCB/SCM		SCM CCB Analyst
SRN	Software/Data Review Notice	3.17	SCM		
SVA	SCM Variance Authorization	3.20	SCM	ECD	CCB

Table 1. Characteristics of Supplemental Documentation Forms.

included in the certified-baseline records-package for each baseline. In addition to the components specified below, a summarizing file-list should accompany each baseline. Inclusion of any of these components into the subject baseline is contingent upon their specification on the associated Life Cycle Specification form.

7.1 Requirements Baseline.

The following components are included into the certified-baseline records-package for a requirements baseline.

- Software Requirements Specification

7.2 Preliminary Design Baseline

The following components are included into the certified-baseline records-package for a preliminary design baseline.

- Software Design Document
- Primary source-code modules

7.3 V&V Plan Baseline

The following components are included into the certified-baseline records-package for a V&V plan baseline.

- V&V Plan and Procedures

7.4 Detailed Design Baseline

The following components are included into the certified-baseline records-package for the Detailed Design Baseline.

- Software Design Document
- Models and Methods Summary
- V&V Plan and Procedures
- Primary source-code modules

7.5 V&V Procedures Baseline

The following components are included into the certified-baseline records-package for the V&V procedures baseline.

- Support source-code modules
- V&V Plan and Procedures

7.6 Implementation Baseline

The following components are included into the certified-baseline records-package for an implementation baseline.

- V&V Plan and Procedures
- Test Results
- V&V Report
- Primary source-code modules
- Support source-code modules
- Users Manual
- Models and Methods Summary
- Version Description Document

7.7 Computational Data Baseline

The following components (if they exist) are included into the certified-baseline records-package for a computational data baseline.

- Data Set Description
- V&V Plan and Procedures
- Test Results
- V&V Report
- Support source-code modules
- Primary interface-tables
- Input interface-tables
- Output interface-tables

8.0 ACCEPTANCE CRITERIA

Acceptance criteria for LANL YMP baselines are specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data Baselines.*

9.0 ATTACHMENTS AND APPENDIXES

Exhibit 1: Standard Continuation Form

Appendix A: Source-Code Documentation-Prolog

Appendix B: Pseudocode Language Description

Appendix C: Data Set Description (DSD)

Appendix D: Models and Methods Summary (MMS)

Appendix E: Software Assessment and Support Document (SAD)

Appendix F: Source-Code Listings (SCL)

Appendix G: Software Design Document (SDD)

Appendix H: Software Requirements Specification (SRS)

Appendix I: Test Results

Appendix J: Users Manual

Appendix K: Version Description Document (VDD)

Appendix L: V&V Plan and Procedures (VPP)

Appendix M: V&V Report (VVR)

ATTACHMENTS
Sample Supplemental Documentation Forms

STANDARD CONTINUATION FORM

DATE	ORIGINATOR	ORGANIZATION	TELEPHONE	SCF-
REFERENCE	SECTION OF FORM CONTINUED			MAIL STOP

COMMENTS

LOS ALAMOS
Yucca Mountain Project

SCF-

APPENDIX A. SOURCE-CODE DOCUMENTATION-PROLOG

The following sections specify a functional outline for the source-code documentation-prolog that is required at the beginning of every source code module. The prolog is implemented as in-line comments using the source-program-language's comment-syntax and semantics. For additional details, refer to the software standards document on source code programming and documentation standards for specific features for the subject programming language.

The following sections describe the contents of each major section of the documentation prolog.

1.0 PURPOSE

This section provides a brief statement of the purpose of the source code module. It should not contain design information and should not be longer than one paragraph.

2.0 REVISION HISTORY

This section contains a tabular summary of the revision history of the module. Each line of the revision history specifies the date, author, authorizing Engineering Change Directive (change reference), and a brief (one sentence) description of the work performed. The table is organized in reverse chronological order, with the description of the most recent revision at the top of the table.

3.0 INTERFACES

This section describes the module's external interfaces. It should be divided into subsections that specify

- Formal Calling-Parameters
- Interface Tables
- Scratch Files

Additional Interfaces subsections may be specified in the software standards document for the subject programming-language, as appropriate.

Each of the above subsections is organized into a table that specifies, at a minimum, the name of each interface; whether it provides input (I), output (O), or bidirectional (I/O) passage of information; and a brief description of the interface.

Within each subsection, the entries are organized alphabetically by interface name.

See TWS-QAS-QP-03.18, *Creation, Management, and Use of Computational Data,* for a description of interface tables.

4.0 GLOBAL OBJECTS

This section is used to describe any entities that are referenced by the module but are defined outside of the module's scope. It should be divided into subsections that specify, at a minimum

- Global Constants
- Global Type Definitions
- Global Variables
- Global Subprograms

Each of the above subsections is organized into a table that specifies, at a minimum, the name of each global entity and a brief description of its use. Within each subsection, the entries are organized alphabetically by name.

5.0 LOCAL OBJECTS

This section is used to describe any entities that are defined and referenced exclusively from within the module. It should be divided into subsections that specify, at a minimum

- Local Constants
- Local Type Definitions
- Local Variables
- Local Subprograms

Each of the above subsections is organized into a table that specifies, at a minimum, the name of each local entity and a brief description of its use. Within each subsection, the entries are organized alphabetically by name.

6.0 FUNCTIONAL DESCRIPTION

This section contains an intermediate-level, narrative description of the algorithm implemented by the module. It should be sufficiently detailed to communicate the overall functional processing performed by the module, but less detailed than the information provided in the Pseudocode section (see below).

7.0 ASSUMPTIONS AND LIMITATIONS

This section contains a list of any assumptions that constrain the design, implementation, performance, application, or use of the module. Known limitations such as processing restrictions, allowed ranges of input data, precision of results, and convergence criteria are also specified in this section.

8.0 SPECIAL COMMENTS

This section is used to document any special features of the module or its operating environment that are not appropriate for inclusion in one of the other sections of the prolog. The structure of special data objects may be included here, as may any other information that the author deems appropriate.

If a Models and Methods Summary is not required for the application under development, any major algorithmic equations shall be discussed in this section.

The format of this section is left to the discretion of the author.

9.0 REQUIREMENTS TRACEABILITY

This section provides a list of the specific requirements, or general classes of requirements that are satisfied by the module. It is organized into a table that specifies the requirement number and name as recorded in the SRS.

In the event that an SRS does not exist for the application of which the module is a component, this section may be omitted.

10.0 REFERENCES

If the module makes use of information (algorithm, data, etc.) that should be referenced, the source is cited in this section.

11.0 PSEUDOCODE

This section contains a detailed description of the algorithm(s) implemented by the module. This information is presented in a standard, block structured program description language (pseudocode).

The details of the LANL YMP pseudocode language are presented in Appendix B.

ATTACHMENTS
Supplemental Documentation Forms

APPENDIX B. PSEUDOCODE-LANGUAGE DESCRIPTION

The LANL YMP pseudocode-language provides a standard, block-structured program design language for describing procedural algorithms. Algorithm descriptions that are rendered in pseudocode are independent of the source programming language in which the algorithm is ultimately implemented.

1.0 STRUCTURE

The LANL YMP pseudocode language is designed to describe two aspects of algorithm design: processing and control structure (control and data flow). Processing is always described with an English-language phrase of the author's choosing. Control structure is specified with a collection of keywords.

A line of pseudocode is organized into two parts: a keyword and a narrative description. Either (or both) may be omitted from the line.

1.1 Narrative Description

The narrative description contains any comments that the author feels are appropriate at this stage of the description of the algorithm.

If there is no accompanying keyword field, the narrative description usually specifies some aspect of the processing performed by the algorithm, e.g.

compute the pressure at the current node

When specified in conjunction with a keyword, the narrative description usually defines a control condition or some other characteristic of the corresponding control structure, such as

IF *convergence has been achieved*

or

END *of the input routine*

The length of the narrative-description field of a pseudocode line is constrained only by the line length supported by the source programming language.

The narrative-description field must be separated from the keyword by at least one space or tab character.

1.2 Keyword

A keyword specifies a control-structure node within the algorithm. Keywords must be chosen from the list in Table 1:

If a keyword is specified in conjunction with a narrative description, the keyword must be the first item on the line and must be separated from the narrative description by at least one blank space or tab character.

2.0 DESCRIPTION OF PSEUDOCODE CONTROL-STRUCTURES

The following sections describe the full complement of pseudocode control structures. All control aspects of any algorithm must be expressed in terms of these structures.

BEGIN	ENDLOOP	LOOP
CASE	ENDSEGMENT	OTHERWISE
ELSE	ENDWHILE	REPEAT
ELSEIF	ERROREXIT	UNTIL
END	ERRORSEGMENT	WHEN
ENDCASE	EXITIF	WHILE
ENDFOR	FOR	
ENDIF	IF	

Table 1. Pseudocode Keywords

The software standards document that describes the coding and documentation standards for the subject source-programming-language must specify how each of the pseudocode control structures is implemented in that language.

2.1 Iteration Structures

The following four block-structured iteration-constructs are supported by the pseudocode language. Each permits an exit condition (EXITIF *condition*) to be located within the body of the loop. When the exit condition is satisfied, control transfers to the pseudocode statement following the ENDFOR, ENDWHILE, ENDLOOP. or UNTIL statement. These constructs are shown schematically in Figure 1.

- **FOR .. ENDFOR** The FOR structure provides a counted loop construct.
- **LOOP .. ENDLOOP** The LOOP construct is the most general iteration structure supported by the pseudocode language.
- **REPEAT .. UNTIL** The REPEAT structure is a standard post-tested loop construct.
- **WHILE .. ENDWHILE** The WHILE structure provides a pre-tested loop construct.

2.2 Block-IF

The Block-IF is the only decision structure supported by the pseudocode language. Typical Block-IF constructs are shown in Figure 2.

2.3 CASE

The CASE construct is the only selection structure supported by the pseudocode language. The CASE structure is shown schematically in Figure 3.

2.4 Other Structures

2.4.1 BEGIN *routine-name*

This pseudocode statement is always the first line of pseudocode in a routine.

2.4.2 END *routine-name*

This pseudocode statement is always the last line of pseudocode in a routine.

```
FOR specify limits here
first statement of loop
        second statement of loop
        ...
        EXITIF specify exit condition
        ...
        last statement of loop
ENDFOR


WHILE specify entry condition          REPEAT
        first statement of loop                first statement of loop
        second statement of loop               second statement of loop
        ...                                    ...
        EXITIF specify exit condition          EXITIF specify exit condition
        ...                                    ...
        last statement of loop         last statement of loop
ENDWHILE                               UNTIL specify exit condition


LOOP
        first statement of loop
        second statement of loop
        ...
        EXITIF specify exit condition
        ...
        last statement of loop
ENDLOOP
```

Figure 1. Iteration Constructs.

2.4.3 ERROREXIT

This line of pseudocode specifies an unconditional branch to an ERRORSEGMENT.

2.4.4 ERRORSEGMENT

This structure delimits a block of pseudocode that describes special error processing features of the routine. Only one ERRORSEGMENT block of pseudocode may be present, and it must be located immediately before the END statement. See Figure 4.

```
IF specify condition
        execute this block when condition is true
        ...
        last statement of block
ELSEIF specify condition
        execute this block when else-if condition is true
        this block may be omitted if no else-if condition
        ...
        last statement of block
ELSEIF specify condition
        execute this block when else-if condition is true
        this block may be omitted if no else-if condition
        ...
        last statement of block
...
ELSE this block is optional
        first statement of block
        ...
        last statement of block
ENDIF
```

Figure 2. Block-IF Construct.

```
CASE description of selection criteria
        WHEN first selection value
                first statement of executable block
                ...
                last statement of executable block
        WHEN next selection value
                first statement of executable block
                ...
                last statement of executable block
        ...
        OTHERWISE optional
                first statement of executable block
                ...
                last statement of executable block
ENDCASE
```

Figure 3. CASE Construct.

```
IF error reading input
        issue "Invalid Input" message
        IF error not recoverable
                ERROREXIT
        ENDIF
ENDIF

. . .

perform more processing

. . .

IF fatal error encountered
        ERROREXIT
ENDIF

. . .

. . .

ERRORSEGMENT
        flush buffers
        close files
ENDSEGMENT

END
```

Figure 4. Typical Use of ERRORSEGMENT.

APPENDIX C. DATA SET DESCRIPTION (DSD)

The Data Set Description is a user-documentation component that describes the interface tables associated with a computational data baseline. It provides information that is targeted for a potential user of the data set.

The following sections describe the contents of each major section of the Data Set Description. In the event that the information required below is already present in an existing document such as a milestone report, the information may be referenced in the external document and need not be included in the Data Set Description.

1.0 PURPOSE

Explain the purpose for which the data was generated.

2.0 REFERENCES

Cite any supporting documents here.

3.0 SCOPE AND DESCRIPTION

To the extent possible, characterize this data. For example, what distinguishes it from other data sets generated by the same software?

4.0 ASSUMPTIONS AND LIMITATIONS

Detail any assumptions that were made in generating the data baseline and any known limitations to its subsequent application.

5.0 VERIFICATION AND VALIDATION SUMMARY

Summarize for the potential user of this data the V&V efforts (and their results). Only those efforts that are unique to the data set need be described here. Omit discussion of the V&V program for the software that generated the data set.

6.0 DATA PRODUCT DESCRIPTIONS

6.1 Name of First Data Product

6.1.1 Purpose

Describe the purpose of this data product.

6.1.2 Scope and Description

Characterize this data with respect to the data baseline (application) as a whole. What is the unifying relationship between the components of this data product?

6.1.3 Assumptions and Limitations

Specify any assumptions or limitations that are unique to the components of the data product.

6.1.4 Heritage of the Data Product

6.1.4.1 Software Source.

For derived data, specify the name and release identifier of the software that was used to generate the data set.

6.1.4.2 Inputs.

For derived data, describe any input interface tables that were used by the software to generate the data set. Include the name and release-id of interface tables from a certified computational- data baseline.

For primary data, describe the data source.

. . .

6.2 Name of Second Data Product

. . .

APPENDIX D. MODELS AND METHODS SUMMARY (MMS)

The Models and Methods Summary is provided to apprise potential users of the details of the mathematical models and numerical methods employed by the software and to comply with the requirements of Section B of NUREG-0856. As such, the Models and Methods Summary has a role both as user documentation and evidential documentation.

The following sections describe the contents of each major section of the Models and Methods Summary. Parenthetical references in the section headings indicate corresponding sections in NUREG-0856 from which the documentation requirements for those sections shall be obtained. In the event that any of the information required below is already present in an existing document such as a milestone report or journal article, the external document may be referenced and the information need not be reproduced here.

1.0 PURPOSE

The Models and Methods Summary provides a detailed description of the mathematical models and numerical methods employed by a software application.

2.0 DEFINITIONS AND ACRONYMS

Terms and acronyms that are used throughout the document are defined here.

3.0 REFERENCES

Supporting documents are cited here.

4.0 STATEMENT AND DESCRIPTION OF THE PROBLEM (B.1)

Describe the overall nature and purpose of the general analysis in which the model will be used.

5.0 STRUCTURE OF THE SYSTEM MODEL (B.2)

Describe the role of any component models of the complete model.

6.0 GENERAL NUMERICAL PROCEDURE (B.3)

Use flowcharts and block diagrams to describe the numerical solution strategy and computational sequence.

7.0 COMPONENT MODELS (B.4)

7.1 Component Model 1

7.1.1 Purpose (B.4.a)

Discuss the purpose and scope of the component model including input to and output from the model and how information is transformed by the model.

7.1.2 Assumptions and Limitations (B.4.b)

Specify any assumptions and limitations upon which the model depends.

7.1.3 Notation (B.4.c)

Identify all algebraic variables used in equations, and associate each with the corresponding computer variable name for the quantity.

7.1.4 Derivation (B.4.d)

Derive the model from generally accepted principles. Justify each step in the derivation. Clearly state the final mathematical form of the model.

7.1.5 Application (B.4.e)

Discuss how the component model may be applied to a geologic repository. Describe any restrictions on the model, and state the validity of the model under extreme conditions.

7.1.6 Numerical Method Type (B.4.f)

Characterize any numerical methods incorporated in the model that go beyond simple algebra.

7.1.7 Derivation of Numerical Model (B.4.g)

Derive the numerical procedure from the mathematical component model, referencing all numerical methods. Present the final form of the numerical model and explain the algorithm.

7.1.8 Location (B.4.h)

State where the component model is used in the software.

7.1.9 Numerical Stability and Accuracy (B.4.i)

Discuss the stability and accuracy of the numerical model, and distinguish between those aspects that have been proven mathematically and those that have not been proven but have been observed in practice.

7.1.10 Alternatives (B.4.j)

Discuss alternatives to the component model and state why this model was chosen.

7.2 Component Model 2

. . .

8.0 EXPERIENCE (B.5)

Discuss the overall performance of the entire model.

APPENDIX E. SOFTWARE ASSESSMENT AND SUPPORT DOCUMENT (SAD)

The Software Assessment and Support Document is evidential documentation that is provided to comply with the requirements of Section D of NUREG-0856. It describes all work that was performed to ensure the functional adequacy and integrity of the software application. The following sections describe the contents of each major section of the Software Assessment and Support Document.

1.0 PURPOSE

State the purpose of the particular Software Assessment and Support Document.

2.0 DEFINITIONS AND ACRONYMS

Terms and acronyms that are used throughout the document are defined here.

3.0 REFERENCES

Supporting documents are cited here.

4.0 MODEL REVIEW

The level of review to which the application's models have been subjected may be established by including copies of all model-related supplemental documentation that was generated during the review/audit process. Alternatively this documentation may be referenced from the Version Description Document (see Appendix K).

Refer to Section D(1) of NUREG-0856 for the applicable documentation requirements.

5.0 VERIFICATION AND VALIDATION

This section may reference the V&V documentation of Section 7.0, which establishes the complete V&V record for the current version of the software application.

Refer to Section D(2) of NUREG-0856 for the applicable documentation requirements.

6.0 MAINTENANCE AND QUALITY ASSURANCE

This section will state that LANL YMP Software Configuration Management policy does not permit creation of multiple, parallel versions of computer software. Consequently no additional documentation need be provided in this section.

The above statement is sufficient to satisfy the requirements of Section D(3) of NUREG-0856.

7.0 VERIFICATION AND VALIDATION DOCUMENTS

The listed documents may be included in this section, or they may be referenced and provided under separate cover.

7.1 V&V Plan and Procedures

7.2 Test Results

7.3 V&V Report and Recommendations

7.4 Support Products

7.5 Review/Audit Report and Recommendations

These documents are already included in the Version Description Document and may be referenced therefrom.

APPENDIX F. SOURCE-CODE LISTINGS (SCL)

The Source-Code Listings document is an evidential-documentation component that provides a compendium of listings of all of the source code that is delivered with the software application.

The Source-Code Listings document shall comply with the requirements of Section E(6) of NUREG-0856.

APPENDIX G. SOFTWARE DESIGN DOCUMENT (SDD)

The Software Design Document is a development document that describes the top-level design of a software application. The following sections describe the contents of each major section of the Software Design Document.

1.0 PURPOSE

A brief (one paragraph) description of the general requirements addressed by the software application is presented here.

2.0 FUNCTIONAL DESCRIPTION

This section provides a narrative description of the overall functional processing capabilities of the software application. A clear representation of the application's segmentation should be provided.

3.0 ASSUMPTIONS AND LIMITATIONS

Any assumptions and limitations inherent to the software application are clearly stated in this section. List-format is recommended for presentation of these items.

4.0 PRIMARY PRODUCT DESCRIPTIONS

This section (and its subordinate subsections) provides detailed descriptions of each primary product (program or reuse component) associated with the application.

4.1 First Product

The name of the program or reuse component is specified here.

4.1.1 Purpose

A brief (one paragraph) description of the general requirements satisfied by this product is presented here.

4.1.2 Functional Description

This section provides a narrative description of the overall functional processing capabilities of the product. A clear representation of the software product's segmentation should be provided.

4.1.3 Assumptions and Limitations

Any assumptions and limitations inherent to the product are clearly stated in this section. List format is recommended for presentation of these items.

4.1.4 Input/Output

All of the software product's input/output interfaces are presented in this section, organized into the subsections described below:

4.1.4.1 Configuration Interface-Table

A representation of the product's configuration interface-table is provided in this section. The name and description of each entry is described.

4.1.4.2 Other Input Data Elements

Data elements that must be obtained from interface tables other than the product's configuration interface-table are described in this section. The name, structure, size, data type, bounds and description of each data element are provided.

4.1.4.3 Prompted Input

Each prompt issued by the product is specified in this section. The size, type, bounds, and any other restrictions on the allowed responses are also specified.

4.1.4.4 Output Interface Tables

A representation of each of the product's output interface-table(s) is provided in this section. The name, structure, size, data type, bounds, and description of each data element are provided.

4.1.4.5 Displays and Reports

A representation of each display or report generated by the product is provided in a manner that specifies format and content.

4.1.4.6 Messages

The identifier and text of each message issued by the product is specified in this section. Conditions that are expected to result in the issuance of each message are described.

4.1.4.7 Other Input/Output

Any other formal input/output mechanisms (e.g. data bases, files, menus, command language, etc.) are described in detail in this section.

4.2 Second Product

. . .

APPENDIX H. SOFTWARE REQUIREMENTS SPECIFICATION (SRS)

The Software Requirements Specification documents the functional and performance requirements of the application and describes external interfaces and design constraints. ANSI/IEEE Std 830-1984, *IEEE Guide to Software Requirements Specifications*, was used a resource in specifying this document.

The following sections provide a standard format for, and describe the contents of, each major section of the Software Requirements Specification. Parenthetical references in the section headings indicate sections in ANSI/IEEE Std 830-1984 from which additional description may be obtained.

1.0 INTRODUCTION (6.1)

1.1 Purpose (6.1.1)

This section specifies the purpose of the Software Requirements Specification and identify its intended audience.

1.2 Scope (6.1.2)

This section identifies the software by name, explains what the software will do, and describes the application of the software being specified.

1.3 Definitions and Acronyms (6.1.3)

All terms and acronyms required to understand the Software Requirements Specification are defined in this section.

1.4 References (6.1.4)

All documents referenced elsewhere in the Software Requirements Specification are cited in this section.

2.0 GENERAL DESCRIPTION

2.1 Software Perspective (6.2.2)

This section describes the relationship of the software being specified to existing systems.

2.2 Software Functions (6.2.3)

This section describes the major functions that the software must perform.

2.3 User Characteristics (6.2.3)

Identify any constraints imposed by the user environment, such as the level of experience of potential users.

2.4 General Constraints (6.2.4)

Any other issues that constrain the developer's options for designing the system are identified here.

2.5 Assumptions and Dependencies (6.2.5)

List specific assumptions and dependencies (such as the hardware and software operating environment) here.

3.0 FUNCTIONAL REQUIREMENTS (6.3.1.1)

This section specifies the processes that transform the software inputs into outputs.

3.1 Major Function 1

3.1.1 Functional Requirement 1

3.1.1.1 Introduction

3.1.1.2 Inputs

3.1.1.3 Processing

3.1.1.4 Outputs

3.1.2 Functional Requirement 2

...

3.2 Major Function 2

...

4.0 EXTERNAL INTERFACE REQUIREMENTS (6.3.1.1)

This section specifies the interfaces that must be supported by the software.

4.1 User Interfaces (6.3.1.5.1)

This section specifies the software characteristics required to support each human interface. It also specifies any requirements for optimizing these interfaces.

4.2 Hardware Interfaces (6.3.1.5.2)

This section specifies the logical characteristics of each interface between the software and the hardware environment within which it operates. It also specifies details of specific device support and required protocols.

4.3 Software Interfaces (6.3.1.5.3)

This section identifies other required software components with which the software is required to operate. It specifies the logical interfaces between these components and defines the requirements for any information interchange between them.

4.4 Communications Interfaces (6.3.1.5.4)

If interfaces to communications resources such as local area networks or data acquisition buses are required, they are specified here.

5.0 PERFORMANCE REQUIREMENTS (6.3.1.2)

Performance requirements such as number of users to be supported, number of files and records, sizes of tables and files, and transaction rates, if known, are specified in this section.

6.0 DESIGN CONSTRAINTS

6.1 Standards Compliance (6.3.1.3.1)

Specify any special standards that constrain the design or implementation of the software. Routine organizational standards need not be explicitly identified in this section.

6.2 Hardware Limitations (6.3.1.3.2)

If hardware constraints exist for the operation of the software, they are enumerated in this section.

7.0 SECURITY (6.3.1.4.2)

Special requirements to protect the software from accidental or malicious access, use, modification, destruction, or disclosure are specified here.

8.0 OTHER REQUIREMENTS

8.1 Data Base (6.3.1.6.1)

If a data base is to be developed as part of the project, specific requirements such as information content, frequency of use, data base access, organization, and data retention requirements are defined here.

8.2 Operations (6.3.1.6.2)

The requirements for routine or special operations required by the user such as operating modes, support functions, and backup and recovery operations are specified here.

9.0 VALIDATION CRITERIA

Any requirements for validating mathematical models or numerical methods employed by the software are specified in this section.

9.1 Validation Criterion 1

9.2 Validation Criterion 2

. . .

APPENDIX I. TEST RESULTS (TR)

The Test Results document is development documentation that contains a record of the execution of the V&V procedures, i.e. the Test Results contains the output generated when the test procedures are executed on the target computer. As such it constitutes the primary record of the results of the software testing activity.

The Test Results document may be distributed among many separate documents. Each test suite may have a separate Test Results document, or each test driver may update a common Test Results document. The organization of the Test Results document is left to the discretion of the developer, but it must be acceptable to the CCB.

APPENDIX J. USERS MANUAL (UM)

The Users Manual provides a user of the software application with information necessary to install and run the application. As such the Users Manual is one of the principal components of user documentation. The Users Manual is also evidential documentation that must be supplied to the U. S. Nuclear Regulatory Commission to meet the requirements of Section C of NUREG-0856.

The following sections describe the contents of each major section of the Users Manual. Parenthetical references in the section headings indicate corresponding sections in NUREG-0856 from which the documentation requirements for those sections shall be obtained.

1.0 PURPOSE

Specify the purpose of the Users Manual here.

2.0 DEFINITIONS AND ACRONYMS

Any terms or acronyms used throughout the document are defined in this section.

3.0 REFERENCES

Any documents referenced within the Users Manual are cited here.

4.0 PROGRAM CONSIDERATIONS

4.1 Program Options (C.1.a)

Each major program option (and combinations of options) is described in this section.

4.2 Program Paths (C.1.b)

The purpose of each subroutine and the major paths through the code are discussed in this section.

4.3 Data Structures (C.1.c)

Discuss the scope, organization, size, and use of all significant data structures here.

4.4 Initialization (C.1.d)

Initialization values must be specifically identified in this section.

4.5 Restart Procedures (C.1.e)

Describe the restart capabilities of the software.

4.6 Error Processing (C.1.f)

Describe error messages, error paths, and abnormal termination sequences in this section.

5.0 INTERFACE TABLES AND DATA FILES

5.1 Interface Tables (C.2)

5.1.1 Name of First Interface Table

5.1.1.1 Content (C.2.a).

Describe the content, purpose, and organization of the interface table. Specify the interface table type (Configuration or Data)

5.1.1.2 Use by Program (C.2.b).

Specify whether the interface table is used for input or output, describe the role of the information in the interface table and identify at what stage during program execution it is used.

5.1.1.3 Auxiliary Processing (C.2.c).

Identify any auxiliary programs used to create, modify, reformat, or interpret the data in the interface table.

5.1.2 Name of Second Interface Table

. . .

5.2 Data Files (C.2)

5.2.1 Name of First Data File

5.2.1.1 Content (C.2.a).

Describe the content, purpose, and organization of the data file.

5.2.1.2 Use by Program (C.2.b).

Specify whether the data file is used for input or output, describe the role of the information in the data file, and identify at what stage during program execution it is used.

5.2.1.3 Auxiliary Processing (C.2.c).

Identify any auxiliary programs used to create, modify, reformat, or interpret the data in the data file.

5.2.2 Name of Second Data File

. . .

6.0 INPUT DATA

6.1 General Considerations

6.1.1 Techniques (C.3.a.i)

Any special input techniques or requirements are described in this section.

6.1.2 Consecutive Cases (C.3.a.ii)

Give conditions for retention of input data between cases, if any.

6.1.3 Defaults (C.3.a.iii)

Explain any conventions regarding default values.

6.2 Individual Input Records or Parameters

6.2.1 Record/Parameter 1

6.2.1.1 Record Identifier (C.3.b.i).

Provide the line identifier or data object label for this type of record.

6.2.1.2 Input Variables (C.3.b.ii).

Identify the internal variables that are assigned values from data provided in this record.

6.2.1.3 Format (C.3.b.iii).

Specify the format of the record, if any.

6.2.1.4 Need (C.3.b.iv).

Specify whether input is necessary or optional for each variable.

6.2.1.5 Repetition (C.3.b.v).

Discuss how many of these records are required or may be used optionally.

6.2.1.6 Units (C.3.b.vi).

Provide the dimensional units for each input field.

6.2.1.7 Default (C.3.b.vii).

Provide the default value, if any, for each field.

6.2.1.8 Description (C.3.b.viii).

Define the meaning of each variable and discuss its use within the code.

6.2.1.9 Range (C.3.b.ix).

State the acceptable limits for each variable.

6.2.2 Record/Parameter 2

. . .

7.0 SYSTEM INTERFACE

7.1 System-Dependent Features (C.4.a)

Identify the external references that must be supplied by the system.

7.2 Compiler Requirements (C.4.b)

Identify the compilers that have been successfully used, and specify any special load options.

7.3 Hardware Requirements (C.4.c)

Describe any special hardware features or environments required by the software.

7.4 Control Sequences or Command Files (C.4.d)

Describe any special command sequences required by the software.

7.5 Installation Instructions

Provide a comprehensive set of instructions for installing the software on platforms for which it has been designed. In a separate command file or script, provide an executable procedure for compiling and/or linking the application. Reference the name of the file here.

8.0 OUTPUT(C.5)

Discuss the code output with respect to input options, and state the origin and meaning of output variables. Describe any graphical capabilities of the software.

9.0 EXAMPLES AND SAMPLE PROBLEMS (C.6)

Furnish a suite of sample problems that demonstrate how the software is used. Include all input data and sample output.

10.0 USER SUPPORT

Specify that users should contact the LANL SCM Organization for user and maintenance support.

APPENDIX K. VERSION DESCRIPTION DOCUMENT (VDD)

The Version Description Document describes the content and capabilities of each delivered version of the system. As such, it is a primary user's documentation component. The Version Description Document is also evidential documentation that shall be supplied to the U. S. Nuclear Regulatory Commission (upon request) to meet requirements specified in Section E of NUREG-0856.

The following sections describe the contents of each major section of the Version Description Document.

1.0 VERSION IDENTIFICATION

This section specifies the release identifier for the application or data described by this document.

2.0 REFERENCES

Any documents referenced in the Version Description Document are cited here.

3.0 CHANGE SUMMARY

3.1 Release Notes

This section presents a description of the new features of the application. In addition, this section identifies any compatibility issues with respect to previous versions and identifies any known errors that are present in the released version.

3.2 SCRs and SIRs Satisfied

This section contains final copies of (or references to) any Software Change Requests and/or Software Incident Reports that are satisfied by the release of this version of the software.

4.0 CHRONOLOGICAL RECORD OF DEVELOPMENT

This section is a compendium (beginning with the authorizing Engineering Change Directive) of all of the supplemental-documentation forms that were generated in support of the development of this version.

This section may be omitted from the Version Description Document that is distributed to users of the software.

APPENDIX L. V&V PLAN AND PROCEDURES (VVP)

The V&V Plan and Procedures document is development documentation that encapsulates the V&V plan and the V&V procedures that are derived from the plan. ANSI/IEEE Std 829-1983 was used as a resource in specifying this document.

The V&V-plan components of this document may be rendered as text documents, documentation prologs of the test software, or a combination of each, depending upon the information that must be represented. However, the test plan information (e.g. Section 4.1ff) must be specified within the documentation prologs of the support modules that execute the testing. In this manner the test plan is closely associated with the procedures that are derived from them.

The V&V procedures are always implemented in command language within the particular V&V Plan and Procedures document component that contains the corresponding V&V plan documentation.

The following sections describe the contents of each major section of the V&V Plan and Procedures.

1.0 PURPOSE

A brief (one paragraph) description of the goals of the V&V effort is presented here.

2.0 FUNCTIONAL DESCRIPTION

This section presents an overview of the organization and proposed execution of the V&V effort.

3.0 ASSUMPTIONS AND LIMITATIONS

Any assumptions and limitations inherent to the V&V effort are clearly stated in this section. Hardware and operating system environment must be specified in this section.

4.0 VERIFICATION AND VALIDATION PLAN

This section provides detailed descriptions of the V&V effort including the role of formal testing, and any other methods such as inspection, analysis, and demonstration. If the formal testing is organized into test suites, one subsection is included for each test suite.

4.1 Name of First Test Suite

4.1.1 Purpose

A brief (one paragraph) description of the requirements fulfilled by this test suite is presented here.

4.1.2 Functional Description

This section specifies, in narrative format, the overall organization of this test suite.

4.1.3 Assumptions and Limitations

Any assumptions and limitations inherent to the test suite are clearly stated in this section.

4.1.4 Summary of Test Cases

This section describes each test case in the test suite. It is organized into the following subsections:

4.1.4.1 Identifier for Test Case 1.

This section specifies a unique identifier for the test case.

4.1.4.1.1 Function Tested. This section provides a brief narrative description of the function under test.

4.1.4.1.2 Test Scope. This section specifies whether the test case is a verification, validation, regression, or acceptance (installation) test.

4.1.4.1.3 Requirements Tested. This section provides a list of the specific requirements (referenced by SRS paragraph number) that are verified by the test.

4.1.4.1.4 Required Inputs. This section describes the inputs necessary to configure the test.

4.1.4.1.5 Expected Outputs. This section defines specific criteria that must be met to pass the test.

4.1.4.2 Identifier for Test Case 2.

. . .

4.2 Name of Second Test Suite

. . .

APPENDIX M. V&V REPORT (VVR)

The V&V Report presents a critical analysis of the Test Results with respect to the expected results specified in the V&V Plan and Procedures. The V&V Report is development documentation.

ANSI/IEEE Std 829-1983 was used as a resource in specifying this document.

The following sections describe the contents of each major section of the V&V Report.

1.0 SCOPE OF V&V ACTIVITIES

Describe the overall V&V effort and the V&V philosophy. Specify why they are appropriate.

2.0 REFERENCES

Cite any references to standard works or data sources here.

3.0 DESCRIPTION OF ENVIRONMENT

Summarize the hardware and software characteristics of the test environment here.

4.0 DISCUSSION OF TEST RESULTS

Discuss and interpret the Test Results in this section. Particular emphasis is placed upon discrepancies between the actual and expected test results. An analysis of any such discrepancies (as well as an explanation of any mitigating circumstances) is presented in this section.

In the event that no discrepancies are identified for a test suite, that fact may be noted and no further explanation is required.

4.1 Test Suite 1

4.2 Test Suite 2

...

5.0 ADDITIONAL V&V ISSUES

Discuss any aspects of the V&V effort that are outside of the scope of the formal testing effort.

6.0 CONCLUSIONS AND RECOMMENDATIONS

This section contains the author's conclusions regarding the acceptability of the V&V effort. The author may also make recommendations regarding the disposition of discrepancies discovered during the testing program. For example, the author may recommend that a particular discrepancy remain unaddressed pending a future repair operation. The recommendation would require that the error be documented in the Version Description Document and that the application be accepted with the known defect. Recommendations may also be made regarding modified or enhanced test strategies that should be applied to future versions of the application.

SOFTWARE CONFIGURATION MANAGEMENT

Effective Date: ____________________

G. Cort **Preparer**	**Date**
S. L. Bolivar **Quality Assurance Project Leader**	**Date**
R. J. Herbst **Technical Project Officer**	**Date**

SOFTWARE CONFIGURATION MANAGEMENT

1.0 PURPOSE

This plan defines the organization, policies, and procedures necessary to ensure the orderly control of the software and computational data products produced or acquired by the Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP).

2.0 SCOPE

This quality administrative procedure (QP) applies to all software and computational data developed or acquired for use in support of licensing activities. It applies to all phases of the software life-cycle specified in TWS-QAS-QP-03.21, *Software Life Cycle.*

3.0 REFERENCES

ANSI/IEEE Std 828-1983, *IEEE Standard for Software Configuration Management Plans*, June 1983.

ANSI/IEEE Std 1042-1987, *IEEE Guide To Software Configuration Management*, September 1987.

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

QARD *Quality Assurance Requirements Document for the Civilian Radioactive Waste Management Program*, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

NN1-1990-0334 *Software Supporting Scientific Investigations/Licensing*

NUREG-0856 *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, June 1983.

Software Configuration Management: An Investment in Product Integrity. Edward H. Bersoff, Vilas D. Henderson, and Stanley G. Siegel, Prentice-Hall, Inc., 1980.

TWS-QAS-QP-03.2 *Procedure for Preparation and Technical and Policy Review of Technical Information Products.*

TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

TWS-QAS-QP-03.19 *Documentation of Software and Computational Data.*

TWS-QAS-QP-03.21 *Software Life Cycle.*

TWS-QAS-QP-17.3 *Procedure for LANL YMP Records Management.*

4.0 DEFINITIONS

Refer to LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project*, Appendixes C and D, respectively, for a glossary of terms and list of acronyms used throughout this document.

5.0 RESPONSIBILITY

5.1 Technical Project Officer (TPO)

The responsibility of the TPO under this QP is to serve as chair of the CCB.

5.2 Software Configuration Manager

The responsibilities of the Software Configuration Manager under this QP are

- Serve as the agent of the TPO and the Configuration Control Board in implementing and administering this QP;
- Serve as the administrative head of the SCM Organization
- Serve as a permanent member and cochair of the CCB;
- Conduct the business of the SCM Organization, including:

(1) Configuration Control (refer to Section 6.2)

(2) Configuration Status Accounting (refer to Section 6.3)

(3) Configuration Identification (refer to Section 6.1)

(4) SCM Audits (refer to Section 6.4)

(5) Establishment and maintenance of software and computational data baselines.

5.3 Configuration Control Board (CCB)

The responsibilities of the CCB under this QP are:

- Evaluate and assess the technical merit and organizational impact of all proposed changes to LANL software and computational baselines
- Authorize all software development activities that are within the scope of this SQAP
- Specify the life-cycle phases, baselines, baseline components, and formal reviews that are associated with a software development task
- Provide the forum for all formal reviews of software or computational data baselines
- Approve or disapprove all software and computational data baselines submitted for review
- Evaluate requests for variances to the provisions of the SQAP
- Make recommendations to the TPO regarding software management issues.

6.0 PROCEDURE

6.1 Configuration Identification

6.1.1 Labeling of Modules

6.1.1.1 Procedure for the Developer

Record the number of the authorizing Engineering Change Directive in the History section of each source code module's documentation prolog and in the header of each high-level text document.

6.1.1.2 Procedure for the SCM Organization

Upon entry into the CPL record the following data base attributes of each source-code or high-level documentation module:

- Module name
- Module type
- Module version

Retain the module name and type specified by the developer. Employ the identifying number of the associated Baseline Submission Summary for the module version.

6.1.2 Labeling of Releases

The release labeling methodology is shown schematically in the flow chart of Figure 1 (Appendix A) and is described below.

6.1.2.1 Procedure for the SCM Organization

Record the release label of the sanctioned release in the Release Label field of the Engineering Change Notice. For additional information regarding the Engineering Change Notice, refer to Section 6.2.8.1.2. Construct the release label as follows:

6.1.2.1.1 Application Field. Obtain the application field from the name specified in the application's AFL.

6.1.2.1.2 First Release. If this is the first release of the application, set the release number (aa) to 01, set the version number (vv) and the revision number (rr) each to 00, and terminate the process.

6.1.2.1.3 Major Release. If the release incorporates a major functional change to all of the products of the application, construct the release, version, and revision numbers as follows, then terminate the process:

- Increment the release number (aa) found in the release label of the most recent prior release of the application and assign this value to the release number field
- Set the version number field to 00.
- Set the revision number field to 00.

6.1.2.1.4 Functional Release. If the release incorporates changes that do not introduce major new functions at the application level, construct the remainder of the release label as follows:

- Retain the release number found in the release label of the most recent prior release of the product and assign this value to the release number field
- Increment the version number found in the release label of the most recent prior release of the product and assign this value to the version number field.
- Set the revision number field to 00.

6.1.2.1.5 Minor Release. If the release incorporates only minor functional changes, construct the remainder of the release label as follows:

- Retain the release number found in the release label of the most recent prior release of the product and assign this value to the release number field
- Retain the version number found in the release label of the most recent prior release of the product and assign this value to the version number field.
- Increment the revision number found in the release label of the most recent prior release of the product and assign this value to the version number field.

6.1.2.1.6 V&V Deficiencies. If the V&V Report (TWS-QAS-QP-03.19 *Documentation of Software and Computational Data,* Appendix M) specifies that the software has not been adequately verified or that one or more models incorporated into the software have not been satisfactorily validated, append a pound symbol (#) to the end of the release identifier.

6.1.2.1.7 Update the CPL. Record the release label as an attribute of the CPL data base partition containing the corresponding release of the application.

6.2 Configuration Control

6.2.1 Identification of CCB Members

6.2.1.1 Procedure for the SCM Organization

SCM personnel perform the following steps to identify and notify each member of the CCB.

6.2.1.1.1 Selection of Members. In consultation with the TPO, identify each individual to serve on the CCB. Document each selection on a CCB Participation Notice as follows

- General Information. Record the date of issue, prospective member's name, organizational affiliation, telephone number, and Laboratory mail stop or external address in the fields at the top of the form.
- Membership. Check one box that designates the membership status of the candidate. For rotating or temporary members, indicate the date upon which the term of service expires.
- If the Temporary Member box is checked in the Membership field, check all boxes in the Role field that characterize the role of the temporary member. If the SIR/SCR Defense or SIR/SCR Analysis box is checked, provide the identification number of the subject Software Incident Report or Software Change Request in the space provided.
- Check one box in the Status field to record the voting status of the member.
- Record any additional comments or restrictions in the Comments/ Restrictions field of the form.
- Sign and date the form in the space provided.
- If the Temporary Member box is checked in the Membership field of the form, if the candidate is not a LANL YMP member, and if a

current Reviewer Qualifications Summary is not on file for the candidate, initiate the completion of a Reviewer Qualifications Summary as specified in Step 6.2.1.1.2. In the RQS Reference field of the form, record the identification number of the Reviewer Qualifications Summary. Otherwise, proceed to Step 6.2.1.1.3.

6.2.1.1.2 Reviewer Qualifications Summary.

- Transmit a copy of a blank Reviewer Qualifications Summary to the candidate member.
- Upon receipt of the completed form from the candidate member, verify that the form is complete and if so, sign and date it in the space reserved for the SCM Representative. Submit a copy to the CSA Active File. If the Reviewer Qualifications Summary submitted by the candidate member is not complete, return the form to the candidate member to resolve any problems and repeat this step.

6.2.1.1.3 Notification of Members. Transmit a copy of the CCB Participation Notice to the candidate member. Submit a copy to the CSA Active File.

6.2.1.2 Procedure for the Candidate Temporary Member

Perform the following steps to establish credentials with the SCM Organization.

6.2.1.2.1 Documentation. Upon receipt of a blank Reviewer Qualifications Summary from the SCM Organization, complete the form as follows.

- General Information. Furnish the date, the candidate name, organizational affiliation, and telephone number in the space provided. If a LANL employee, provide the Laboratory mail stop. Otherwise, furnish the external mailing address.
- Summary of Qualifications and Experience. Detail all relevant qualifications and experience in this section. Attach any supporting documentation such as a current resume to this form.
- Reviewer's Current Position & Primary Work. Describe the current position and primary job-related responsibilities in this section. Attach any supporting documentation such as a current resume to this form.
- Other Comments. Specify any other relevant information here.
- Sign and date the form in the space provided.

6.2.1.2.2 Submission. Submit the completed form to the SCM Organization.

6.2.2 Notification of CCB Meetings

6.2.2.1 Procedure for the SCM Organization.

6.2.2.1.1 Schedule the Meeting. Determine the date, time, and location for the meeting. Document this information in the corresponding fields of a CCB Meeting Announcement form.

6.2.2.1.2 Identification of Agenda. Record the proposed agenda for the meeting in the Agenda field of the CCB Meeting Announcement.

6.2.2.1.3 Notification of Participants. Sign and date the form. Transmit a copy of the CCB Meeting Announcement to each participant. Submit a copy to the CSA Active File.

6.2.3 CCB Operation

6.2.3.1 Procedure for the CCB Chair

The CCB chair conducts a meeting of the CCB according to the following procedures.

6.2.3.1.1 Call to Order. Establish whether a majority of the voting members are present. If not, terminate the process. Otherwise, call the meeting to order.

6.2.3.1.2 Identify Recorder. Identify the individual who will record the minutes of the meeting on a CCB Meeting Minutes form.

6.2.3.1.3 Certify Minutes of Previous Meeting. Conduct a vote of the CCB to formally accept the CCB Meeting Minutes of the previous meeting. If the motion carries, sign the CCB Meeting Minutes form in the space provided and submit a copy to the CSA Active File.

If the acceptance motion does not carry, identify issues to be addressed and assign a permanent or rotating member to the remedial effort. Schedule another acceptance vote for a subsequent CCB meeting.

6.2.3.1.4 Conduct the Meeting. Execute the agenda documented on the corresponding CCB Meeting Announcement.

6.2.3.1.5 Adjourn the Meeting. Conduct a vote for adjournment of the meeting. If the adjournment motion is carried, adjourn the meeting.

6.2.3.2 Procedure for the Recorder

6.2.3.2.1 Meeting Minutes. Document the business conducted at the meeting on a CCB Meeting Minutes form as follows

- CMA Reference. In the CMA Reference field, record the identification number of the CCB Meeting Announcement that contains the meeting agenda.
- Date. Record the date of the meeting in the Date field.
- CCB Chair. Record the name of the chair for the meeting in the CCB Chair field.
- Recorder. Provide the name of the recorder in the Recorder field.
- Minutes. Record the minutes of the CCB meeting in this field.

6.2.3.2.2 Submission of Minutes. Sign and date the CCB Meeting Minutes form, and submit it for formal acceptance at the next meeting of the CCB (see Section 6.2.3.1.3).

6.2.4 Delegation of Change Control Authority

6.2.4.1 Procedure for the CCB Chair

6.2.4.1.1 Identification of Change Control Authority. Appoint a person or group to act as Change Control Authority. Conduct a vote of the CCB to ratify these appointments.

6.2.4.2 Procedure for the Recorder

6.2.4.2.1 Documentation of Change Control Authority. Document the results of Step 6.2.4.1 in the "Change Control Authority" field of the Review/Audit Report and Recommendations. Record any restrictions or special conditions that are imposed by the CCB on the Change Control Authority.

6.2.5 Computer Program Library Control

6.2.5.1 Procedure for the SCM Organization

6.2.5.1.1 Passwords. Employ password controls to restrict access to the CPL to members of the SCM Organization. Within the SCM Organization, issue passwords only to those individuals that require access to the CPL to perform their job function.

6.2.6 Releases

This section describes the procedures for performing an assessment, engineering, or probation release of information from the CPL. For information on the release of sanctioned baselines, refer to Section 6.2.9.2.4.

6.2.6.1 Procedure for the SCM Organization.

6.2.6.1.1 Verification. Upon receipt of a CPL Transmittal Request, verify that the form is signed by the requestor and that the reference specified in the SCR Reference, SIR Reference, or ECD Reference field specifies an open CSA record that is appropriate to justify the requested release. If verification fails, check the Not Approved box in the Disposition field of the CPL Transmittal Request, and proceed to Step 6.2.6.1.5.

6.2.6.1.2 Evaluation. Determine whether the information provided on the form is complete and consistent with the type of release being requested. Also determine whether the SCM Organization has the authority to issue the release or whether CCB approval must be obtained.

6.2.6.1.3 Disposition. Perform one of the following actions based upon the outcome of Step 6.2.6.1.2.

- If the information is complete and appropriate and the release can be performed as requested, check the Approved box in the Disposition field of the form and proceed to Step 6.2.6.1.4.
- If the release can be performed but requires minor modifications to the request, check Approved with Modifications, explain the

necessary changes in the SCM/CCB Comments field, and proceed to Step 6.2.6.1.4.

- If CCB action is required, check the Requires CCB Action box in the Disposition field, document the reason that CCB Action is required in the SCM/CCB Comments field, place the request on the agenda of the next CCB meeting, and await the CCB decision. Upon obtaining a decision from the CCB, repeat Step 6.2.6.1.3.
- If insufficient information is provided on the request to perform the release, check the Incomplete box, document the nature of the problem in the SCM/CCB Comments field, and proceed to Step 6.2.6.1.5.
- If the release is to be held in suspense, check the Tabled box, provide an explanation for this decision in the SCM/CCB Comments box, and proceed to Step 6.2.6.1.5.
- If the request is not approved for any other reason, check the Not Approved box, document the reason in the SCM/CCB Comments field, and proceed to Step 6.2.6.1.5.

6.2.6.1.4 Executing the Release. Transfer the information specified on the CPL Transmittal Request to the specified destination.

6.2.6.1.5 Closing the Release. Sign and date the CPL Transmittal Request, and return a copy to the requestor. Submit a copy to the CSA Active File, and terminate the process.

6.2.7 Baseline Certification

The baseline certification and sanctioning process is shown schematically in Figure 2 (Appendix A).

6.2.7.1 Procedure for SCM Organization

6.2.7.1.1 Baseline Admission. After the formal review process for a baseline is completed and all review issues are resolved to the satisfaction of the CCB, transfer the baseline from the Certification Environment into the CPL. Transfer into the CPL all components identified with the baseline on the task's Life Cycle Specification form. For additional information on the formal review process and issue resolution, refer to TWS-QAS-QP-03.17, *Reviews of Software and Computational Data Baselines*.

6.2.7.1.2 Documentation. Document the baseline certification process on a Baseline Certification Notice as follows

- General Information. Record the certification date in the Date field and complete the subject field. Use the contents of the title field of the corresponding Life Cycle Specification for the subject. Provide the name of the developer, the developer's organizational affiliation, telephone, and mail stop in the fields provided.
- LCS Reference. Provide the identifier of the Life Cycle Specification that controlled the development of the baseline. If the baseline is a computational data baseline, place N/A in this field.
- Application Name. Furnish the name of the application as specified in its AFL.

- Baseline Identification. Check the appropriate box to identify the baseline that is being certified. If certification follows the completion of a baseline closure review, check the corresponding Baseline/Phase Closed box.
- Furnish any additional comments in the Comments field.
- Sign and date the form.

6.2.7.1.3 Notification of Developer. Transmit one copy of the Baseline Certification Notice to the developer identified in the Developer field. Submit a copy to the CSA Active file.

6.2.8 Baseline Sanctioning

The baseline certification and sanctioning process is shown schematically in Figure 2 (Appendix A).

6.2.8.1 Procedure for the SCM Organization

Subsequent to certifying an implementation or computational data baseline, sanction the baseline as follows

6.2.8.1.1 Technical and Policy Review. Initiate the technical and policy review process for the baseline according to the provisions of TWS-QAS-QP-03.2, *Procedure for Preparation and Technical and Policy Review of Technical Information Products*. For a software baseline, subject the following baseline components to review: Models and Methods Summary, Users Manual Document, and Version Description Document.

For a computational data baseline, subject the Data Set Description to review.

If the Technical and Policy Review requires changes to any of the reviewed documents, initiate Software Change Requests or Software Incident Reports as appropriate to effect the modifications. Suspend the process until the required changes have been processed through the life cycle and approved by the CCB.

6.2.8.1.2 Documentation. Document the baseline sanctioning process on an Engineering Change Notice as follows. The Engineering Change Notice serves as the formal notice of approval to use the sanctioned software in producing technical calculations.

- Date. Record the sanctioning date in the Date field.
- Application Name. Furnish the name of the application.
- ECD Reference. Provide the identifier of the Engineering Change Directive that authorized the development of the baseline. If the baseline is a Computational Data Baseline, place N/A in this field.
- BCN Reference. Provide the identifier of the Baseline Certification Notice that documents the certification of the baseline.
- Release Label. Construct the release label(s) for the application and record in this field. The procedure for constructing release labels is described in Section 6.1.2.1.
- Furnish any relevant comments in the Comments field. In particular, if the software is the product of a conversion or qualification effort and if it was not possible to satisfy all

requirements during the conversion/qualification effort, identify those requirements that remain unmet and provide justification.
- Sign and date the form.

6.2.8.1.3 **Notification of Developer.** Transmit one copy of the Engineering Change Notice to the developer identified in the Developer field. Submit a copy to the CSA Active File.

6.2.8.1.4 **Notification of Registered Users.** Upon sanctioning a new version of a previously sanctioned software-application, notify the registered users of the application by transmitting a copy of the corresponding Engineering Change Notice to each. Registered users of a sanctioned application or computational data baseline are those individuals for whom an approved Software/Data Dissemination Request is on file with the SCM Organization.

6.2.8.1.5 **Notification of National Energy Software Center.** Complete a National-Energy-Software-Center Software-Summary form, and transmit the form to the National Energy Software Center.

6.2.9 Interface Control

6.2.9.1 Procedure for the Requestor

To obtain the latest version of a LANL-YMP-sanctioned software-application or certified data-set, execute the following steps.

6.2.9.1.1 **Formal Request for Software or Data.** Obtain a Software/Data Dissemination Request from the SCM Organization and complete the form as follows

- General Information. Provide the date of request, requestor name, telephone number, and organizational affiliation in the corresponding fields of the Software/Data Dissemination Request. If the request originates from within LANL, provide the Laboratory mail stop in the space provided. Otherwise, furnish the requestor's external address. Check the "YMP Use" box if the software is to be used in support of the Yucca Mountain Project. Otherwise, check the "External" box.
- Application or Data Set Release ID. Provide the release id of the sanctioned baseline being requested. Consult the LANL YMP Software Configuration Manager for assistance in obtaining this name.
- File Transmittal Block. Complete the information in the File Transmittal Block to specify the characteristics of the destination computing environment and details of the transfer process.
  - Provide the name and telephone number of the individual to be contacted with questions about the transmittal, if different from the requestor.
  - Identify the hardware platform (e.g. VAX, Sun SPARC, etc.) and operating system of the destination computing system.
  - Specify the preferred file format for transmission.
  - In the Method of Distribution field, specify the preferred method of transmission by checking one of the Tape, Disk, or Network

boxes. Complete the descriptive information under the checked box.

- Comments. Provide any additional comments, requests, or explanation in the Comments field.

6.2.9.1.2 Submission. Sign and date the Software/Data Dissemination Request in the space reserved for the requestor. Submit the form to the LANL YMP SCM Organization.

6.2.9.1.3 Installation and Checkout. Upon receipt of the distribution package from the SCM Organization, perform the installation according to the installation instructions enclosed. Execute the acceptance tests provided with the distribution package and compare the results to the certified results provided. If discrepancies are discovered, enlist the aid of the SCM Organization to identify the cause and modify the local installation environment to resolve the problem. If the discrepancies cannot be resolved by changes to the local installation environment, submit a Software Incident Report.

6.2.9.2 Procedure for the SCM Organization

Utilize the following procedures for release of a sanctioned baseline to the user community.

6.2.9.2.1 Verification. Upon receipt of a Software/Data Dissemination Request, verify that the form is signed by the requestor and that the application or data set specified on the form exists. If verification fails, check the Not Approved box in the Disposition field, and proceed to Step 6.2.9.2.5.

6.2.9.2.2 Evaluation. Determine whether the information provided on the form is complete and consistent. Also determine whether the SCM Organization has the authority to issue the release or whether CCB approval must be obtained.

6.2.9.2.3 Disposition. Perform one of the following actions based upon the outcome of Step 6.2.9.2.2.

- If the information is complete and appropriate and the release can be performed as requested, check the Approved box in the Disposition field of the form and proceed to Step 6.2.9.2.4.
- If the release can be performed but requires minor modifications to the request, check Approved with Modifications, explain the modifications in the SCM/CCB Comments field, and proceed to Step 6.2.9.2.4.
- If CCB action is required (to approve the release of source code, for example), check the Requires CCB Action box in the Disposition field, document the reason that CCB Action is required in the SCM/CCB Comments field, place the request on the agenda of the next CCB meeting, and await the CCB decision. Upon obtaining a decision from the CCB, repeat Step 6.2.9.2.3.
- If the release is to be held in suspense, check the Tabled box, provide an explanation for this decision in the SCM/CCB Comments box, and proceed to Step 6.2.9.2.5.

- If the request is not approved for any reason, check the Not Approved box, document the reason in the SCM/CCB Comments field, and proceed to Step 6.2.9.2.5.

6.2.9.2.4 Executing the Release. Compose the distribution package as follows:

- For software distributions include the Models and Methods Summary (if mandated for the corresponding software class), Users Manual Document, Version Description Document, installation instructions, acceptance tests (with results for comparison) and binary code.
- If the release is being made to the U. S. Nuclear Regulatory Commission, include all of the above documents. In addition, prepare a Software Summary Form (See *NUREG-0856, Appendix A*) for the application. Create the Software Assessment and Support Document and Source Code Listings in accordance with *TWS-QAS-QP-03.19 Appendixes E and F*, respectively. Complete Section 4 of the Version Description Document in accordance with the provisions of *TWS-QAS-QP-03.19 Appendix K*. Include these documents in the distribution package.
- Compose a data distribution-package of the following components: Data Set Description and universal interface-tables.

Transmit the distribution package to the requestor in accordance with the format and distribution specifications provided in the File Transfer Block of the Software/Data Dissemination Request.

6.2.9.2.5 Closing the Release. Sign and date the Software/Data Dissemination Request, and return a copy to the requestor. Submit a copy to the CSA Active File, and terminate the process.

6.2.9.2.6 Installation and Checkout. If problems arise during the installation and/or checkout of the software by the prospective user, assist in identifying any features of the local installation environment that may be causing the problems.

6.2.10 Variances

6.2.10.1 Procedure for the Requestor

6.2.10.1.1 Documentation. Complete an SCM Variance Authorization form as follows

- General Information. Provide the date of request, general subject of the request, requestor name, telephone number, and organizational affiliation, and Laboratory mail stop in the corresponding fields of the SCM Variance Authorization.
- ECD Reference. Furnish the identifier of the Engineering Change Directive of the development task against which the variance is directed. If the variance is requested against a computational baseline, record N/A in this field.
- Type of Variance. Check one box in this field to indicate the target of the variance. If Other is checked, provide a brief description of the target in the space provided.

- Description. Describe the variance that is being requested. Include a specific reference to a provision of the LANL SQAP, its implementing procedures, or a standards document.
- Justification. Explain why this variance is necessary. Characterize the special situation that requires it. Justify in detail why this variance does not contravene any provisions of the QARD.

6.2.10.1.2 Submission. Sign and date the SCM Variance Authorization in the space reserved for the requestor. Submit the form to the SCM Organization.

6.2.10.2 Procedure for the SCM Organization.

6.2.10.2.1 Scheduling. Place the SCM Variance Authorization on the agenda for consideration at a future CCB meeting. Identify the requestor as a temporary member of the CCB for the meeting at which the SCM Variance Authorization is considered.

6.2.10.3 Procedure for the CCB.

6.2.10.3.1 Evaluation. Determine whether the information provided on the form is complete and consistent. Assess the merit of the request and decide upon its disposition. In particular assess the requested variance with respect to any applicable provisions of *QARD Quality Assurance Requirements Document for the Radioactive Nuclear Waste Management Program.*

6.2.10.3.2 Disposition. Perform one of the following actions based upon the outcome of Step 6.2.10.3.1.

- If the variance is authorized exactly as requested, check the Approved box in the Disposition field of the form and proceed to Step 6.2.10.3.3.
- If the variance is granted in a modified form, check Approved with Modifications, explain the modifications in the SCM/CCB Comments field, and proceed to Step 6.2.10.3.3.
- If insufficient information is provided, check the Insufficient Information box, explain the omission in the SCM/CCB Comments field, and proceed to Step 6.2.10.3.3.
- If the request is not granted, check the Not Approved box, document the reason in the SCM/CCB Comments field, and proceed to Step 6.2.10.3.3.

6.2.10.3.3 Return to SCM. Sign and date the SCM Variance Authorization, and return a copy to the SCM Organization for submission to the CSA Active File, and terminate the process.

6.3 Configuration Status Accounting (CSA)

6.3.1 CSA Records Collection

6.3.1.1 Procedure for the SCM Organization.

6.3.1.1.1 Marking. Upon receipt of a supplemental documentation form, assign a unique, serial numeric identifier to the form, and record the identifier in the identification field located in the upper right corner of the form.

6.3.1.1.2 **Archiving.** Ensure that the information provided on the form is recorded in the CSA data base.

6.3.1.1.3 **Updating the CSA Active File.** When a supplemental-documentation form is closed, place a copy of the form in the CSA Active File pending its incorporation into a records package for transfer to the LANL YMP Records Processing Center.

6.3.1.1.4 **CSA Reports.** Upon generation of a CSA Report, place a copy in the CSA Active File pending its incorporation into a records package for transfer to the LANL YMP Records Processing Center.

6.3.2 CSA Records Maintenance and Storage

6.3.2.1 Procedure for the SCM Organization.

6.3.2.1.1 **Updates to CSA Records.** Upon receipt of an updated supplemental documentation form, ensure that the update information is recorded in the CSA data base.

6.3.2.1.2 **Updating the CSA Active File.** If the form is closed, place a copy in the CSA Active File pending its incorporation into a records package foı transfer to the LANL YMP Records Processing Center.

6.3.2.1.3 **Records Packages.** Employ only closed CSA records in a records package.

6.3.3 Reports

6.3.3.1 Procedure for the Requestor.

6.3.3.1.1 **Documentation.** Request generation of a CSA report by completing a CSA Information Request as follows:

- General Information. Furnish the date of the request and the requestor's name, organizational affiliation, telephone number, and Laboratory mail stop in the corresponding fields of the form.
- Report Name. Propose a name for the report.
- Report Content. If the CSA Information Request specifies a new report that has not been previously issued, check the New box. Otherwise, if the request is for issuance of an update to an existing report, check the Update box.
- Report Type. Specify a periodic report by checking one of the boxes that designates the issuing period. Specify an on-demand or ad hoc report by checking the corresponding box. Check only one box.
- Description. If the New box is checked in the Report Content field, furnish a description of the proposed report here.

6.3.3.1.2 **Submission.** Sign and date the CSA Information Request in the space reserved for the requestor. Submit the form to the LANL YMP SCM Organization.

6.3.3.2 Procedure for the SCM Organization.

6.3.3.2.1 Verification. Upon receipt of a CSA Information Request, verify that the form is signed by the requestor. If verification fails, check the Not Approved box in the Disposition field, and proceed to Step 6.3.3.2.5.

6.3.3.2.2 Evaluation. Determine whether the CSA data base contains sufficient and appropriate information to generate the report. Also assess whether the SCM Organization has sufficient resources to generate the report within the time constraints or at the frequency requested.

6.3.3.2.3 Disposition. Perform one of the following actions based upon the outcome of Step 6.3.3.2.2.

- If the evaluation indicates that the report can be generated as requested, check the Approved box in the Disposition field of the form and proceed to Step 6.3.3.2.4.
- If generation of the report is to be held in suspense, check the Tabled box, provide an explanation for this decision in the SCM Comments box, and proceed to Step 6.3.3.2.5.
- If the report is not approved, check the Not Approved box, document the reason in the SCM Comments field, and proceed to Step 6.3.3.2.5.

6.3.3.2.4 Generation and Distribution. Generate the report and distribute copies to each person/organization designated on the distribution list specified in the Description field. Submit a copy to the CSA Active File. For periodic reports, repeat this step at the period specified in the Report Type field of the CSA Information Request.

6.3.3.2.5 Notify Requestor. Sign and date the CPL Transmittal Request, and return a copy to the requestor. Submit a copy to the CSA Active File, and terminate the process.

6.4 Configuration Auditing

6.4.1 Functional Configuration Audit (FCA)

6.4.1.1 Procedure for the Software Configuration Manager.

6.4.1.1.1 Allocate Resources. Assign sufficient and appropriate resources to conduct the FCA.

6.4.1.2 Procedure for SCM Auditor(s).

6.4.1.2.1 Assessment. Evaluate the functional characteristics of the baseline. Identify major functional inadequacies that preclude conducting a subsequent review.

6.4.1.2.2 Documentation. Document each major issue on a Review/Audit Item Disposition form. See TWS-QAS-QP-03.17, *Reviews of Software and Computational Data,* for instructions on completing this form.

6.4.1.2.3 FCA Summary. Summarize the findings of the auditors on a Review/Audit Report and Recommendations form. See TWS-QAS-QP-03.17, *Reviews of Software and Computational Data*, for instructions on completing this form.

6.4.1.2.4 Notification of Developer. Sign and date the Review/Audit Report and Recommendations in the space reserved for the SCM/CCB Representative. Provide a copy of the form and all attendant Review/Audit Item Disposition forms to the developer. Submit the originals to the CSA Active File.

6.4.1.2.5 Verification of Issue Resolution. Upon resubmittal of a baseline that previously failed the audit, verify that each issue identified on a Review/Audit Item Disposition is resolved to the auditor's satisfaction. For each such issue, sign and date the corresponding Review/Audit Item Disposition, transmit a copy to the developer, and submit a copy to the CSA Active File. Repeat this step until all outstanding issues are resolved.

6.4.1.3 Procedure for the Developer

6.4.1.3.1 Issue Resolution. Resolve the issues identified on Review/Audit Item Disposition forms. As each issue is resolved, sign and date the corresponding Review/Audit Item Disposition form in the space reserved for the developer. Upon completion, resubmit the updated baseline into the formal audit/review process.

7.0 QUALITY ASSURANCE DOCUMENTATION

7.1 Records

The following documents are Project QA records.

- All components of a certified baseline as specified in TWS-QAS-QP-03.19, *Documentation of Software and Computational Data*
- All LANL YMP supplemental documentation forms that meet the acceptance criteria of Section 8.0
- All CSA reports issued by the SCM Organization and for which a CSA Information Request has been accepted.

All records are combined into records packages for submission to the Records Processing Center in accordance with the provisions of TWS-QAS-QP-17.3, *Procedure for LANL YMP Records Management.*

7.2 Records Packages

This procedure implements six distinct records packages that compose the complete suite of QA documentation for software and computational data baselines and the SQA effort. The SCM Organization produces and submits each records package to the LANL YMP Records Processing Center.

7.2.1 Certified Baseline Records-Package

This records package documents all aspects of the development, assessment, and certification of a baseline. It is produced by the SCM Organization after it formally certifies (issues a Baseline Certification Notice for) the subject baseline. It comprises the following components:

- the baseline components specified in Section 7.0 of TWS-QAS-QP-03.19, *Documentation of Software and Computational Data,* for the corresponding baseline
- any CPL Transmission Request forms that were issued for software releases that supported the development of the baseline
- any SCM Variance Authorizations that were issued in support of the development, assessment, or certification of the baseline
- the Baseline Submission Summary form that accompanied the proposed baseline into the formal audit/review process
- all Software Review Notice forms, Review/Audit Report and Recommendations forms and the associated Review/Audit Item Description forms that describe the formal audits and reviews to which the baseline was subjected
- the Baseline Certification Notice form that documents the certification of the baseline
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

7.2.2 CCB Meeting Records-Package

This records package documents a meeting of the CCB. It is produced by the SCM Organization after acceptance of the minutes of a CCB meeting by the CCB. It consists of the following closed supplemental documentation forms:

- the CCB Meeting Minutes form
- the CCB Meeting Announcement form that is referenced on the CCB Meeting Minutes
- Any SCM Variance Authorizations that are not associated with a particular development task
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

7.2.3 Change-Initiation Records-Package

This records package documents a collection of functionally related formal change-proposals that have been made against LANL YMP software and computational data. It is produced by the SCM Organization after the constituent change proposals are closed. It consists of the following closed supplemental documentation forms:

- one or more Software Change Requests
- one or more Software Incident Reports
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

7.2.4 Interface Records-Package

This records package describes and documents the disposition of a formal request to release sanctioned LANL YMP software or computational data to an external entity. It is produced by the SCM Organization after the subject Software/Data Dissemination Request is closed. It consists of the following closed supplemental documentation forms:

- one or more Software/Data Dissemination Requests
- any SCM Variance Authorization forms that are issued to implement the release
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

7.2.5 SCM Records-Package

This records package describes and documents the routine operation of the SCM Organization. It is produced by the SCM Organization at regular intervals as specified by the Software Configuration Manager. It consists of any CSA Reports generated and distributed during the interval and any of the following supplemental documentation forms that are closed during the interval:

- CCB Participation Notices
- any CSA Information Requests that have been executed
- any Reviewer Qualifications Summaries that have been received
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

7.2.6 Task Records-Package

This records package describes and documents a particular software development or computational data-generation task. It is produced by the SCM Organization after the Engineering Change Notice for the subject task is issued. For software development tasks it contains the documents that authorize the work and configure the life cycle. For software and computational data tasks, the document that closes the task is also included. The Task Records Package consists of the following closed supplemental documentation forms:

- Engineering Change Directive (software development tasks only)
- Life-Cycle Specification (software development tasks only)
- Engineering Change Notice
- all Standard Continuation Forms referenced by any of the above supplemental documentation forms.

8.0 ACCEPTANCE CRITERIA

Acceptance criteria for LANL YMP baselines are specified TWS-QAS-QP-03.17, *Reviews of Software and Computational Data* and in TWS-QAS-QP-03.19, *Documentation of Software and Computational Data.*

Supplemental Documentation Forms are formally accepted when they are closed.

CSA Reports are formally accepted upon issuance by the SCM Organization. Furthermore, to be accepted, a closed CSA Information Request must exist for the CSA Report.

9.0 ATTACHMENTS AND APPENDIXES

Exhibit 1: Baseline Certification Notice

Exhibit 2: CCB Meeting Announcement

Exhibit 3: CCB Meeting Minutes

Exhibit 4: CCB Participation Notice

Exhibit 5: CSA Information Request

Exhibit 6: Engineering Change Notice

Exhibit 7: Reviewer Qualifications Summary

Exhibit 8: Software/Data Dissemination Request

Exhibit 9: SCM Variance Authorization

Appendix A: Flow Charts

ATTACHMENTS
Supplemental Documentation Forms

BASELINE CERTIFICATION NOTICE

DATE	SUBJECT			BCN-
DEVELOPER	ORGANIZATION		TELEPHONE	MAIL STOP
LCS REFERENCE	APPLICATION NAME			

REQUIREMENTS PHASE	☐ REQUIREMENTS BASELINE	☐ BASELINE/PHASE CLOSED
DESIGN PHASE	☐ PRELIMINARY DESIGN BASELINE ☐ V & V PLAN BASELINE ☐ DETAILED DESIGN	☐ BASELINE/PHASE CLOSED
IMPLEMENTATION PHASE	☐ V&V PROCEDURES BASELINE ☐ IMPLEMENTATION BASELINE	☐ BASELINE/PHASE CLOSED
DATA	☐ COMPUTATIONAL DATA BASELINE	☐ BASELINE CLOSED

COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

SCM REPRESENTATIVE DATE

CCB MEETING ANNOUNCEMENT			
MEETING DATE	MEETING TIME	MEETING LOCATION	CMA-
AGENDA			
			SCF-

LOS ALAMOS Yucca Mountain Project	SCM REPRESENTATIVE / DATE

CCB MEETING MINUTES

CMA REFERENCE	DATE	CCB CHAIR	RECORDER	CMM-

MINUTES

SCF-

LOS ALAMOS
Yucca Mountain Project

RECORDER (SUBMISSION) DATE

CCB CHAIR (ACCEPTANCE) DATE

CCB PARTICIPATION NOTICE

DATE	NAME	ORGANIZATION	CPN-

RQS REFERENCE	TELEPHONE	MAIL STOP	EXTERNAL ADDRESS

MEMBERSHIP

- ☐ PERMANENT MEMBER
- ☐ ROTATING MEMBER ______ TERM EXPIRES
- ☐ TEMPORARY MEMBER ______ TERM EXPIRES
- ☐ OBSERVER

ROLE OF TEMPORARY MEMBER

- ☐ REVIEW(S)
- ☐ SIR/SCR DEFENSE ______ REFERENCE
- ☐ SIR/SCR ANALYSIS ______ REFERENCE
- ☐ OTHER (SEE COMMENTS)

STATUS

- ☐ VOTING
- ☐ NON-VOTING

COMMENTS/RESTRICTIONS

SCF-

LOS ALAMOS
Yucca Mountain Project

______ SCM REPRESENTATIVE ______ DATE

CSA INFORMATION REQUEST

DATE	REQUESTOR	ORGANIZATION	TELEPHONE	MAIL STOP	CIR-

REPORT NAME	REPORT CONTENT	REPORT TYPE
	☐ UPDATE ☐ NEW	PERIODIC ☐ WEEKLY ☐ BI-WEEKLY ☐ MONTHLY ☐ OTHER SPECIFY ____ ☐ ON-DEMAND ☐ AD-HOC

DESCRIPTION

SCF-

DISPOSITION	SCM COMMENTS
☐ APPROVED ☐ NOT APPROVED ☐ TABLED ☐ OTHER (SEE COMMENTS)	SCF-

LOS ALAMOS
Yucca Mountain Project

REQUESTOR ____ DATE ____

SCM REPRESENTATIVE ____ DATE ____

ENGINEERING CHANGE NOTICE

DATE	APPLICATION NAME		ECN-
ECD REFERENCE	**SCN REFERENCE**	**RELEASE LABEL**	

COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

SCM REPRESENTATIVE

DATE

REVIEWER QUALIFICATIONS SUMMARY

DATE	REVIEWER'S NAME	EXTERNAL ADDRESS	RQS-
ORGANIZATION	MAIL STOP		TELEPHONE

SUMMARY OF QUALIFICATIONS & EXPERIENCE

SCF-

REVIEWER'S CURRENT POSITION & PRIMARY WORK

SCF-

OTHER COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

REVIEWER   DATE

SCM REPRESENTATIVE   DATE

SOFTWARE/DATA DISSEMINATION REQUEST

DATE	APPLICATION OR DATA RELEASE ID		SDDR-
REQUESTOR	TELEPHONE	ORGANIZATION	MAIL STOP
EXTERNAL ADDRESS			☐ YMP USE ☐ EXTERNAL USE

FILE TRANSMITTAL BLOCK

CONTACT	PHONE	MAIL STOP
HARDWARE PLATFORM	OPERATING SYSTEM	
FILE FORMAT (ASCII, TAR, CPIO, VMS BACKUP, ETC.)		

METHOD OF DISTRIBUTION

☐ TAPE	☐ DISK	☐ NETWORK FILE TRANSFER
TAPE TYPE ______	DISK TYPE ______	☐ CFS
DENSITY ______	DENSITY ______	☐ FTP NODE NAME ______
LABEL ______	FORMAT ______	☐ DECNET
FILE NAME ______	FILE NAME ______	FULL PATHNAME ______

COMMENTS

SCF-

DISPOSITION	SCM/CCB COMMENTS
☐ APPROVED ☐ APPROVED WITH MODIFICATIONS ☐ REQUIRES CCB ACTION ☐ TABLED ☐ NOT APPROVED	SCF-

LOS ALAMOS
Yucca Mountain Project

REQUESTOR ______ DATE ______

SCM REPRESENTATIVE ______ DATE ______

SCM VARIANCE AUTHORIZATION

DATE	SUBJECT			SVA-
ECD REFERENCE	REQUESTOR	TELEPHONE	ORGANIZATION	MAIL STOP

TYPE OF VARIANCE

- ☐ SCM PROCEDURE
- ☐ DOCUMENTED STANDARD
- ☐ REVIEW PROCEDURE
- ☐ V & V PROCEDURE
- ☐ DATA MANAGEMENT PROCEDURE
- ☐ OTHER ______________

DESCRIPTION (IDENTIFY SPECIFIC SECTIONS OF SQAP, QP, AND/OR STANDARDS DOCUMENT)

SCF-

JUSTIFICATION

SCF-

DISPOSITION

- ☐ APPROVED
- ☐ APPROVED WITH MODIFICATIONS
- ☐ INSUFFICIENT INFORMATION
- ☐ NOT APPROVED

SCM/CCB COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

______________ REQUESTOR ______ DATE

______________ CCB CHAIR ______ DATE

APPENDIX A
Flow Charts

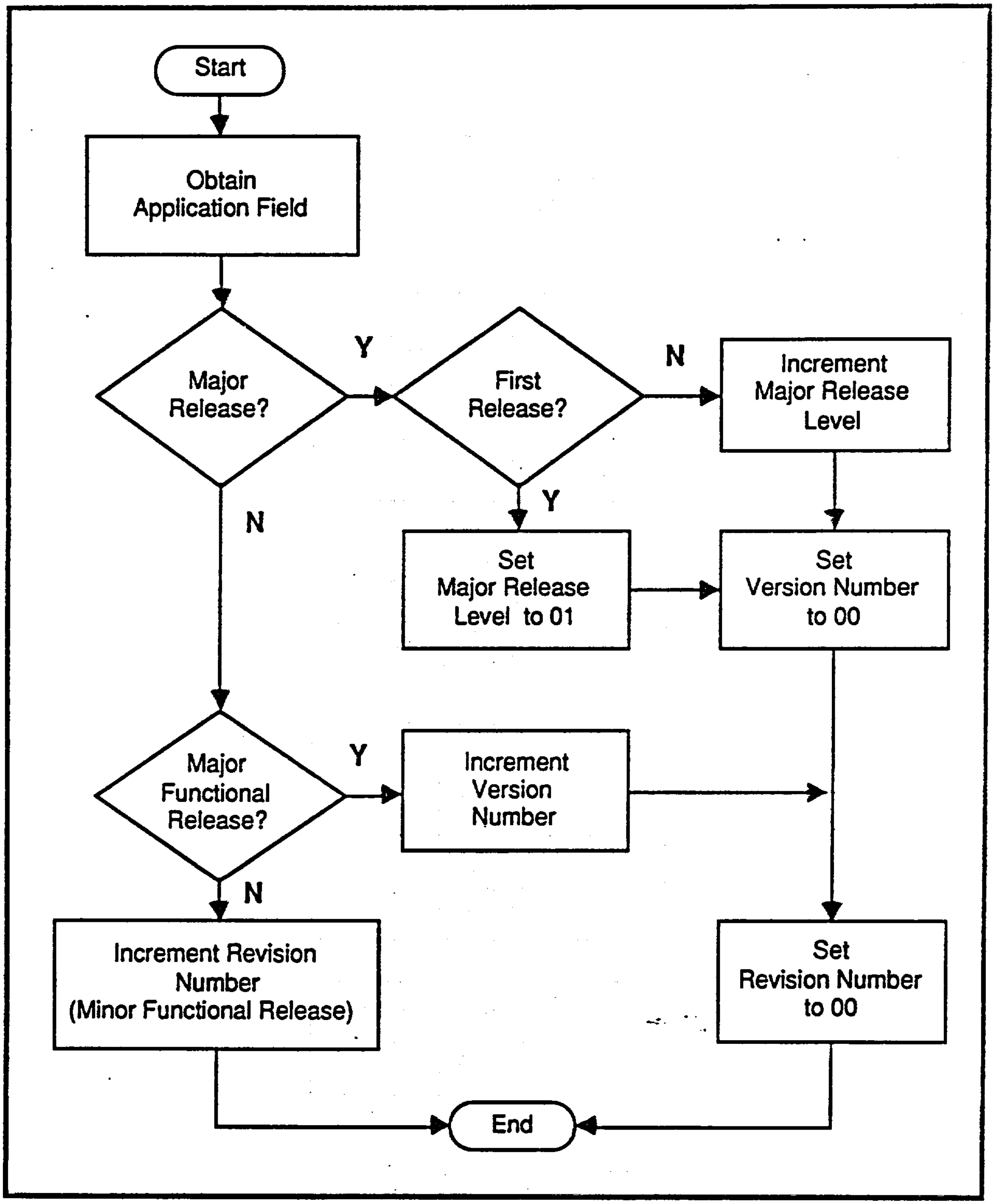

Figure 1. Release Labeling Methodology

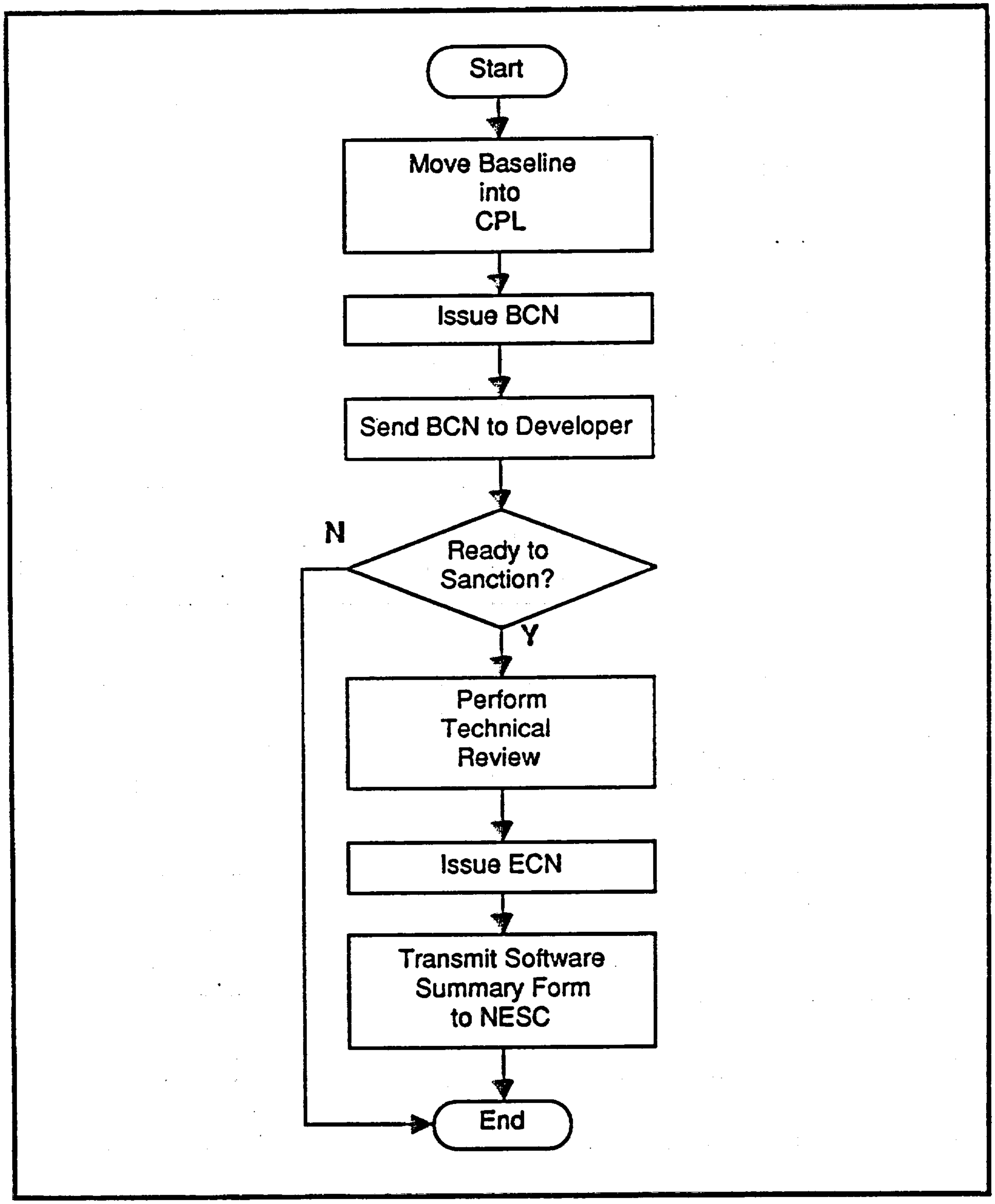

Figure 2. Baseline Certification and Sanctioning

SOFTWARE LIFE CYCLE

Effective Date: ____________________

D. R. Hines **Preparer**	**Date**
S. L. Bolivar **Quality Assurance Project Leader**	**Date**
R. J. Herbst **Technical Project Officer**	**Date**

SOFTWARE LIFE CYCLE

1.0 Purpose

This document describes the software life-cycle model implementation as it applies to software developed for the Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP).

2.0 Scope

This procedure applies to all LANL YMP software development activities that are performed to support licensing.

3.0 References

ANSI/IEEE Std 829-1983, *IEEE Standard for Software Test Documentation,* August 1983.

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

QARD *Quality Assurance Requirements Document for the Civilian Radioactive Waste Management Program,* U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

NN1-1990-0334 *Software Supporting Scientific Investigations/Licensing*

TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

TWS-QAS-QP-03.19 *Documentation of Software and Computational Data.*

TWS-QAS-QP-03.20 *Software Configuration Management.*

TWS-QAS-QP-03.21 *Software Life Cycle.*

TWS-QAS-QP-03.22 *Verification and Validation of Software and Computational Data.*

TWS-QAS-QP-15.2 *Deficiency Reporting.*

4.0 Definitions

See LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project,* Appendixes C and D, respectively for a glossary of terms and list of acronyms used throughout this document.

5.0 Responsibilities

5.1 Developer

The responsibilities of the developer under this procedure are

- Adhering to the software life cycle specified by the Configuration Control Board (CCB) for the software development task
- Producing the baselines and baseline components specified for the software development task

5.2 Software Configuration Management (SCM) Organization

The responsibilities of the SCM Organization under this procedure are

- Evaluating and assessing baselines (control points within the life cycle) through a program of formal audits of the baseline documents
- Certifying and sanctioning baselines after CCB approval
- Closing baselines
- Closing life-cycle phases

5.3 Configuration Control Board (CCB)

The responsibilities of the CCB under this procedure are

- Authorizing software development, enhancement, or repair
- Specifying the life-cycle configuration for any authorized development task
- Assessing the baselines produced by the development organization through a program of formal reviews of the baseline documents

6.0 Procedure

6.1 Procedure for the Change Initiator

Any LANL YMP member may be the initiator of a Software Change Request or Software Incident Report for software or computational data. The procedures for the change initiation are described in the following subsections.

6.1.1 Software Change Requests

The Software Change Request form provides a means for proposing enhancements to existing software, for requesting authorization to develop new software, or for requesting authorization to convert pre-existing software to comply with the provisions of the Los Alamos YMP software quality assurance program. As such, the Software Change Request is the mechanism for requesting the development of the first version of a software application or for initiating perfective or adaptive maintenance operations on the latest version of an existing application.

A Software Change Request may be submitted:

- Before the initiation of the formal software life-cycle for the development of the first version of a software application;
- Before the initiation of the formal software life-cycle for the conversion of pre-existing development software or acquired noncommercial software.
- During the Design, or Implementation Phase to request CCB-approval to revisit a prior (closed) life-cycle phase;
- During the Requirements, Design, or Implementation Phase to document formally an enhancement suggested for incorporation later, outside of the scope of the current development activity; or
- During the Operation Phase to initiate a perfective or adaptive maintenance activity.

The change initiator (requestor) prepares the Software Change Request as follows:

- General Information. Enter the date, name, telephone number, organization, and mail stop of the requestor.

- Subject. Provide a brief summary of the proposed change.
- Description of Proposal. Provide a detailed description of the proposed change. If enhancements to existing software are being proposed, be specific in identifying the affected software. Restrict the discussion to change description, leaving justification to the next section.
- Justification. Describe the merits of the proposed change.
- Sign and date the form.

Return the form to the SCM Organization and await notification concerning the disposition of the request.

6.1.2 Software Incident Reports

The Software Incident Report form provides a means for reporting discrepancies or problems in existing software or computational data. As such, the Software Incident Report is the mechanism for initiating corrective maintenance operations on the latest version of an existing software application or computational-data set.

A Software Incident Report may be submitted:

- During the Requirements, Design, or Implementation to document formally a known error repair of which is recommended for later, outside of the scope of the current development activity;
- During the Operation Phase to initiate a corrective maintenance activity.

The change initiator (originator) prepares the Software Incident Report as follows:

- General Information. Enter the date, name, telephone number, organization, and mail stop of the originator.
- Subject. Provide a brief summary of the problem.
- Program or Module Name. Enter the name of the module in which the problem was discovered.
- When First Occurred. Enter the date the problem was first noticed.
- Recoverable. Enter yes or no depending upon whether you were able to recover from the condition that is being reported.
- Repeatable. Enter yes or no based upon whether the condition is repeatable.
- DR Reference. If the originator has submitted a Deficiency Report (see TWS-QAS-QP-15.2 *Deficiency Reporting*) in conjunction with this Software Incident Report, provide the Deficiency Report number here.
- Description of Problem. Provide a description of the problem. Do not rely on attachments or enclosures as a complete description of the problem. The main discussion should be provided here, referencing any attachments when necessary.
- Sign and date the form.

Return the form to the SCM Organization and await notification concerning the disposition of the request.

6.2 Procedure for the SCM Organization

6.2.1 Software Change Requests and Software Incident Reports

Upon receipt of a Software Change Request or Software Incident Report

- Inspect the form for completeness. If the information supplied is adequate, continue on to the next step in the process.
- If the form is not complete, under "Disposition", check the box marked "Insufficient Information", and explain in the "Analysis" section. Return the form to the originator and exit this procedure.
- Assign a unique identifying number to the form.
- Log the form into the Configuration Status Accounting (CSA) data base.
- Add the Software Change Request or Software Incident Report to the agenda for a future CCB meeting. If the form was returned by an analyst, exit this procedure.

6.2.2 CPL Transmittal Requests

Upon receipt of a CPL Transmittal Request, determine the disposition of the request as follows:

- Approved. Check this box if the request is approved. Sign and date the form.
- Approved With Modifications. If the request is approved, but the original request has been modified, check this box and supply explanation in the "SCM/CCB Comments" box. Sign and date the form.
- Requires CCB Action. If the request is of such a scope and nature that the SCM Organization requires input from the CCB, check this box. As appropriate, supply explanation in the "SCM/CCB Comments" box. Add the request to the agenda of a future CCB meeting.
- Incomplete. If there was insufficient information to enable the SCM organization to grant the request, check the "Incomplete" box. Supply an explanation in the "SCM/CCB Comments" box. Sign and date the form and return it to the requestor.
- Not Approved. Check this box if the request is rejected. Supply an explanation in the "SCM/CCB Comments" box. Sign and date the form and return it to the requestor.

6.2.3 Life-Cycle Support

Perform SCM audits on all baselines submitted for formal review. Perform all assessment and engineering releases authorized by the CCB in support of the development task. Certify each baseline after completion of the corresponding baseline-closure review. Sanction the implementation baseline and distribute the sanctioned software to the user community.

6.2.4 Discrepancy-Analysis Support

Utilize the resources of the SCM Organization (in particular the CSA Database, the Computer Program Library, and the LANL YMP Computational-Data Archive) to provide support to the CCB and analyst in determining the cause, impact on previous calculations, and possible corrective actions for discrepancies reported on a Software Incident Report. Cooperate in the generation of on-demand CSA reports to establish the scope of impact of the discrepancy and supply the mechanism for notifying affected users of suspect software and/or data. In determining the impact of the discrepancy on computational data, restrict the scope of the inquiry to certified computational-data baselines resident in the LANL YMP Data Archive.

6.3 Procedure for the CCB

The CCB specifies the disposition of all Software Change Requests and Software Incident Reports.

6.3.1 Evaluation and Analysis

Evaluate the proposed Software Change Request or Software Incident Report. If sufficient expertise exists on the CCB to determine the nature, impact, and scope of the proposed change or problem, assign the CCB as analyst and perform the analysis in accordance with the provisions of Section 6.4.2. If there is insufficient expertise at the meeting to make this determination or if it is inappropriate to perform the analysis within the context of the CCB meeting, assign an analyst to perform additional evaluation and schedule further consideration of the Software Change Request or Software Incident Report for a subsequent meeting.

6.3.2 Disposition

6.3.2.1 Software Change Requests

Determine the disposition of the Software Change Request as follows:

- Insufficient Information. Check this box if there was insufficient information to analyze the Software Change Request. Sign and date the form and return it to the SCM Organization.
- Previously Requested. Check this box if the proposed change is already described on another Software Change Request and provide the form number of the existing Software Change Request. Sign and date the form, and return it to the SCM Organization.
- Not Approved. If the request is rejected by the CCB, check this box, sign and date the form, and return it to the SCM Organization.
- Approved, Approved With Modifications. If the CCB approves the request, check the appropriate box. If work can begin immediately, check the box marked "Assigned" and provide the form number of the authorizing Engineering Change Directive; otherwise table the Software Change Request by leaving the box marked "Assigned" unchecked. Sign and date the form, and return it to the SCM Organization.

6.3.2.2 Software Incident Reports

Determine the disposition of the Software Incident Report as follows:

- No Error Found. Check this box if no error exists. Sign and date the form, and return it to the SCM Organization.
- Insufficient Information. Check this box if there was insufficient information to analyze the Software Incident Report. Sign and date the form and return it to the SCM Organization.

- Previously Reported. Check this box if the problem is already described on another Software Incident Report and provide the form number of the existing Software Incident Report. Sign and date the form and return it to the SCM Organization.
- Error Acknowledged. If analysis indicates that a problem exists, check this box. If work can begin immediately, check the box marked "Assigned" and provide the form number of the authorizing Engineering Change Directive; otherwise table the Software Incident Report by leaving the box marked "Assigned" unchecked. Sign and date the Software Incident Report and return it to the SCM Organization.

6.3.3 Life-Cycle Configuration

Following approval and assignment of a Software Change Request or Software Incident Report, proceed as follows:

6.3.3.1 Engineering Change Directive (General Information)

Initiate an Engineering Change Directive and prepare the form as follows:

- Date. Enter the date of the current CCB meeting.
- Title. Enter a descriptive title for the development task.
- Developer Information. Enter the developer's name, telephone number, organization, and mail stop.
- Software Class. Determine the software class and enter the designation in this box. For a description of the various software classes, refer to Section 5.2.2.1 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*
- Heritage. Determine the software heritage and enter the designation in this box. For a description of the various software heritages, refer to Section 5.2.5 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*
- SCR References. Supply the form numbers of all Software Change Requests that initiated the Engineering Change Directive.
- SIR References. Supply the form numbers of all Software Incident Reports that initiated the Engineering Change Directive.

6.3.3.2 Life-Cycle Specification

Initiate a life-cycle specification process by preparing a Life Cycle Specification form as described below. Regardless of the software heritage designation specified on the ECD, prepare the Life Cycle Specification *as though the development task is for new development software.*

6.3.3.2.1 General Information. Enter the date, title, ECD reference, and the developer's name, telephone number, organization, and mail stop.

6.3.3.2.2 Life Cycle Phases. Identify the life-cycle phases that must be traversed for this development task. Check the corresponding boxes on the Life Cycle Specification form. Refer to Table 1 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project* to determine the minimum set of life-cycle phases that must be specified.

6.3.3.2.3 Baselines and Baseline Components. Identify the documentation components that must be developed for this task and allocate each component to the appropriate life-cycle phase. Refer to Table 2 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project* to determine the minimum set of documentation components required for the subject software class. Table 3 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project* specifies how to allocate the documentation components among life-cycle phases.

Allocate each documentation component into one (and only one) of the baselines associated with the phase. For each baseline to which one or more documentation components are assigned, check the corresponding box on the Life Cycle Specification form. Also check the box(es) that correspond to the allocated components within the baseline. Always check the File List, Primary Modules, and/or Support Modules box(es) for any baseline that is specified.

6.3.3.2.4 Reviews. Identify the reviews that will be performed to certify the products of the development task. If the Requirements, Design, and/or Implementation baselines are specified, select the corresponding baseline-closure reviews (SRR, CDR, and SAR, respectively) by checking the appropriate box(es) on the Life Cycle Specification form. Specify a target date for each review in the space provided on the form. Optionally, an in-process review may be specified for any or all of these baselines by checking the corresponding In-Process Review box(es) and indicating a target date for each such review in the space provided.

If the Preliminary Design, V&V Plan, and/or V&V Procedures baselines are specified, select the corresponding in-process reviews by checking the appropriate box(es) on the Life Cycle Specification form. Specify a target date for each review in the space provided on the form.

6.3.3.2.5 Authorization. Sign and date the Life Cycle Specification, and return it to the SCM Organization.

6.3.3.3 Engineering Change Directive (Additional Information)

Complete the Engineering Change Directive as follows:

- Comments. Provide a description of the development task here. If the task involves qualification of acquired noncommercial software or pre-existing development software, specify which of the development approaches specified in Section 5.2.5.1.2 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project* shall be employed.
- Sign and date the Engineering Change Directive, and return it to the SCM Organization.

6.3.4 Life-Cycle Reviews

Perform all reviews specified on the Life Cycle Specification as the appropriate baselines are completed and audited by the SCM Organization. Refer to TWS-QAS-QP-03.17 *Reviews of Software and Computational Data* for additional information.

6.4 Procedure for the Analyst

Upon evaluation of a Software Change Request or a Software Incident Report, the CCB may determine that there are insufficient resources at the meeting for analysis of the proposed change or problem, and may assign one or more analysts to examine the proposed change or problem in more detail.

6.4.1 Assessment Release

Obtain the Software Change Request or a Software Incident Report from the SCM Organization. If an existing software application or computational data baseline is affected by the Software Change Request or a Software Incident Report, obtain an assessment release from the SCM Organization by preparing and submitting a CPL Transmittal Request form. Refer to Section 6.5.1 for instructions for preparing the form.

6.4.2 Analysis

Evaluate the scope and nature of the Software Change Request or Software Incident Report. Assess the impact of the proposed changes or discrepancies on design, other baselines, or applications. Determine whether the discrepancy affects the results of previous calculations (restrict the scope of this investigation to the contents of the LANL YMP Computational Data Archive). Also establish whether the discrepancy compromises results published in any formal reports.

Formulate a plan of corrective action to eliminate the discrepancy and mitigate any problems with affected software or data baselines or formal reports. Document the results of the analysis and proposed corrective action plan in the "Analysis" portion of the respective form, and include an estimate of the number of person-hours expended in the analysis effort. Sign and date the form and return the form to the SCM Organization.

For discrepancies (reported on a Software Incident Report) determine whether the discrepancy constitutes a condition-adverse-to-quality or a significant-condition-adverse-to-quality. If so, initiate a Deficiency Report within the framework of TWS-QAS-QP-15.2 *Deficiency Reporting* and annotate the "DR Reference" section of the Software Incident Report with the identifying number of the resulting Deficiency Report.

6.5 Procedure for the Developer

Upon issuance of the Engineering Change Directive and Life Cycle Specification by the CCB, the developer may begin the software development task.

6.5.1 Engineering Release

If the associated Engineering Change Directive authorizes work on existing software, initiate an engineering release by preparing a CPL Transmittal Request form as follows:

- General Information. Enter the date, title, and requestor's name, telephone number, organization, and mail stop.
- SCR Reference, SIR Reference. These boxes apply only to assessment releases performed by an analyst. The developer ignores these boxes. The analyst supplies the appropriate references for the Software Change Request(s) or Software Incident Report(s) that initiated the analysis effort.
- ECD Reference. Enter the number of the Engineering Change Directive that authorizes the development effort. This box does not apply to an analyst requesting an assessment release.
- Action. Check the box marked "Engineering Release". If the release is being requested by an analyst to assess a Software Change Request or Software Incident Report, mark "Assessment Release".
- Content. Characterize the general content of the release by checking the appropriate box.
- File Transmittal Block. Complete the File Transmittal Block. Completion of this section provides the SCM Organization with information necessary to transmit the proposed baseline to the requestor. For additional information on completing the File Transmittal Block, refer to TWS-QAS-QP-03.20, *Software Configuration Management*, Section 6.2.9.1.1.
- Sign and date the form.

Submit the form to the SCM Organization and await receipt of the requested material.

6.5.2 Traversal of the Software Life Cycle

Proceed through the life-cycle phases in the order that they are specified on the Life Cycle Specification form.

Within each phase, develop the baselines and baseline components that are specified on the Life Cycle Specification form. Employ a development strategy that effectively addresses the relevant technical issues and produces baseline components that comply with TWS-QAS-QP-3.19, *Documentation of Software and Computational Data.*

Omit any phases, baselines, and baseline components that are not specified on the Life Cycle Specification form.

6.5.2.1 Development Philosophy

LANL YMP software development policies allocate the majority of the life cycle to unconstrained development activity, the goal of which is to develop specific software and documentation components (baselines). The rigorous controls imposed on the acceptance of any baseline (refer to TWS-QAS-QP-3.17, *Reviews of Software and Computational Data,* and to TWS-QAS-QP-3.19, *Documentation of Software and Computational Data*) eliminate the need to mandate specific development methodologies or procedures. Consequently, the experience and expertise of the developer can be focused upon the solution of the problem, the creative process is not compromised, and the technical quality of the final product is assured. Figure 1 illustrates this process.

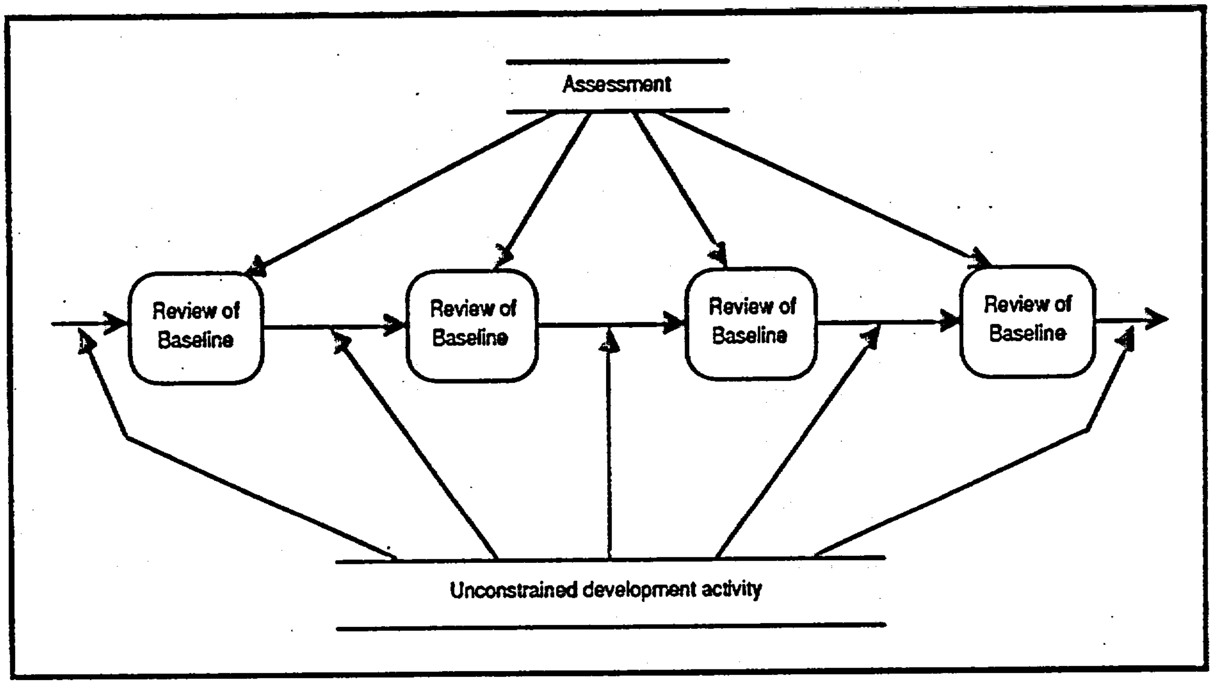

Figure 1. Software Development and Reviews.

6.5.2.2 Life-Cycle Phase Execution

Direct all activities conducted within the scope of a life-cycle phase toward:

(1)Generation of the baseline documents specified on the associated Life Cycle Specification form for the phase.

(2)Completion of all reviews specified for the life-cycle phase on the associated Life Cycle Specification form and resolution of all review/audit issues to the satisfaction of the change control authority.

6.5.2.3 Design Iteration

If it is necessary to revisit a prior life-cycle phase for the purpose of updating an associated baseline, the following procedures shall be executed.

6.5.2.3.1 Prior Phase Open Concurrently. If the baseline-closure review has not yet been completed for the prior phase, perform the necessary updates to the appropriate components of the associated baseline(s).

6.5.2.3.2 Prior Phase Already Closed. If the baseline-closure review has already been completed for the prior phase, perform the following steps.

- Submit a Software Change Request that identifies the changes to be made to the appropriate components of the associated certified baseline(s).
- If the Software Change Request is approved by the CCB, submit a CPL Transmittal Request to the SCM Organization to obtain the components to be changed.
- Proceed through the Life Cycle Specification for the task as specified by the CCB to accomplish the changes. Modify the designated documentation components and submit the resulting updated baselines to all reviews specified on the LCS.

6.5.2.3.3 Updates to Current-Phase Software and Documentation. Upon completion of the updates to prior phase documents, ensure that all information developed during the currently open life-cycle phase is consistent with the updates, or modify the appropriate documents to re-establish consistency.

6.5.2.4 Rapid Prototyping

During software development, it may be necessary to perform a rapid prototyping activity. Rapid prototyping is a process that allows the developer to suspend the current development activity and investigate informally alternative design approaches, algorithms, or other issues critical to the specification, design or implementation of the software application. Rapid prototyping permits tasks (e.g., coding) to be performed that would normally take place during a future development phase.

Rapid prototyping is not a substitute for the formal life-cycle-based development cycle, or any phase thereof. A rapid prototyping activity suspends the normal development life-cycle. The results of the informal investigation are then employed to guide the subsequent formal development efforts.

The procedure for rapid prototyping is given below and is illustrated in Figure 2.

- Suspend the normal, life-cycle-based development activity.
- Begin a rapid prototyping effort to investigate issues critical to the specification, design or implementation of the software application.
- Upon completion of the rapid prototyping effort, return to the development phase at the point of departure, employing the results of the rapid prototyping effort to guide the subsequent life-cycle-based development activities.

6.5.2.5 Closing a Life-Cycle Phase

The initiating event for the closure of a life-cycle phase is a baseline closure review. Refer to LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project*, for a discussion of baseline closure reviews. The procedure for closing a life-cycle phase is given below and is illustrated in

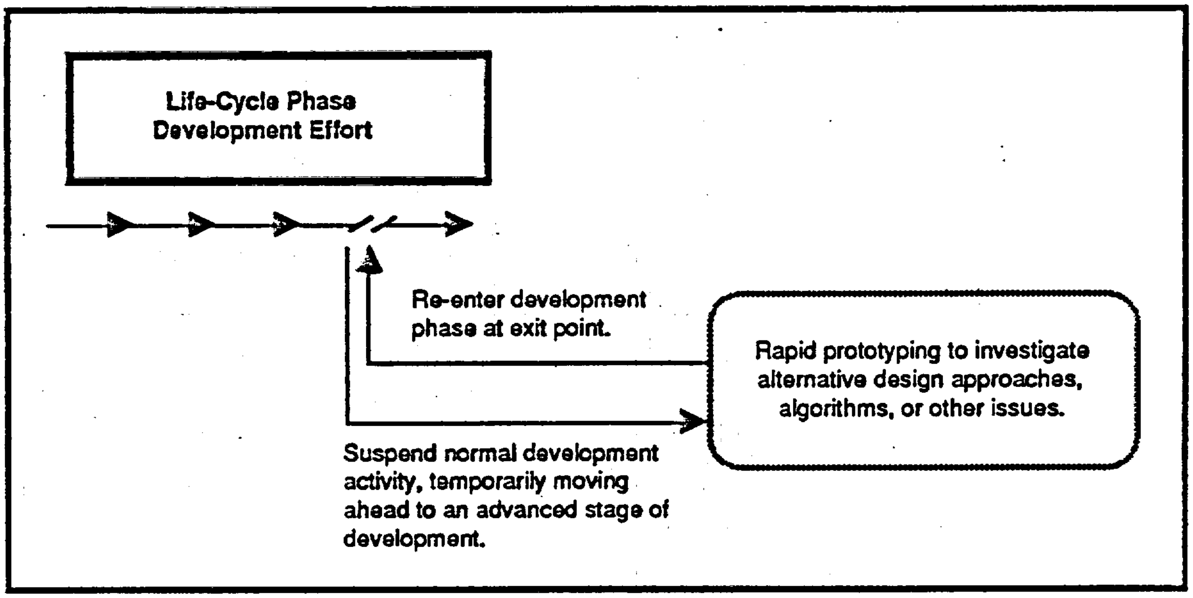

Figure 2. Rapid Prototyping.

Figure 3. Table 1 summarizes the baseline closure reviews as they apply to the life-cycle phases.

- If the life-cycle phase is not specified on the Life Cycle Specification form, exit the procedure; otherwise proceed to the next step.
- If any prior phases are open, exit the procedure; otherwise proceed to the next step.
- Prepare the baseline, submit it for review, and resolve all review issues to the satisfaction of the change control authority.

When the software has passed the baseline closure review at the end of the life-cycle phase, certification of the baseline by the SCM Organization closes the life-cycle phase.

Life-Cycle Phase	Baseline Closure Review	Review of
Requirements	Software Requirements Review (SRR)	Requirements Baseline
Design	Critical Design Review (CDR)	Detailed Design Baseline
Implementation	Software Acceptance Review (SAR)	Implementation Baseline

Table 1. Life-Cycle Phase Closure.

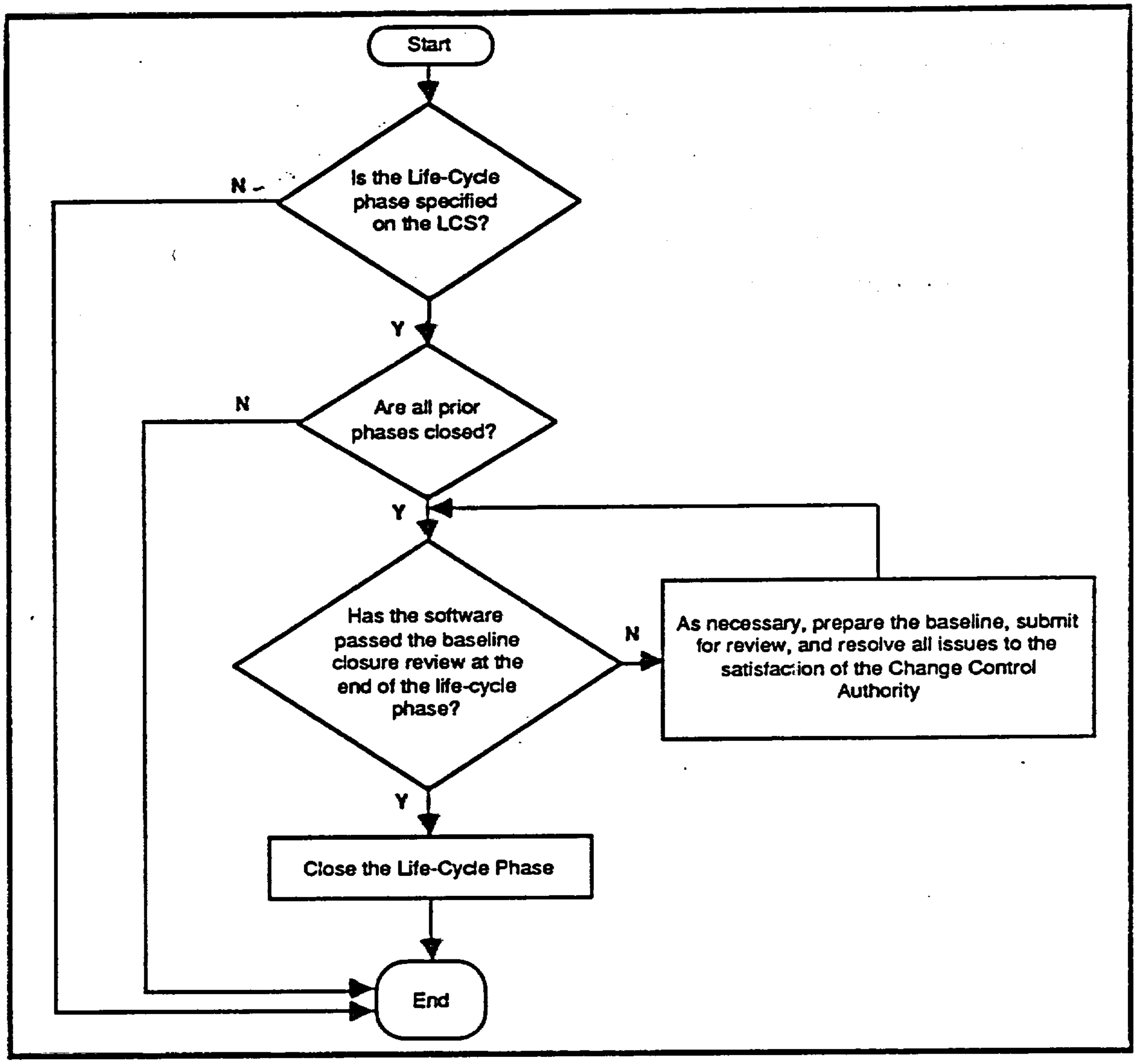

Figure 3. Closing a Life-Cycle Development Phase.

7.0 Quality Assurance Documentation

Execution of this procedure results in no formal Project QA records or records packages. However, as described in TWS-QAS-QP-03.20, *Software Configuration Management*, after certification, the corresponding baselines and supplemental-documentation are incorporated into records packages by the SCM Organization. The supplemental documentation forms that are included into these records packages are listed in Section 9.0.

8.0 ACCEPTANCE CRITERIA

LANL YMP software baselines developed during the life cycle are considered to have met acceptance criteria when reviewed and approved by the CCB in accordance with TWS-QAS-QP-3.17, *Reviews of Software and Computational Data*.

9.0 ATTACHMENTS

Exhibit 1: CPL Transmittal Request

Exhibit 2: Engineering Change Directive

Exhibit 3: Life Cycle Specification

Exhibit 4: Software Change Request

Exhibit 5: Software Incident Report

ATTACHMENTS
Supplemental Documentation Forms

CPL TRANSMITTAL REQUEST

DATE	TITLE	CTR-

REQUESTOR	TELEPHONE	ORGANIZATION	MAIL STOP

SCR REFERENCE	SIR REFERENCE	ECD REFERENCE

CONTENT ☐ SOURCE ☐ EXECUTABLE ☐ DATA ☐ OBJECT ☐ DOCUMENTATION ☐ OTHER

ACTION ☐ ASSESSMENT RELEASE ☐ ENGINEERING RELEASE ☐ PROBATION RELEASE ☐ OTHER

FILE TRANSMITTAL BLOCK

CONTACT	PHONE	MAIL STOP

HARDWARE PLATFORM	OPERATING SYSTEM

FILE FORMAT (ASCII, TAR, CPIO, VMS BACKUP, ETC.)

METHOD OF DISTRIBUTION

☐ TAPE
TAPE TYPE ______
DENSITY ______
LABEL ______
FILE NAME ______

☐ DISK
DISK TYPE ______
DENSITY ______
FORMAT ______
FILE NAME ______

☐ NETWORK FILE TRANSFER
☐ CFS
☐ FTP NODE NAME ______
☐ DECNET
FULL PATHNAME ______

DISPOSITION
☐ APPROVED
☐ APPROVED WITH MODIFICATIONS
☐ REQUIRES CCB ACTION
☐ INCOMPLETE
☐ NOT APPROVED

SCM/CCB COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

______ REQUESTOR ______ DATE

______ SCM REPRESENTATIVE ______ DATE

ENGINEERING CHANGE DIRECTIVE

DATE	TITLE				ECD-
DEVELOPER		TELEPHONE	ORGANIZATION		MAIL STOP
SOFTWARE CLASS	HERITAGE	SCR REFERENCES		SIR REFERENCES	

COMMENTS

SCF-

LOS ALAMOS
Yucca Mountain Project

CCB CHAIR

DATE

LIFE CYCLE SPECIFICATION

DATE	TITLE			LCS-
ECD REFERENCE	DEVELOPER	TELEPHONE	ORGANIZATION	MAIL STOP

☐ REQUIREMENTS PHASE — REVIEW — TARGET DATE

- ☐ REQUIREMENTS BASELINE
  - ☐ FILE LIST ☐ SRS
- Review: ☐ IN-PROCESS ________
- Review: ☐ SRR ________

☐ DESIGN PHASE — REVIEW — TARGET DATE

- ☐ PRELIMINARY DESIGN BASELINE
  - ☐ FILE LIST ☐ SDD ☐ PRIMARY MODULES
  - Review: ☐ IN-PROCESS ________
- ☐ V & V PLAN BASELINE
  - ☐ FILE LIST ☐ VVP (PLAN ONLY)
  - Review: ☐ IN-PROCESS ________
- ☐ DETAILED DESIGN BASELINE
  - ☐ FILE LIST ☐ SDD ☐ VVP (PLAN ONLY) ☐ PRIMARY MODULES
  - ☐ MMS
  - Review: ☐ IN-PROCESS ________
  - Review: ☐ CDR ________

☐ IMPLEMENTATION PHASE — REVIEW — TARGET DATE

- ☐ V & V PROCEDURES BASELINE
  - ☐ FILE LIST ☐ VVP ☐ SUPPORT MODULES
  - Review: ☐ IN-PROCESS ________
- ☐ IMPLEMENTATION BASELINE
  - ☐ FILE LIST ☐ VVP ☐ TEST RESULTS
  - ☐ USERS MANUAL ☐ MMS ☐ VDD
  - ☐ PRIMARY MODULES ☐ SUPPORT MODULES ☐ VVR
  - Review: ☐ IN-PROCESS ________
  - Review: ☐ SAR ________

LOS ALAMOS
Yucca Mountain Project

________________________ CCB CHAIR ________ DATE

SOFTWARE CHANGE REQUEST

DATE	SUBJECT			SCR-
REQUESTOR	TELEPHONE	ORGANIZATION		MAIL STOP

DESCRIPTION OF PROPOSAL

SCF-

JUSTIFICATION

SCF-

DISPOSITION

- ☐ INSUFFICIENT INFORMATION
- ☐ PREVIOUSLY REQUESTED SCR NO. ______
- ☐ NOT APPROVED
- ☐ APPROVED
- ☐ APPROVED WITH MODIFICATIONS
- ☐ ASSIGNED ECO NO. ______

ANALYSIS

ANALYSIS EFFORT (PERSON HOURS) ______

SCF-

LOS ALAMOS
Yucca Mountain Project

REQUESTOR	DATE
ANALYST	DATE
CCB CHAIR	DATE

SOFTWARE INCIDENT REPORT

DATE	SUBJECT			SIR-
ORIGINATOR	TELEPHONE	ORGANIZATION		MAIL STOP
PROGRAM OR MODULE NAME	WHEN FIRST OCCURRED	RECOVERABLE ☐ YES ☐ NO	REPEATABLE ☐ YES ☐ NO	DR REFERENCE:

DESCRIPTION OF PROBLEM

SCF-

ANALYSIS

ERROR SCOPE: ☐ SYSTEM ☐ APPLICATION ☐ DOCUMENT ☐ DATA

ERROR TYPE: ☐ DATA REFERENCE ☐ DATA DECLARATION ☐ COMPUTATION ☐ COMPARISON ☐ CONTROL-FLOW ☐ INTERFACE ☐ INPUT/OUTPUT ☐ OTHER (SEE COMMENTS)

DISPOSITION

☐ NO ERROR FOUND

☐ INSUFFICIENT INFORMATION

☐ PREVIOUSLY REPORTED

SIR NO. ______

☐ ERROR ACKNOWLEDGED

☐ ASSIGNED ______ ECD NO.

ANALYSIS COMMENTS

ANALYSIS EFFORT
(PERSON HOURS) ______

SCF-

LOS ALAMOS
Yucca Mountain Project

ORIGINATOR	DATE
ANALYST	DATE
CCB CHAIR	DATE

VERIFICATION AND VALIDATION OF SOFTWARE AND COMPUTATIONAL DATA

Effective Date: ____________________

G. Cort **Preparer**	**Date**
S. L. Bolivar **Quality Assurance Project Leader**	**Date**
R. J. Herbst **Technical Project Officer**	**Date**

VERIFICATION AND VALIDATION OF SOFTWARE AND COMPUTATIONAL DATA

1.0 PURPOSE

The purpose of this procedure is to provide a comprehensive, independent, and traceable verification and validation (V&V) process for all software and data developed or used to support licensing. This goal is achieved through an aggressive program of formal testing, evaluation, and independent assessment.

2.0 SCOPE

This quality administrative procedure applies to all Los Alamos National Laboratory (LANL) Yucca Mountain Project (YMP) software and computational data developed or acquired to support licensing activities.

3.0 REFERENCES

ANSI/IEEE Std 829-1983, *IEEE Standard for Software Test Documentation*, August 1983.

LANL-YMP-QAPP *Los Alamos National Laboratory Quality Assurance Plan for the Yucca Mountain Project.*

LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project.*

QARD *Quality Assurance Requirements Document for the Civilian Radioactive Waste Management Program*, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, 1990.

NN1-1990-0334 *Software Supporting Scientific Investigations/Licensing*

4.0 DEFINITIONS

See LANL-YMP-SQAP *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project*, Appendixes C and D, respectively, for a glossary of terms and list of acronyms used throughout this QP.

5.0 RESPONSIBILITIES

The LANL YMP V&V strategy charges the development organization with the major responsibility for V&V activities, specifies an independent oversight and authentication role to the SCM Organization, and grants approval authority to the CCB.

The developer formulates the V&V strategy, implements the process, and documents and evaluates the results.

The SCM Organization provides independent assessment of the V&V effort through a series of formal audits of the V&V baselines and documents. Thereafter, the SCM Organization physically controls the V&V information until the formal review process is complete. In this manner, SCM provides an independent assessment of the V&V effort.

Formal reviews are conducted by the CCB, which has the authority to approve or reject the V&V documents under review. Hence, the CCB imposes another set of independent constraints upon the V&V process.

6.0 PROCEDURE

6.1 Verification of Software

The software verification process is represented schematically Figure 1 of Appendix A and is described below.

6.1.1 Requirements Traceability

6.1.1.1 Procedure for the Developer.

The developer demonstrates the traceability of requirements into the software design and implementation as follows:

6.1.1.1.1 Requirements Phase. If no Software Requirements Specification is specified for the task, then proceed to Step 6.1.1.1.3. Otherwise, to promote traceability, specify software requirements in a manner that allows them to be easily identified and tracked through subsequent baselines. Ensure that the Software Requirements Specification clearly states and uniquely identifies each software requirement.

Emphasize the development of testable requirements. A requirement that can be specifically and objectively tested of necessity must be clearly enough stated for later identification in the Design or Implementation Baseline.

6.1.1.1.2 Design Phase. During the Design Phase, demonstrate traceability of the software requirements into the software design as follows.

For the preliminary design, establish that major requirements (or groups of requirements) are allocated into the Software Design Document, thereby demonstrating that the overall architecture of the software is adequate to accommodate the requirements specified in the Software Requirements Specification. For the detailed design, map each Software Requirements Specification requirement into one or more source code modules.

Specify (in the Requirements Traceability section of each source-code documentation-prolog) the identifying number of each software requirement satisfied by the module. Ensure that each requirement in the Software Requirements Specification is implemented within one or more modules of the software design (as embodied in the documentation prolog of each software module). Further ensure that each module of the design addresses at least one software requirement.

6.1.1.1.3 Implementation Phase. During the Implementation Phase, establish that the software requirements are traceable into the software implementation (code). Demonstrate that the source code is a faithful rendition of the detailed design by comparing the source code to the corresponding pseudocode.

6.1.1.2 Procedure for the SCM Organization.

After depositing the subject baseline in the Certification Environment, confirm that the requirements are traceable into the baseline as follows

6.1.1.2.1 Design Baseline. Verify traceability of the software requirements into the software design as follows. If no Software Requirements Specification is specified for the development task, proceed to Step 6.1.1.2.2.

As part of the Functional Configuration Audit ensure that each requirement in the Software Requirements Specification is implemented within one or more modules of the software design (as embodied in the documentation prolog of each software module). Further ensure that each module of the design addresses at least one software requirement.

6.1.1.2.2 Implementation Baseline. As part of the Functional Configuration Audit, establish that the requirements specified in the Software Requirements Specification are traceable into the software implementation (code). Verify that the source code is a faithful rendition of the detailed design by comparing the source code to the corresponding pseudocode.

6.1.1.2.3 Identification and Resolution of Issues. If Steps 6.1.1.2.1 or 6.1.1.2.2 expose significant requirements traceability errors, document and resolve the issues in accordance with the provisions of TWS-QAS-QP-03.20, *Software Configuration Management.*

6.1.1.3 Procedure for the CCB.

As part of the formal review process, evaluate whether traceability requirements are met by the proposed baseline. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.1.2 Formal Testing

6.1.2.1 Procedure for the Developer.

The developer implements a program of formal testing as follows:

6.1.2.1.1 Software Requirements. To facilitate subsequent testing, emphasize the development of testable requirements.

6.1.2.1.2 Test Plan. Develop the test plan in accordance with the provisions of TWS-QAS-QP-03.19, *Documentation of Software and Computational Data.* If sufficient resources are available, develop the test plan concurrently with the detailed design, and employ personnel who are not otherwise associated with the design effort.

6.1.2.1.3 Test Execution and Assessment. Execute the program of formal testing as follows:

- Test Procedures. Derive the test procedures from the test plan in accordance with the provisions of TWS-QAS-QP-03.19, *Documentation of Software and Computational Data.*

- Test Results. Generate the test results by executing the test procedures and capturing the output in a file.
- Assessment. Compare the test results to the success criteria identified for each test in the test plan.
- Resolution. Correct any errors discovered in the previous step. If additional tests are required, repeat this procedure starting at Step 6.1.2.1. If errors are discovered in the requirements, design, or implementation, re-enter the appropriate life-cycle phase to correct the problem. (Note: this may require initiation of a formal change processing activity as described in TWS-QAS-QP-03.21, *Software Life Cycle*. Repeat Step 6.1.2.1.3 until all tests are passed.

6.1.2.1.4 Update the V&V Report. Include the results of the verification testing effort in the V&V Report and interpret the results to develcp a recommendation regarding whether the results are adequate to support verifying the software. If, due to circumstances beyond the control of the developer, the software cannot be adequately verified, provide a justification for this position in Section 6.0 of the V&V Report (TWS-QAS-QP-03.19 *Documentation of Software and Computational Data*, Appendix M). Also in this section, document a proposed schedule for completion of the verification effort at a level commensurate with the extent to which the software will be used to support a license application.

6.1.2.2 Procedure for the SCM Organization.

As part of the Functional Configuration Audit, re-execute the test procedures within the certification environment, thereby regenerating the test results. Compare the regenerated test results to those produced by the developer. If this procedure fails to reproduce the developer's test results to a reasonable degree of accuracy, document and resolve the issues in accordance with the provisions of TWS-QAS-QP-03.20, *Software Configuration Management*.

6.1.2.3 Procedure for the CCB.

As part of the formal review process, evaluate whether the testing program for the proposed baseline is satisfactory. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17 *Reviews of Software and Computational Data.*

6.2 Model Validation

The model-validation process is represented schematically in Figure 2 of Appendix A and is described below.

6.2.1 Procedure for the Developer

For each model incorporated into the application, perform the following validation steps.

6.2.1.1 Validation History.

Determine whether the model has been validated previously as a reuse component. If so, establish the reference to the V&V Report in which the validation results are described and resume the process at Step 6.2.1.5.

6.2.1.2 Identify Validation Resources.

Identify the resources that exist to support the validation effort. The most authoritative resources are independent data from YMP-approved sources. Examples of such data sources include

- Laboratory experiments,
- Field experiments and observations, and
- In situ testing.

In the event that independent data is not available to support the validation effort, consider alternative methods such as comparison of model results with analytical models, checking boundary values, and comparison with independent results produced by certified LANL YMP software.

As a last resort, employ qualified technical experts to review the model. The formal review mechanism described in TWS-QAS-QP-03.17, *Review of Software and Computational Data Baselines*, should be employed to implement this approach.

6.2.1.3 Develop the Validation Plan.

Develop a strategy for utilizing the validation resources identified in the previous step in a plan for validating the model. Specifically identify any verified, traceable data sets that are employed for comparison in the validation process and provide a justification for the use of each. Incorporate this validation plan into the V&V Plan and Procedures document.

6.2.1.4 Perform the Validation Analysis.

Implement the validation plan to determine whether the model can be validated. If the results of the validation analysis are not adequate to justify validating the model, decide whether additional validation resources exist to supplement the effort. If additional resources exist, resume the process at Step 6.2.1.2, otherwise reject the model and terminate the process.

6.2.1.5 Update the V&V Report.

Include the results of the validation analysis in the V&V Report and interpret the results to develop a recommendation regarding whether the results are adequate to support validating the model. If, due to circumstances beyond the control of the developer, the model cannot be adequately validated, provide a justification for this position in Section 6.0 of the V&V Report (TWS-QAS-QP-03.19 *Documentation of Software and Computational Data*, Appendix M). Also in this section, document a proposed schedule for completion of the validation effort at a level commensurate with the extent to which the software will be used to support a license application.

6.2.2 Procedure for the CCB

As part of the formal review process, evaluate the validation plan, validation analysis, and validation results encapsulated in the V&V Plan and Procedures document and V&V Report. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.3 Verification of Computational Data

6.3.1 Verification of Derived Data

6.3.1.1 Procedure for the Producer of the Data

Document the results of the computational data verification effort in the V&V Report for the proposed computational data baseline.

6.3.1.2 Procedure for the SCM Organization

As part of the Functional Configuration Audit, regenerate the computational data within the certification environment using certified software and input interface tables. Compare the regenerated data to the data produced by the developer. If this procedure fails to reproduce the developer's test results to a reasonable degree of accuracy, document and resolve the issues in accordance with the provisions of TWS-QAS-QP-03.20, *Software Configuration Management.*

6.3.1.3 Procedure for the CCB

As part of the formal review process of the proposed computational data baseline, establish whether the V&V Report adequately demonstrates verification of the data. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.3.2 Verification of Primary Data

6.3.2.1 Procedure for the Producer of the Data

Document the results of the computational data verification effort in the V&V Report for the proposed computational data baseline.

6.3.2.2 Procedure for the CCB

As part of the formal review process of the proposed computational data baseline, establish whether the V&V Report adequately demonstrates verification of the data. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.4 Validation of Computational Data

6.4.1 Procedure for the Producer of the Data

Evaluate the veracity of the computational data set through

- Assessment of fundamental conclusions that can be drawn from the data
- Examination of boundary behavior
- Evaluation of consistency with previously established computational, laboratory, or field results.

Document the results of the computational data validation effort in the V&V Report for the proposed baseline.

6.4.2 Procedure for the CCB

As part of the formal review process, evaluate the computational data validation effort as documented in the V&V Report. Document and resolve any problems in accordance with the provisions of TWS-QAS-QP-03.17, *Reviews of Software and Computational Data.*

6.5 The LANL YMP Certification Environment

6.5.1 Procedure for the Submitter

To initiate the transfer of a proposed baseline into the certification environment, complete the Baseline Submission Summary as described in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data*, and submit the completed form to the SCM Organization.

6.5.2 Procedure for the SCM Organization

6.5.2.1 Verification

Upon receipt of a completed Baseline Submission Summary, verify that the form is signed by the submitter and that the reference specified in the LCS Reference field is accurate. If verification fails, check the Not Accepted box in the SCM Disposition field of the form, and proceed to Step 6.5.2.6.

6.5.2.2 Disposition

If the information is complete and appropriate and the proposed baseline can be admitted to the certification environment as requested, proceed to Step 6.5.2.3. Otherwise, if the information provided on the form is inaccurate or incomplete, check the Not Accepted box, document the nature of the problem in the SCM/CCB Comments field, and proceed to Step 6.5.2.6.

6.5.2.3 Admitting the Proposed Baseline

Transfer the information specified on the Baseline Submission Summary into the certification environment according to the instructions in the File Transmittal Block. If technical difficulties obstruct the admission process, confer with the technical contact identified in the Contact field for the File Transmittal Block of the Baseline Submission Summary to resolve the problems.

6.5.2.4 Execution

Perform the following operations to authenticate the V&V results produced by the development organization.

- For computational data baselines, regenerate the output interface tables using only certified applications and input data. Compare the regenerated data to the interface tables that were admitted to the certification environment with the proposed baseline. Proceed to Step 6.5.2.5. Otherwise, proceed to Step 6.5.2.7.
- Repeat the requirements-traceability activities described in Section 5.3.1.1 of LANL-YMP-SQAP, *Los Alamos National Laboratory Software Quality Assurance Plan for the Yucca Mountain Project* as appropriate for the proposed baseline. If errors are exposed, proceed to Step 6.5.2.5. If no errors are discovered, and if the proposed baseline is not an implementation baseline, proceed to Step 6.5.2.7.
- Rebuild all primary and support products that compose the application. If errors are exposed, proceed to Step 6.5.2.5.
- Regenerate all support data that is required for the execution of the V&V effort. If errors are exposed, proceed to Step 6.5.2.5.
- Re-execute the V&V procedures to reproduce the Test Results. Employ the rebuilt primary and support software in this effort. Compare the regenerated test results to the results that were admitted to the certification environment with the proposed baseline. If errors are exposed, proceed to Step 6.5.2.5.

6.5.2.5 Discrepancies

If major discrepancies exist between the information provided by the developer and the information regenerated in the certification environment, reject the submission by checking the Not Accepted box on the Baseline Submission Summary. Otherwise, check the Accepted box on the form.

6.5.2.6 Notification

Sign and date the Baseline Submission Summary, and return a copy to the requestor. Submit a copy to the CSA Active File.

6.5.2.7 Issue Resolution

If discrepancies were identified in Step 6.5.2.5, perform the following steps. Otherwise, proceed to Step 6.5.2.8.

Work with the submitter to explore the nature of the discrepancy and its cause. If it is determined that the discrepancy is caused by the incorrect handling or composition of the submission, the use of an uncontrolled version of the software, or some other easily correctable condition, then instruct the submitter to correct the condition, recreate the proposed baseline in the developer environment, and resubmit the corrected proposed-baseline as in Step 6.5.1.

If the discrepancy is determined to be caused by an inexact duplication of the local computer's working environment, then (in consultation with the submitter) decide whether the discrepancy is significant and whether it jeopardizes the integrity of the proposed baseline. If the discrepancy is judged to be inconsequential, then document it on a Review/Audit Item Disposition form in accordance with the provisions of Section 6.4.1 of TWS-QAS-QP-03.20, *Software Configuration Management*, for later consideration by the full CCB at the formal review.

If the discrepancy is judged to seriously undermine the integrity of the proposed baseline, then take steps to duplicate the local working environment or advise the submitter on actions that can be taken to make the local environment conform to that of the certification environment. Instruct the submitter to correct the condition, recreate the proposed baseline in the developer environment, and resubmit the corrected proposed-baseline at Step 6.5.1.

6.5.2.8 Review Scheduling

If no discrepancies of consequence exist, schedule the formal review of the proposed baseline.

7.0 QUALITY ASSURANCE DOCUMENTATION

Execution of this procedure results in no formal Project QA records or records packages. However, after certification of the proposed baseline of which they are components, the V&V documents developed as a consequence of this procedure are incorporated (by the SCM organization) into the baseline's certified-baseline-records-package as described in Section 7.2.1 of TWS-QAS-QP-03.20, *Software Configuration Management*.

8.0 ACCEPTANCE CRITERIA

V&V documentation is evaluated and assessed according to the requirements for reviews and audits specified in TWS-QAS-QP-03.17, *Reviews of Software and Computational Data*, and TWS-QAS-QP-03.20, *Software Configuration Management*, respectively.

9.0 ATTACHMENTS AND APPENDIXES

Appendix A. Flow Charts

APPENDIX A
Flow Charts

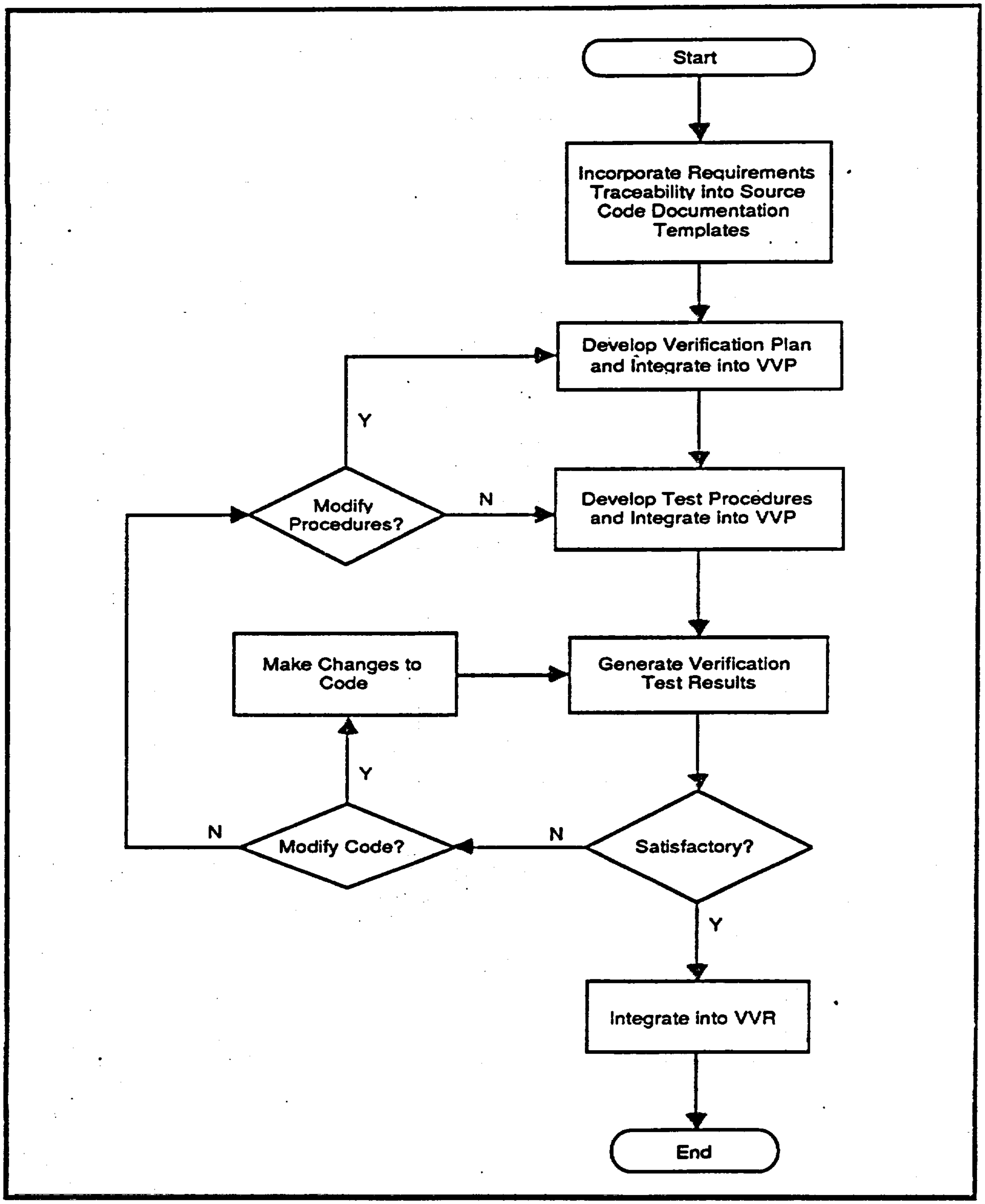

Figure 1. Software Verification

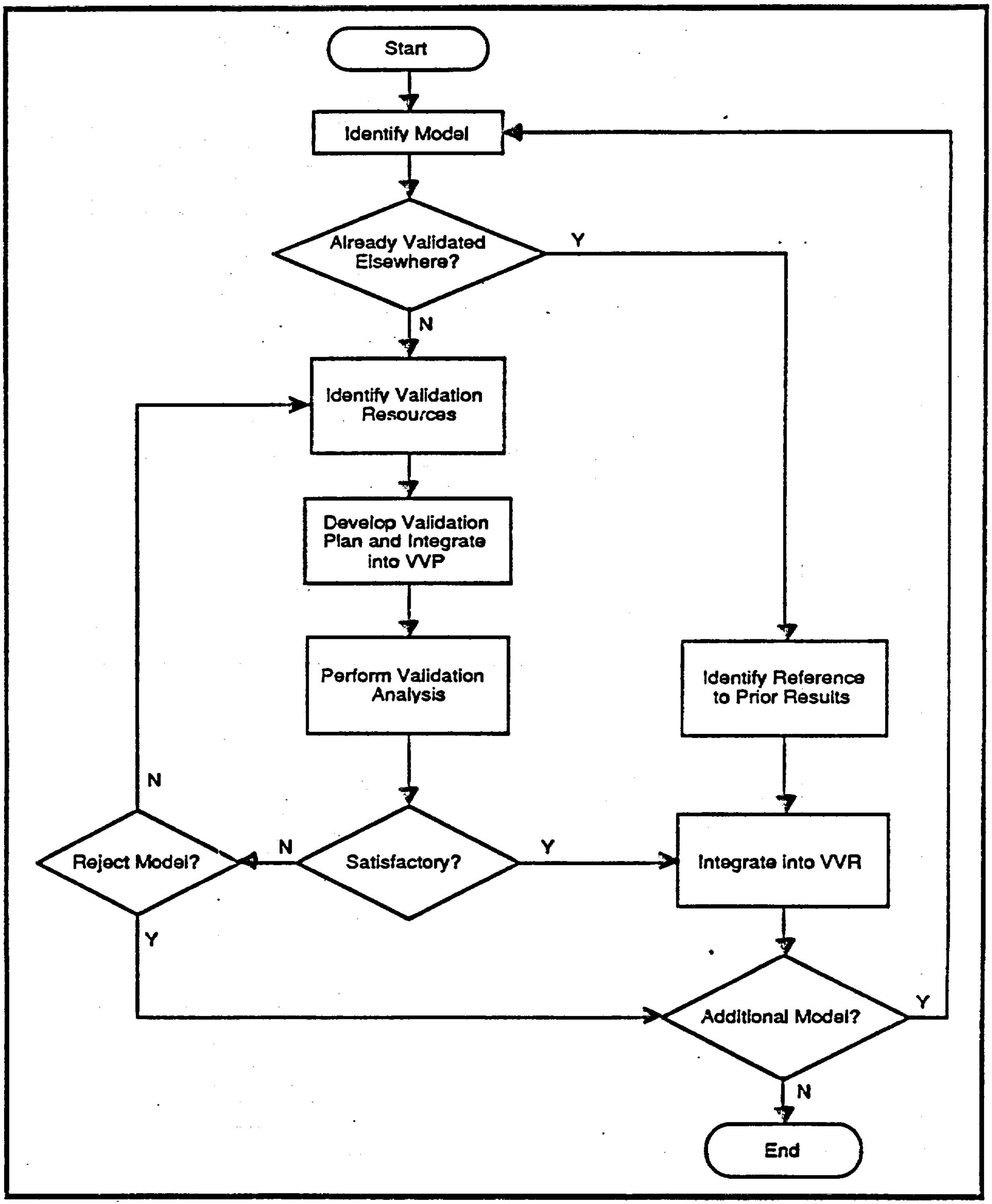

Figure 2. Software Validation

TWS-EES-5-4-91-02
WBS 1.2.3.4.1.5.1
May 2, 1991

Interim Report: Sensitivity Analysis of Integrated Radionuclide Transport Based on a Three-Dimensional Geochemical/Geophysical Model

Milestone R746

by

Kay H. Birdsell, Katherine Campbell, Kenneth G. Eggert,
and Bryan J. Travis

ABSTRACT

This report presents preliminary transport calculations for radionuclide movement at Yucca Mountain. These calculations are used to study the sensitivity of radionuclide migration to uncertainties in several factors that affect transport through porous media. These factors include spatial distribution of sorption coefficients, recharge rate, dispersivity length scale, radionuclide species, and source term. The simulations were run with TRACRN (Travis and Birdsell, 1991), a finite-difference porous flow and radionuclide transport code developed for the Yucca Mountain Site Characterization Project. Approximately 30,000 nodes are used to represent the unsaturated and saturated zones underlying the repository in three dimensions. Transport calculations for ^{99}Tc, ^{135}Cs, and ^{129}I are presented. Calculations such as these are used to study the effectiveness of the site's geochemical barriers at a mechanistic level, to determine the sensitivity of radionuclide transport to various transport mechanisms and parameters, and to help guide the geochemical site characterization program.

INTRODUCTION

One of the tasks of the geochemistry program for the Yucca Mountain Site Characterization Project is to provide a geochemical retardation model for the site to those charged with performance assessment calculations. Therefore, a goal of the geochemical characterization program is to understand the effect of site geochemistry on far-field transport calculations from the potential repository to the accessible environment. We also wish to understand the sensitivity of these calculations to assumptions regarding hydrologic properties, sorption processes, transport properties, and site mineralogy. One method selected for this task is to formulate a transport model for the site and use that model to integrate results from hydrologic and geochemical site characterization studies. This model will also allow estimation of the changes in retardation that may occur due to changes in scenarios assumed by performance assessment. This report discusses the formulation of this model and presents preliminary sensitivity analyses based on the model.

The calculations described in this report are repository-scale, three-dimensional simulations of radionuclide migration from the repository horizon through the unsaturated zone and into the saturated zone. The simulations were run with the computer code TRACRN (Travis and Birdsell, 1991). A three-dimensional geochemical/geophysical model of the tuffs below the repository horizon at Yucca Mountain was constructed for the calculations. The hydrologic component of the model is based on the 3-D hydrological reference stratigraphy developed at Sandia National Laboratories (SNL) (Ortiz et al., 1985) from the Topopah Spring welded unit (TSw2) down to the Bullfrog welded unit (BFw). Dipping beds, which are offset along the Ghost Dance Fault, and a nonhorizontal water table are included. Composite characteristic curves developed by Peters and Klavetter (1988; Peters et al., 1984) describe the hydrologic properties of the units. The geochemical model includes spatially distributed sorption coefficients that are functions of local mineral assemblage. Six different realizations of sorption coefficient fields are used to study the sensitivity of the transport of ^{99}Tc and ^{135}Cs to inhomogeneities and uncertainties in this retardation process. Calculations for the transport of ^{99}Tc, ^{135}Cs, and ^{129}I under steady recharge rates of 0.1 and 0.5 mm/yr are presented. The calculations are used to study the sensitivity of radionuclide migration to several factors that affect transport: spatially distributed sorption coefficients, recharge rate, dispersivity length scale, nuclide species, and source term.

CONCEPTUAL MODEL

The conceptual model used for these simulations is made up of four main components: a mathematical model, a hydrologic model, a geochemical model, and a min/pet model. These models are intimately related, e.g., the mathematical model describes the equations of flow and transport for the hydrologic and geochemical models, and the sorption coefficients used in the geochemical model are derived from the mineral distribution developed in the mineralogic/petrologic (min/pet) model.

Mathematical Model

The simulations were run with the computer code TRACRN (Travis and Birdsell, 1991). A subset of the equations embodied within TRACRN form the mathematical model describing flow and transport through the Yucca Mountain tuffs. These equations include conservation of mass for the liquid phase,

$$\frac{\partial}{\partial t}(\varepsilon\sigma\rho) + \nabla\bullet(\rho\hat{u}) = \varepsilon\dot{S} \qquad ; \qquad (1)$$

conservation of momentum for the liquid phase (Darcy's Law),

$$\hat{u} = \frac{-k}{\mu}(\nabla P + \rho\hat{g}) \qquad ; \qquad (2)$$

and conservation of contaminant,

$$\frac{\partial}{\partial t}(\varepsilon\sigma\rho C_\alpha) + \nabla\bullet(\rho\hat{u}C_\alpha) = \nabla\bullet(\varepsilon\sigma\tau_c D_\alpha\rho\nabla C_\alpha) + \varepsilon C_\alpha\dot{S} + \nabla\bullet(\varepsilon\sigma\bar{D}\nabla(\rho C_\alpha))$$
$$-\varepsilon\lambda_\alpha\sigma\rho C_\alpha - \rho\rho_m(Kd_\alpha(\frac{\partial}{\partial t}C_\alpha + \lambda_\alpha C_\alpha)) \qquad ; \qquad (3)$$

where ε is the porosity, σ is the saturation, ρ is the liquid density, $\hat{u}$ is the Darcy velocity, $\dot{S}$ is a source or sink, k is the permeability, P is the liquid pressure, C is the contaminant concentration, τ_c is the constrictivity, D is the molecular diffusivity, $\bar{D}$ is the dispersion tensor, λ is the half-life, ρ_m is the rock density, Kd is the equilibrium sorption coefficient, and the subscript α is the contaminant. Equation (3) describes diffusive, dispersive, and advective transport of any number of radioactive contaminants undergoing equilibrium sorption. Solution of the flow equations is obtained by an implicit, integrated finite-difference algorithm. The transport equation can be solved using either an implicit or explicit, integrated finite-difference algorithm. To control numerical dispersion of the transport solution, a tensor anti-diffusion correction is available with the explicit solution algorithm. This approach uses centered differencing of the spatial derivatives, which is the most accurate but is also unstable, with an added term that estimates the time truncation error to stabilize the solution. The matrix equations formulated by the implicit schemes are solved using a preconditioned conjugate-gradient method.

Hydrologic Model

The hydrologic model includes the stratigraphy, the hydrologic properties of the units, the imposed recharge rates, and the position of the water table. The stratigraphy is based on the three-dimensional reference stratigraphic model of Yucca Mountain developed by Ortiz et al. (1985). The stratigraphic units included in the model are those from the repository horizon down to the Bullfrog welded unit. From top to bottom these units include

Topopah Spring welded, lithophysae-poor (TSw2);
Topopah Spring welded, vitrophyre (TSw3);
Calico Hills and Lower Paintbrush nonwelded, vitrophyre (CHnv);
Calico Hills and Lower Paintbrush nonwelded, zeolitized (CHnz);
Prow Pass welded (PPw);
Upper Crater Flat nonwelded (CFUn); and
Bullfrog welded (BFw).

The CHnv and CHnz units incorporate the three Calico Hills units (CHn1, CHn2, and CHn3) and are differentiated by the position of the zeolitized zone (TZZ) given by Ortiz et al. (1985). The position of the water table is also taken from their model. Data from Nevada coordinates 757,000 ft to 772,000 ft north and 557,000 ft to 566,000 ft east are included in the modeled area. The units dip at about 6^o from west to east. The Ghost Dance Fault zone is located at approximately 562,400 ft east and dips from 5 to 10 degrees.

Composite characteristic curves developed at SNL (Peters and Klavetter, 1988; Peters et al., 1984; Dudley et al., 1988) were used to describe the hydrologic properties of the units. The curves represent composite-porosity properties, i.e., matrix and fracture properties are combined to form a single characteristic curve for each unit. The composite-porosity model is a simplified dual-porosity model that assumes equivalent pressures locally and parallel flow in the matrix and fractures (Peters and Klavetter, 1988; Dudley et al., 1988). Figures 1 and 2 show conductivity curves for the TSw2 and PPw units, respectively. The double-plateaued composite curve (Fig. 1) is a typical curve for a tuff with a high fracture porosity and a high fracture conductivity. The single-plateaued composite curve (Fig. 2) is typical of a sparsely fractured tuff with a high matrix saturated conductivity. Composite properties are available for TSw2, TSw3, CHnv, CHnz, and PPw (Dudley et al., 1988). Matrix conductivity curves are reported (Peters et al., 1984) for the CFUn and BFw units. Composite curves were constructed for these units by using the fracture properties of the CHnz and PPw units respectively, because of the similarity in fracture characteristics between the CFUn unit and the CHnz unit and between the BFw and the PPw unit.

Recharge rates of 0.1 and 0.5 mm/yr were used to establish steady flow fields through the mountain. These rates are estimates of possible high recharge rates that could occur at Yucca Mountain. To simulate this recharge, a constant flux was applied to the upper boundary, which corresponds to the repository horizon.

Geochemical model

The main constituent of the geochemical model focused on for this set of calculations is the spatial distribution of sorption coefficients as a function of mineral assemblage. The min/pet model described below explains the geostatistical analysis of mineral distributions that was subsequently used to construct fields of spatially distributed sorption coefficients. Six different sorption fields were generated for each of the two radionuclide species, ^{99}Tc and ^{135}Cs. These Kd fields are used to study the sensitivity of radionuclide transport to uncertainties in this sorption property. Other important constituents of the geochemical model are the magnitude of the longitudinal and transverse dispersivity length scales, the source terms for the radionuclides as they are released from the repository along with the position and shape of the repository itself, and diffusion coefficients for the radionuclides in the different tuffs.

Simulations of the transport of technetium ^{99}Tc for a 5,000-yr period and cesium ^{135}Cs for a 10,000-yr period were run with spactially distributed sorption coefficients. The sorption coefficient Kd for ^{99}Tc depends on the abundance of the minerals hematite and mica,

$$Kd_{Tc} = Kd_{hem}X_{hem} + Kd_{mica}X_{mica} \quad , \tag{4}$$

where $Kd_{hem} = 5.3$ ml/g is the sorption coefficient of ^{99}Tc on pure hematite, $Kd_{mica} = 3.4$ ml/g is the sorption coefficient of Tc on pure mica, and X is the weight fraction of the respective mineral. Kd for Cs varies with the abundance of clinoptilolite, montmorillonite, mordenite, analcime, and glass in the tuff (Daniels et al., 1982)

$$Kd_{Cs} = Kd_{clin}\sum W_i X_i \quad , \tag{5}$$

where $Kd_{clin} = 3.8 \times 10^4$ ml/g is the sorption coefficient for Cs on pure clinoptilolite, and the Wi's are weighting factors for each mineral. The Wi's represent the ratio of the mineral's Kd to that of clinoptilolite. They range from 0.50 for montmorillonite to 0.016 for glass. These species were chosen for the simulations because of their different transport properties. Tc forms the anion TcO_4^- , which will not cation exchange with the zeolites or clays in the tuffs. Because the abundance of hematite and mica in the tuffs is low, its sorption coefficient is low. Cs acts as a simple cation. It is thought to undergo cation exchange with the zeolitic tuffs and consequently has a very high sorption coefficient. Sorption coefficients for most other radionuclides should lie between those of Cs and Tc. One calculation assuming no sorption was performed to investigate the effect of technetium's low sorptivity compared to no sorptivity at all. Table I shows the mean and range of the six simulated Kd realizations for Cs and Tc in the seven min/pet layers discussed below. The values shown provide an indication of the variability between realizations, as well as the inhomogeneity within each realization. A set of calculations was also run for Cs with homogeneous sorption coefficients based on the hydrologic units. These Kd's are shown in Table I as Realization No. 7. Some simulations for ^{129}I were also run. It was assumed to be nonsorbing.

TABLE I. VARIATION AMONG Kd REALIZATIONS
(Mean and range within units and realizations)

Unit	Realiz Number	Cesium Mean	Cesium (Range)	Technetium Mean	Technetium (Range)
TSw2	1			0.037	(0.009,0.096)
	2			0.034	(0.009,0.108)
	3			0.037	(0.010,0.108)
	4			0.031	(0.008,0.085)
	5			0.032	(0.010,0.090)
	6			0.027	(0.009,0.073)
	7	100	(-)		
Zi	1	2802	(971,7482)	0.031	(0.011,0.061)
	2	3341	(911,12162)	0.030	(0.006,0.080)
	3	3108	(933,8334)	0.040	(0.009,0.095)
	4	3669	(807,13967)	0.051	(0.015,0.139)
	5	2338	(662,5681)	0.036	(0.010,0.094)
	6	3162	(744,8640)	0.034	(0.003,0.133)
	7	100	(-)		
Vitric	1	757	(344,1839)	0.023	(0.001,0.084)
	2	744	(381,3509)	0.020	(0.001,0.080)
	3	792	(420,2838)	0.026	(0.001,0.093)
	4	870	(440,3377)	0.026	(0.001,0.104)
	5	709	(225,2307)	0.024	(0.001,0.093)
	6	715	(401,1657)	0.020	(0.001,0.094)
	7	0	(-)		
CHnz	1	16828	(822,36792)	0.043	(0.001,0.791)
	2	19950	(364,37772)	0.034	(0.001,0.631)
	3	18249	(226,37712)	0.050	(0.001,0.636)
	4	19797	(185,37509)	0.039	(0.001,0.478)
	5	20556	(843,37716)	0.033	(0.000,0.499)
	6	21171	(595,36727)	0.039	(0.001,0.772)
	7	3000	(-)		
PPw	1			0.018	(0.006,0.052)
	2			0.021	(0.005,0.061)
	3			0.015	(0.002,0.066)
	4			0.014	(0.004,0.039)
	5			0.016	(0.005,0.046)
	6			0.021	(0.006,0.080)
	7	200	(-)		
CFUn	1	11799	(701,33291)		
	2	11206	(692,30239)		
	3	10409	(538,34239)		
	4	12501	(552,33185)		
	5	10382	(966,33546)		
	6	10916	(747,33606)		
	7	400	(-)		
BFw	1			0.101	(0.025,0.269)
	2			0.089	(0.024,0.235)
	3			0.096	(0.022,0.281)
	4			0.094	(0.017,0.253)
	5			0.103	(0.029,0.319)
	6			0.087	(0.029,0.233)
	7	100	(-)		

These radionuclides have long half-lives of order 10^5 to 10^6 years.

The dispersivity length scales are unknown for field-scale transport through the Yucca Mountain tuffs. The simulations were run using different longitudinal and transverse dispersivities to study their effect on radionuclide migration. Longitudinal dispersivities of 10 m and 1 m, and transverse dispersivities of 1 m and 0.1 m were run with a ratio of longitudinal to transverse dispersivity of 10:1. The large dispersivity values assumed here result from scaling up data from column studies to repository scale.

Release rates from the repository vary with time. Estimates of these release rates were not available at the time these simulations were started. A steady source of $C_o = 1$ released at the recharge rate was used to calculate relative concentrations for the first few sets of ^{99}Tc and ^{135}Cs calculations. The transport equations are linear so the results can be scaled. Estimated source terms were used for the ^{129}I and the subsequent ^{135}Cs calculations. Two types of source terms were used, moist-continuous and flow-through. Figures 3 and 4 show the source terms that were used (Apted et al., in preparation) over the 10,000 yr time frame that was modeled. Both ^{129}I and ^{135}Cs have rapid release fractions as well as alteration-rate-controlled releases. For release by the moist-continuous scenario, the spent-fuel container is assumed to be in contact with the borehole, release occurs by molecular diffusion through the partially saturated rock matrix, and complete containment is assumed for the first thousand years. This source term is fairly independent of recharge rate. For release by the flow-through scenario, the spent-fuel container is surrounded by a 3-cm air gap. Water drips from the borehole wall into a perforation in the container and out through holes in the bottom of the container. This scenario does depend on recharge rate and assumes 0.5 mm/yr. For the transport calculations presented, this source was used for both recharge rates despite this inconsistency.

The release area roughly follows the proposed shape and position of the repository (MacDougall et al., 1987). Release is homogeneous from the repository (i.e., panels of canisters or individual canisters are not considered). With the steady source term, actual quantities of radionuclides released to the accessible environment can not be estimated, but the effectiveness of the site's geochemical barriers can be investigated and some sensitivity analysis calculations can be performed. Breakthrough curves can be estimated with the more realistic source terms.

The same diffusion coefficient was used for the two radionuclides in the various tuffs. Typical aqueous diffusion coefficients are on the order of 10^{-5} $(cm)^2/s$. Diffusion experiments in saturated cores show that the tortuosity decreases the effective diffusion coefficient by a factor of approximately 0.05 in the Topopah Spring core samples and by 0.07 in the Calico Hills samples (Rundberg et al., 1987). The effective diffusion coefficient also decreases with saturation, but this dependence is not yet known for the Yucca Mountain tuffs. Tortuosity values of 0.05 were used for all of the tuffs and diffusion coefficients of 10^{-5} $(cm)^2/s$ were used for all of the nuclides.

Mineralogic/Petrologic Model

For the purposes of simulating mineral distributions, the block (excluding the Ghost Dance fault) was divided into seven units. Five of these are the hydrologic units TSw2, CHnz, PPw, CFUn, and BFw. The vitric units TSw3 and CHnv are combined into a sixth unit, except for a thin smectite-bearing zeolitized layer at the top of the basal vitrophyre of the Topopah Spring Member (Bish and Vaniman, 1985) that is treated as a separate, seventh unit.

The available mineralogical data consist of x-ray diffraction measurements of between 6 (for the smectite-bearing unit) and 75 samples per unit from 12 drill holes near the target-development area. Alkali-feldspar and at least some of the silica polymorphs (quartz, tridymite, and cristobalite) are observed in almost all samples. Glass, clinoptilolite, mordenite, smectite, mica, calcite, and hematite also occur in measurable quantities in some of the units.

The geochemical model requires average Kd values (based on mineralogy) for each of some 30,000 blocks. The available data are therefore used to estimate the parameters of spatial trend and covariance models for the logarithmic ratios $r(i)=log(m(i)/a(i))$, where $a(i)$ is the abundance of the ubiquitous mineral alkali-feldspar at the i-th location in the block, and $m(i)$ is the abundance of one of the other minerals present in the unit under consideration (Aitchison, 1986). (It should be noted that although we have selected one model for each ratio in each unit, the range of models that are consistent with the relatively sparse observations is extremely broad.) These models are then used to generate six possible spatial distributions for the minerals throughout the block, each of which is consistent with the observations that exist but is elsewhere constrained only by the statistical requirements of the stochastic model. The over 30,000 block-averaged mineral compositions of each realization are then converted to average sorption coefficients for each grid block using the geochemical model described above.

SIMULATIONS

Grid

The bedded tuffs dip at approximately 6^o from west to east. The stratigraphic data was rotated upward 6^o and translated to facilitate gridding of the units. The data was also converted to meters to match input requirements for TRACRN. A nonvertical gravity vector compensates for the rotation of the beds. The grid is made up of 30,870 finite-difference zones. This quantity was chosen because it was near the maximum problem size that could be run with TRACRN using the memory allocated per user on the Cray Y-MP's running the CTSS operating system at Los Alamos National Laboratory (about 4.2 million words out of 5.0 million words allowed). There are 15 300-m blocks in the north-south direction, 37 73-m blocks in the east-west direction with 5 finer blocks near the Ghost Dance Fault zone, and 49 blocks from an elevation of 50 m to 450 m. The Ghost Dance Fault zone is located at 1695 m east and is 5-m wide. The vertical zones range in thickness from 2 m to 18 m. The beds vary in thickness and in elevation throughout the modeled region. The grid captures much of this variation. Offset along the fault zone is not explicitly modeled as a different material (i.e., it has the material properties of the adjacent unit).

Source Terms

The recharge rate was treated as a source term for the simulations. Each of the finite-difference blocks at the upper boundary supplied water at the 0.1-mm/yr or the 0.5-mm/yr recharge rate. The radionuclide source term was treated similarly, except that only finite-difference cells within the boundary of the repository block supplied radionuclide at a concentration of either 1.0 g/g fluid, for the steady source, or concentrations corresponding to the source terms shown in Figs. 3 and 4. The release area has roughly the same shape and position as that planned for the potential repository block (MacDougall et al., 1987). The leachate rate was considered to be the same as the recharge rate. The flow field was brought to steady state. The transport simulations were then run under steady flow conditions.

Hydrologic Properties

Characteristic curves of capillary pressure and relative permeability as functions of saturation were constructed for each hydrologic unit based on the composite properties discussed previously. The curves (see Fig. 1) are highly nonlinear as the fractures saturate, which generally occurs at composite saturations greater than 0.999. Because both the saturated and the unsaturated zones are considered in these simulations, calculational difficulties occurred in finite-difference zones adjacent to the water table due to the extreme nonlinearity of these curves. For these preliminary calculations, the curves were consequently linearized from composite saturations of 0.99 to 0.9999 for units TSw2 and TSw3 and from 0.99 to 0.99999 in units CFUn and CHnz to help the simulations converge more readily. The effect of this linearization is that the fractures saturate over a larger saturation range. This causes the relative permeability to increase more gradually although the increase begins at a lower composite saturation value.

Water Table

The water table at Yucca Mountain rises sharply to the northwest. It was included in these calculations because the distance from the repository to the water table varies significantly with position. A planar, but nonhorizontal, surface was initially defined based on the water table surface included in the stratigraphic model (Ortiz et al.,1985) used for these simulations. Constant-pressure boundary conditions hold the water table at its initial level at the boundaries. It fluctuates some with recharge rate, but is artificially held close to its initial position by the imposed pressures at the bottom and side boundaries. Because the stratigraphic data was rotated upward along the dipping beds in the east-west cross sections and because the vertical scale is elongated with respect to the horizontal scale, the simulated water table appears to be far from horizontal in the results that follow. Figure 5 shows schematically how the rotation and elongation skews the figures that follow.

Boundary Conditions

Constant-pressure boundary conditions were used along the side and bottom boundaries. As mentioned above, this created a stagnant saturated zone that kept the water table at its current position. For the first set of transport calculations (see *Spatially Distributed Kd*), saturations and pressures along the side boundaries in the unsaturated zone were held at their initial values. The flow field was run to steady state, based on boundary values that ultimately were inconsistent with the internal values. For the rest of the calculations presented, the saturation and pressure values for the side boundaries in the unsaturated zone were updated to make them consistent with the internal values. This was done by reinitializing the boundary values for the previous steady-state flow calculation to the values in the adjacent internal zones and reestablishing a new steady-state flow field based on the new boundary values. This process was repeated (4 or 5 times) until the reinitialization no longer changed the flow results. A no-flow boundary condition was used for the upper boundary with the water and contaminant sources located in the zones directly beneath the upper boundary. A zero gradient boundary condition was used for the transport solution.

RESULTS

Flow Results

Figures 6 through 8 show steady-state pressure, saturation, and velocity plots at the 0.1-mm/yr flow rate through an east-west cross section of the mountain. The stratigraphy used for the calculations is superimposed on the pressure plot to show its strong influence on the flow and transport solutions. The simulated water table is nonhorizontal because it is rotated to offset the rotation of the stratigraphic data in the east-west planes (see Fig. 5) and also because it mimics the northwesterly rise observed at the mountain. Down-gradient flow does not occur beneath the water table because its position is over constrained by the constant-pressure boundaries along the sides and bottom. In the velocity vector plot (Fig. 8), strong lateral flow can be identified in the CHnv and PPw units, and the finer gridding along the fault zone at 1695 m east is evident. Although the fault has no explicit properties of its own, the offset of beds along the fault causes some of the lateral flow along bedding planes to be diverted downward. A circulation pattern is evident along the boundaries. This seems incorrect and is again related to the artificially constrained boundary conditions. Figure 9 shows saturation profiles through a north-south cross section of the mountain with the stratigraphy superimposed. By comparing Figs. 7 and 9, the 3-dimensionality of the flow field becomes apparent. The east-west cross section cuts the repository at a point approximately three-quarters of the way north from its southernmost tip. The north-south cross section cuts the repository slightly east of its midpoint. The flow solutions were assumed to be at steady state when the largest pressure change over the entire grid for a 50,000 yr time period was about 1 part in 10^7. The steady flow solution was then used for subsequent transport calculations. These figures show the flow solution obtained after the boundary conditions in the unsaturated zone had been updated a few times.

Transport Results

Spatially Distributed Kd - Figures 10 through 15 show log-scale fluid concentration plots for ^{99}Tc at 5,070 yr for the various realizations of *Kd* at the two cross sections shown above. Figures 10 and 11 represent the "worst case" scenario of zero sorption. Figures 12 and 13 show the plumes for the east-west cross section for *Kd* realizations No. 1 and No. 6, which, respectively, migrated the least and the most of the six realizations. Figures 14 and 15 show overlay plots of the plumes for *Kd* realizations No. 2 through 6 for the east-west and north-south cross sections, respectively. (Realization No. 1 was left off the overlay plots because it makes them confusing.) The steady source concentration of 1.0 g/g fluid was assumed for this set of calculations. These solutions were obtained by solving the transport equation explicitly with the tensor anti-diffusion option. This approach considerably decreased numerical dispersion seen in the implicit calculation. Run times, however, increased by a factor of about 10 when using the explicit solution. The runs were stopped at 5,070 yrs (rather than to 10,000 yrs) to save on computer costs.

The effect of technetium's low sorptivity can be studied by comparing Fig. 10 with Figs. 12, 13, and 14 and Fig. 11 with Fig. 15. Transport of ^{99}Tc is retarded by a factor of 10% to 30% for the sorbing cases vs. the nonsorbing case. This retardation factor is reasonable assuming the upper four units have an average Kd of about 0.03 (see Table I). In Figs. 14 and 15, the different sorption realizations do not produce significant variability in the simulated results under the 0.1-mm/yr recharge rate at 5,070 yr. More significant variability may be seen, however, with increasing recharge, time, and dispersivity values. Some other cross sections show more variability with the different Kd fields and also more nonuniformity in space, indicating a more three-dimensional structure than shown in the cross sections presented. A downward dip in the 10^{-12} C_o concentration plumes is evident in the east-west plots along the region offset by the fault zone at 1695 m east. This dip occurs because the lateral flow, which carries the ^{99}Tc along the CHnv/CHnz interface (see Fig. 8) toward the fault from the west, stops abruptly at the offset and is diverted downward. The downward dip does not occur for realization No. 1 (Fig. 12) because the 10^{-12} contour has not reached the lateral flow region at the 300-m elevation.

Figures 16 and 17 show overlays of log-scale fluid concentration plots for ^{135}Cs at 10,000 yr for the six realizations of Kd. These solutions were generated using the implicit solution of the transport equation. Numerical dispersion did not significantly affect the calculation of the slow moving Cs. The figures show that cesium's high sorptivity successfully retards its migration over the 10,000-yr period. The concentration contours are identical in the TSw2 unit because no sorption of ^{135}Cs occurs in that unit. A slight spreading of the contours with realization occurs below TSw2, but the spreading is insignificant for not only these two cross sections but also for all other cross sections that were checked.

Recharge Rate and Dispersivity Length Scale - Figures 18 through 21 show log-scale fluid concentration plots for ^{99}Tc at 10,000 yr at a 0.1-mm/yr recharge rate for the two cross sections shown above. The position of the water table is also given for each cross section. Kd realization No. 1 for ^{99}Tc was used for this set of simulations. Two sets of dispersivity length scales are presented for the calculations shown. For Figs. 18 and 20, a longitudinal dispersivity of 10 m (used in the vertical direction) with a transverse dispersivity (used in the horizontal direction) of 1 m was used. For Figs. 19 and 21, a longitudinal value of 1 m and a transverse value of 0.1 m were used. The constant source term is again used for these calculations. At this flow rate, the assumed dispersivity strongly affects the transport solution. Technetium concentrations as high as 10^{-9} C_o for the high dispersivity case (Figs. 18 and 20) and 10^{-11} and $10^{-10} C_o$ for the lower dispersivity case (Figs. 19 and 21) intercept the water table. A factor of 10 difference in the dispersivity length scale resulted in a factor of up to 100 difference in the concentration breaking through to the water table for these particular cross sections. Other cross sections show concentrations reaching the water table up to 1,000 times larger for the higher dispersivity case than for the lower dispersivity case. Vertical flow occurring along the fault zone is evident in these plots at 1695 m east by the downward dip in the concentration plumes at that position.

Figures 22 through 25 show log-scale fluid concentration profiles at the 0.5-mm/yr recharge rate. Figures 22 and 23 are for the east-west cross section, and Figs. 24 and 25 are for the north-south cross section. Concentration profiles for the two dispersivity length scales are presented. Larger concentrations occur for the 0.5-mm/yr cases than for the 0.1-mm/yr cases. (Remember that the constant source concentration of 1.0 g/g fluid is used for both flow rates.) For the cross sections shown, concentrations on the order of 10^{-5} C_o reach the water table for the high dispersivity case

(Figs. 22 and 24), and concentrations on the order of 10^{-7} to 10^{-8} C_o reach the water table for the low dispersivity case (Figs. 23 and 25). Here again a factor of 10 increase in the value of the dispersivity length scale produced a factor of 100 to 1000 increase in concentrations reaching the water table.

Figures 26 and 27 show log-scale fluid concentration plots for ^{135}Cs for the two cross sections at the fastest flow rate. *Kd* realization No. 1 for ^{135}Cs was used for this set of simulations. Results using the high dispersivity length scale are presented here so that these plots show the most rapid migration of cesium of any of the calculations run. The figures show that cesium's high sorptivity successfully retards its migration.

Dimensionality - Figure 28 shows two three-dimensional visualizations of the ^{99}Tc plume at 10,000 yrs for a recharge rate of 0.1 mm/yr, the low dispersivity length scales, the constant source, and *Kd* realization No. 1. The plume is highly three-dimensional. The shape of the repository is evident in the first figure. Both figures show fast paths along the left (western) side and along the fault. This particular simulation is presented because it is transported the least of the *Tc* simulations and still demonstrates this high degree of three-dimensionality. The other *Tc* and the *I* simulations are even more highly three-dimensional.

Figure 29 shows two three-dimensional visualizations of the entire ^{135}Cs plume at 20,000 yrs for a recharge rate of 0.5 mm/yr, the high dispersivity length scales, *Kd* realization No. 1, and the constant source term. This plume was chosen because it is transported the most of the *Cs* simulations and yet its structure can probably be adequately represented in two dimensions. The plumes for the other *Cs* simulations show even less three-dimensionality than this one. It should be noted that for this *Kd* realization, the TSw2 unit is nonsorbing. Any sorption in this unit slows the migration even further and makes the plumes structure less three-dimensional. The layer just below the repository shown in the first figure is a deeper shade of red than the corresponding layer for the *Tc* simulation. *Cs* stays more concentrated near the source because its migration is limited.

Recharge Rate and Source Term - Figures 30 through 33 show concentration contours for ^{129}I transport from the repository at 10,000 yrs using a recharge rate of 0.1 m/yr. Results based on the moist-continuous source term are presented in Figs. 30 and 31, and results based on the flow-through source term are presented in Figs. 32 and 33. The larger dispersivity length scale (10 m longitudinal and 1 m transverse) is used for this set of calculations. ^{129}I is assumed to be nonsorbing.

Several observations can be made by comparing these results with results presented in the previous sections. First, by comparing Figs. 30 and 32 with Fig. 20 and Figs. 31 and 33 with Fig. 22, the influence of the source term and sorption is demonstrated. The source terms used for the *I* simulations are lower than the continuous source used for the *Tc* simulations. The difference in the source is reflected in the higher concentration contours located near the top of the figures. Despite the lower source concentration, slightly higher concentrations reach the water table for the *I* case using the moist-continuous source (Figs. 30 and 31) than for the *Tc* case (Figs. 20 and 22) because *I* is nonsorbing while *Tc* is slightly sorbing.

Breakthrough concentrations at the water table are substantially different for the two variable source terms. For the 0.1-mm/yr flow rate, results using the moist-continuous source term (Figs. 30 and 31) show *I* concentrations on the order of 10^{-9} compared to *I* concentrations on the order of 10^{-14} for the flow-through source term (Figs. 32 and 33).

Figures 34 through 37 show ^{129}I concentration contours at 10,000 yrs at the 0.5 mm/yr recharge rate. Figs. 34 and 35 represent results for the moist-continuous source term, and Figs. 36 and 37 represent results for the flow-through source term. Again the larger dispersivity length scale is used, and *I* is assumed nonsorbing. Comparing these results with results for the constant source *Tc* calculations (Figs. 24 and 26) at the same flow rate shows lower concentrations at the water table for the *I* simulations because of the lower source and despite *Tc*'s sorbtive capacity in contrast to the comparison done at the 0.1-mm/yr flow rate using the moist-continuous source term for *I*.

Concentrations at the water table for the two source terms are again substantially different at this higher recharge rate. They are approximately four orders of magnitude higher for the case which uses the moist-continuous source term (Figs. 34 and 35) than for the case which uses the flow-through source term (Figs. 36 and 37).

A comparison between results for like source terms at the two recharge rates shows significant differences in break-through concentrations depending on recharge rate. For the moist-continuous source term, *I* concentrations at the water table are two to three orders of magnitude higher for the 0.5-mm/yr recharge rate (Figs. 34 and 35) than for the 0.1-mm/yr recharge rate (Figs. 30 and 31). For the flow-through source term, *I* concentrations are four orders of magnitude higher for the 0.5-mm/yr rate (Figs. 36 and 37) than for the 0.1-mm/yr rate (Figs. 32 and 33).

Figures 38 through 41 show *Cs* concentration contours at 10,000 yrs for the north-south cross section for the two source terms and at the two flow rates. Sorption coefficients are based on unit (see Realization No. 7 in Table I) rather than using the spatially distributed realizations used in the other *Cs* calculations. The contours are wider and the concentrations higher for the calculations using the moist-continuous source (Figs. 38 and 40) than for the calculations using the flow-through source (Figs. 39 and 41) simply because the source concentration is larger. Sorption is so strong that transport is limited in these simulations to less than 50 m from the source region. The TSw2 unit contributes to the retardation of *Cs* here, while it did not in the previous sets of calculations.

CONCLUSIONS AND RECOMMENDATIONS

This paper describes our first attempts at modeling transport at Yucca Mountain using spatially distributed stratigraphic, geochemical, and mineralogic data in three dimensions. Work will continue to improve this model based on the recommendations given below and as further information from site characterization becomes available. Some conclusions regarding the sensitivity of radionuclide transport to various transport parameters can be made based on the results presented in the previous sections.

Spatially Distributed Kd - For *Tc*, the different realizations of *Kd* fields did not produce significant variability in the simulated results. Geochemical studies during site characterization are expected to provide refinement in geochemical retardation process assumptions and in their relation to the min/pet models. The current set of simulations uses only a handful of realizations of mineral distribution. Many more are required to obtain statistically realistic results. Plume variations due to variations in the *Kd* realization may be magnified as flow rates and dispersivities change. Therefore, radionuclide migration at other recharge rates (both steady and unsteady) and with larger dispersivity length scales as a function of sorption field must also be considered. The scale of the spatial variability of the sorption parameters may be much smaller than the size of the grid blocks used for these calculations. A smaller volume should be considered to see if the calculated results are size dependent. Cumulative totals of radionuclides crossing a given surface will be calculated to determine whether the different realizations produce statistically different results. If further studies indicate that the results of transport calculations run with detailed sorption data do not depend much on the variation in the sorption coefficients, such detailed data may not need to be gathered even for fast moving species like *Tc*.

For *Cs*, the different realizations of *Kd* fields produced almost no variability in the simulated results. It seems that for highly sorptive radionuclides like *Cs* , detailed information regarding sorption as a function of mineralogy is not required to properly model its migratory behavior. The sorption task proposes investigating a minimum *Kd* approach for strongly sorbing radionuclides. The approach is based on estimating a minimum sorption coefficient for the units underlying the repository block. Subsequent calculations will test this hypothesis.

Recharge Rate and Dispersivity Length Scale - For *Tc*, both the recharge rate and the dispersivity length scales strongly affected the simulated transport results.
Improvements in the hydrologic model will help to better determine the dependence of transport on hydrology and on recharge rate at the site. Site characterization studies will provide a better understanding of the site conceptual hydrologic model, as well as improve estimates of hydrologic parameters. The composite-porosity method, as implemented for these simulations, may be inadequate for transport calculations when fracture flow exists. The method smears out the faster fracture velocities by combining them with matrix velocities. Modeling studies will be done to determine the effect that the individual components of matrix and fracture flow have on radionuclide migration under different recharge scenarios. Results of these studies will be incorporated into the model. Further, the Ghost Dance Fault zone will be modeled explicitly, and flow in the saturated zone will be modeled more realistically. Recharge should be modeled from the ground surface to the water table rather than by assuming a constant flux at the repository level. Higher flow rates will obviously change the simulated results, although calculations performed by Prindle and Hopkins (1989) indicate increasing lateral diversion around the repository with increasing recharge.

Studies will be conducted to better understand the dispersion process. Dispersivity length scales may need to be coupled to recharge scenarios, functions of grid block size, and time variant. Saturation effects and flow regime (i.e., matrix- vs. fracture-dominated flow) can also strongly effect dispersivity values.

Dimensionality - The calculations demonstrate that migration from the potential repository is three dimensional, especially for less sorptive species. For weakly sorbing species like technetium, more three-dimensional studies are required to understand how heterogeneities and uncertainties in hydrologic and transport properties affect predictions of breakthrough to the accessible environment. For strongly sorbing species like cesium, two-dimensional simulations may be sufficient to simulate transport through the mountain.

Source Term - For iodine, the simulated results were strongly dependent on the source term. For weekly sorbing nuclides like *I* or *Tc*, accurate source terms are essential in evaluating the effectiveness of the site's geochemical barriers and in predicting quantities of radionuclides that may reach the accessible environment.

For *Cs*, the simulated results were fairly independent of source term. Retardation was so strong that transport was limited to less than 50 m from the respository. For strong sorbers, such as *Cs*, migration to the accessible environment may not occur even based on extreme release scenarios. An accurate description of the source term for these types of nuclides may not be needed.

ACKNOWLEDGMENT

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The software documented in this report was not verified, validated, or otherwise subjected to the controls of a Yucca Mountain Site Characterization Project Office-approved quality program.

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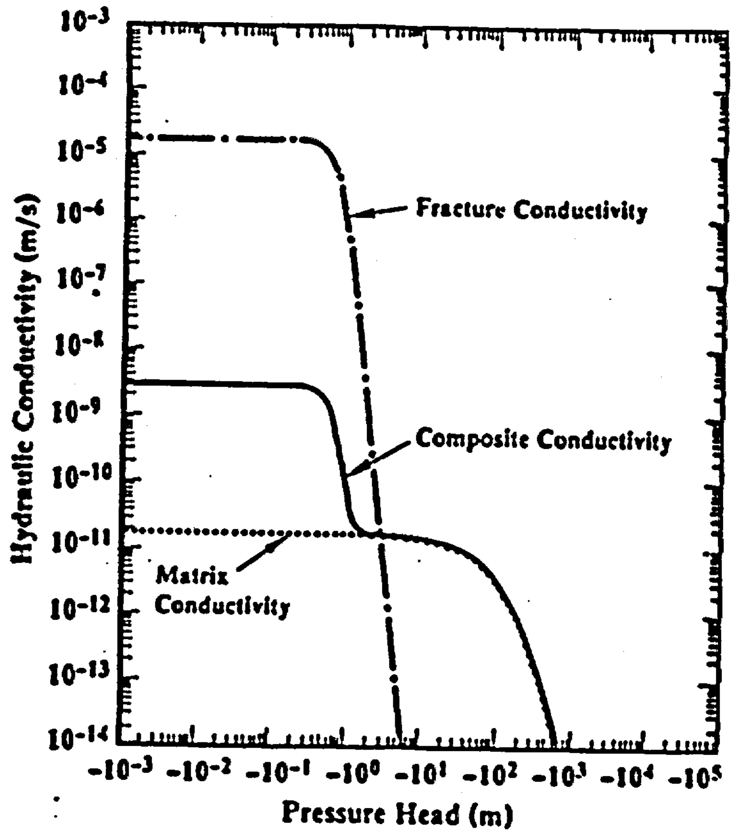

Fig. 1. Conductivity curve for TSw2.

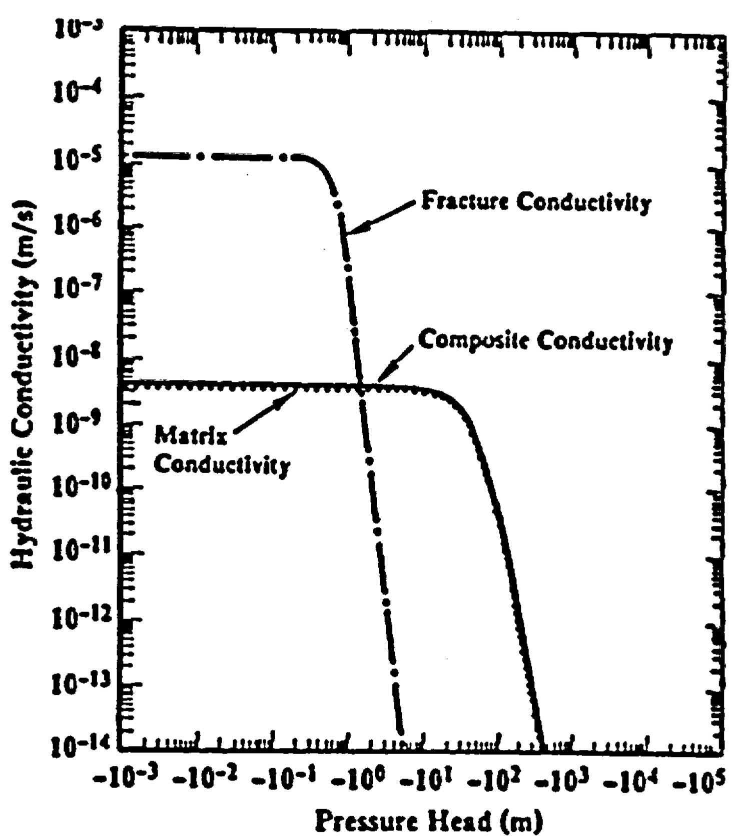

Fig. 2. Conductivity curve for PPw.

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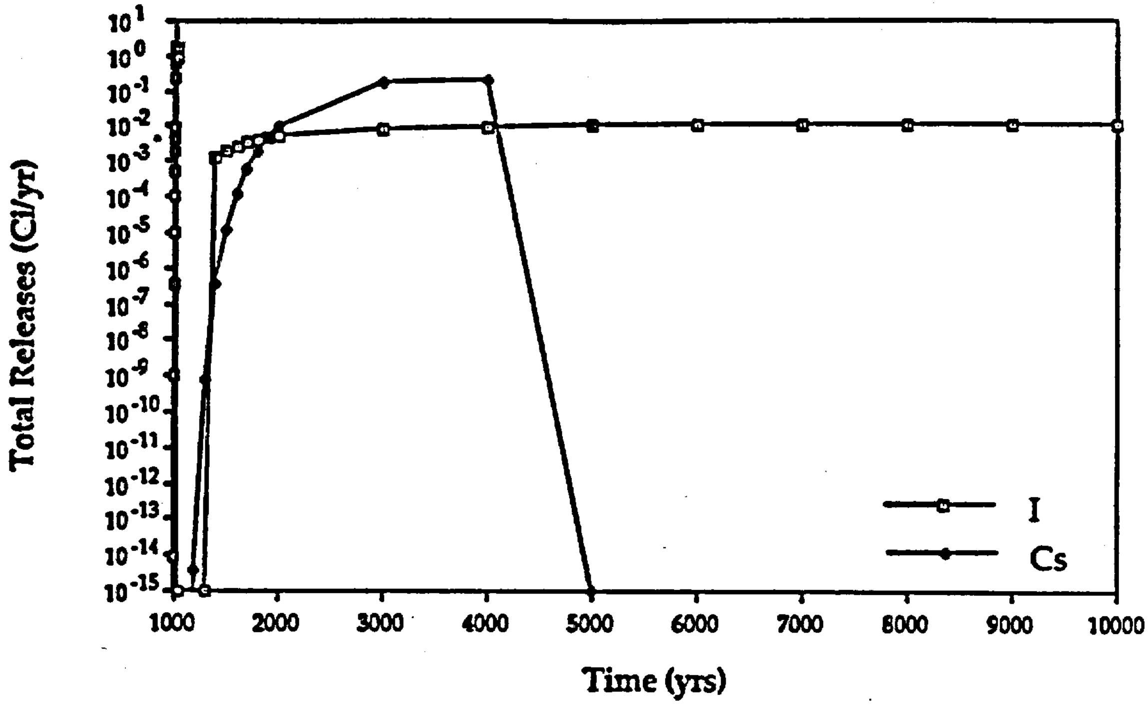

Fig. 3. Moist-continuous source term for ^{129}I and ^{135}Cs.

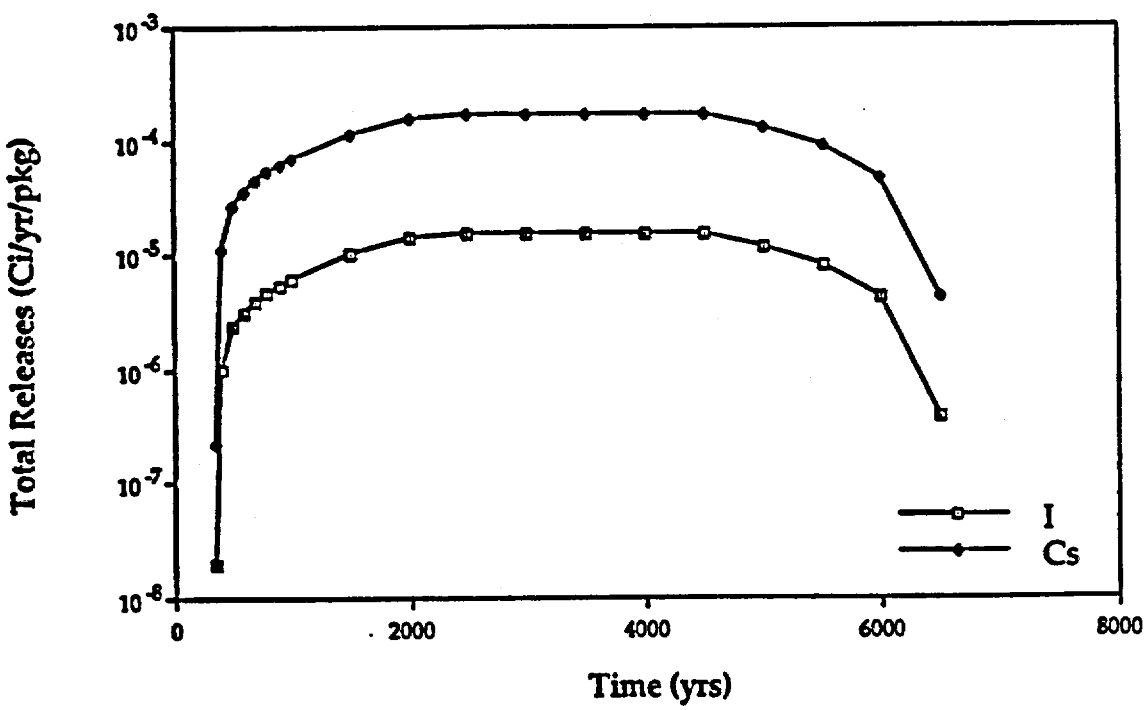

Fig. 4. Flow-through source term for ^{129}I and ^{135}Cs.

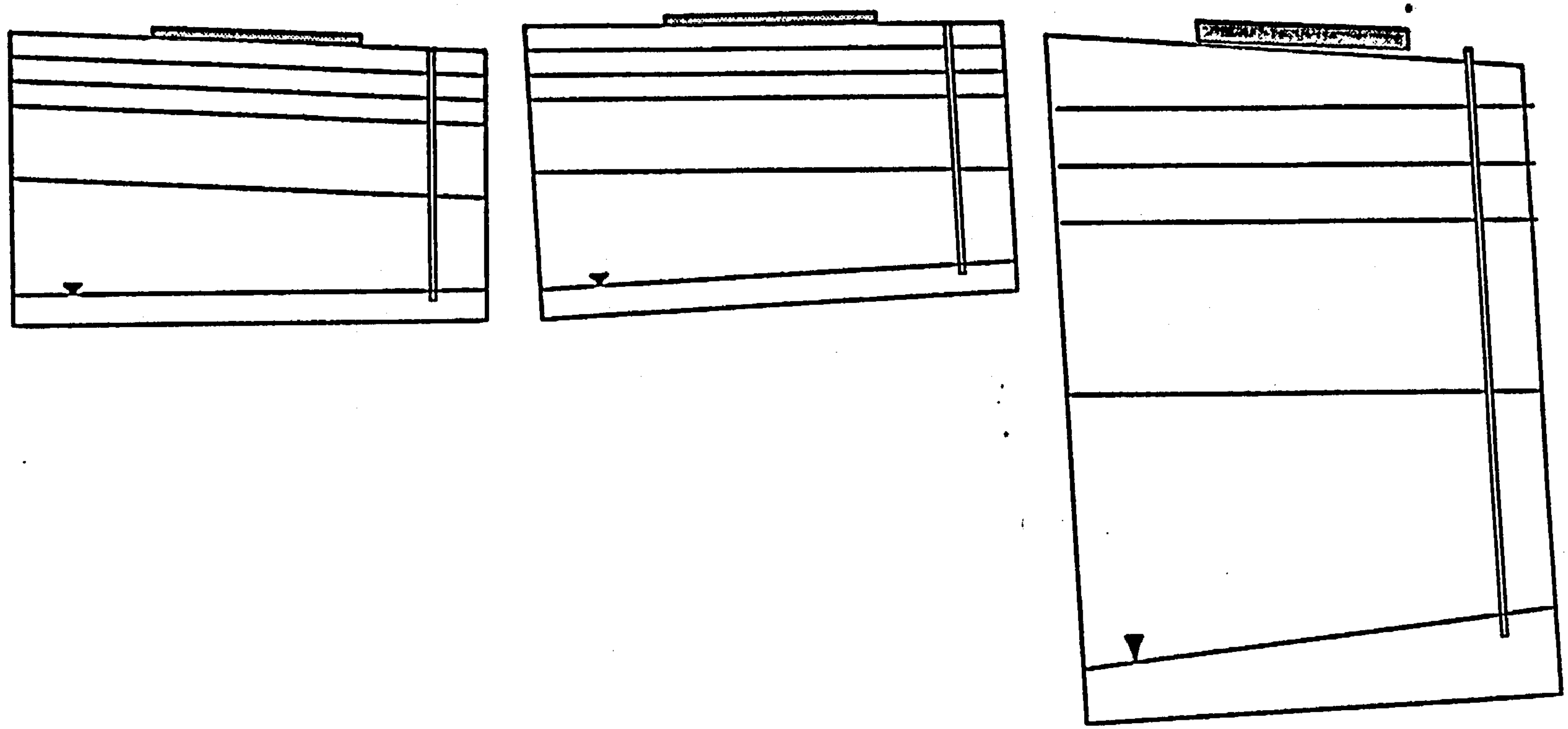

Fig. 5. Effect of grid rotation and axis elongation on water table appearance.

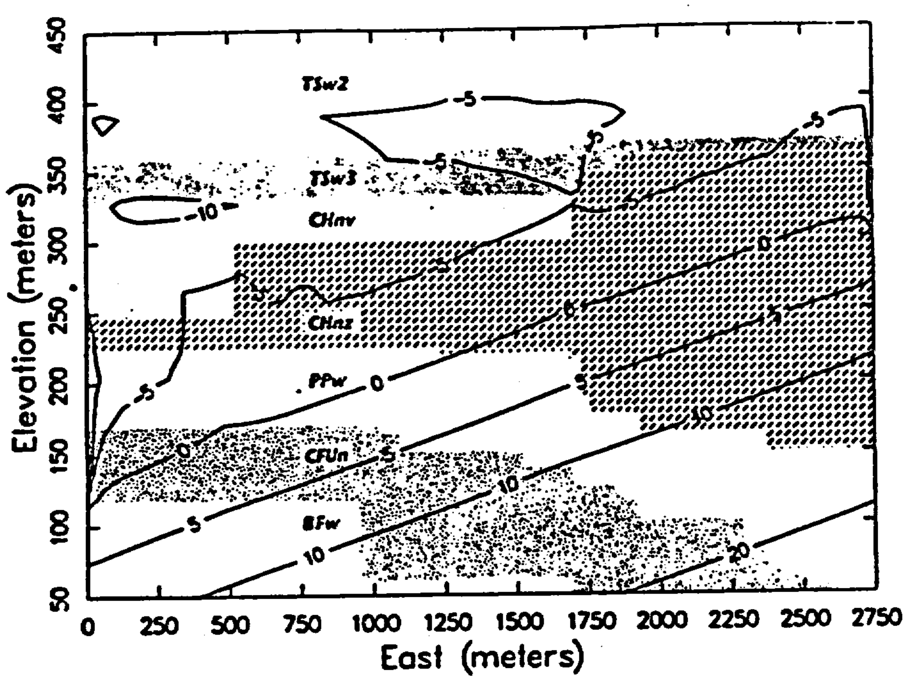

Fig. 6. Steady-state liquid pressure contours (10^6 dynes/cm ^{2}) at a constant recharge of 0.1 mm/yr, east-west cross section (North 3450 m).

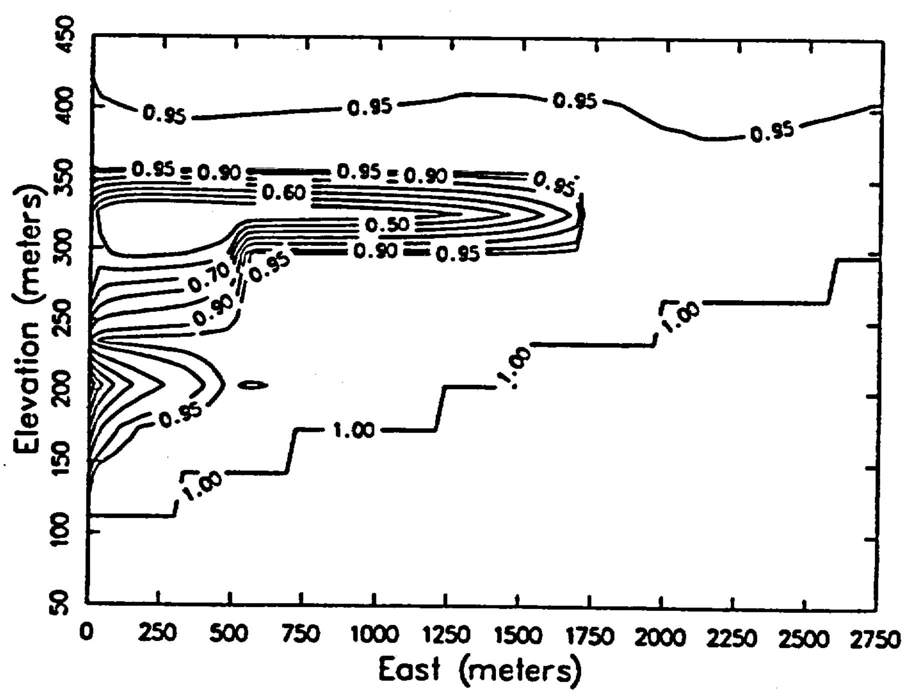

Fig. 7. Steady-state saturation contours at a constant recharge of 0.1 mm/yr, east-west cross section (North 3450 m).

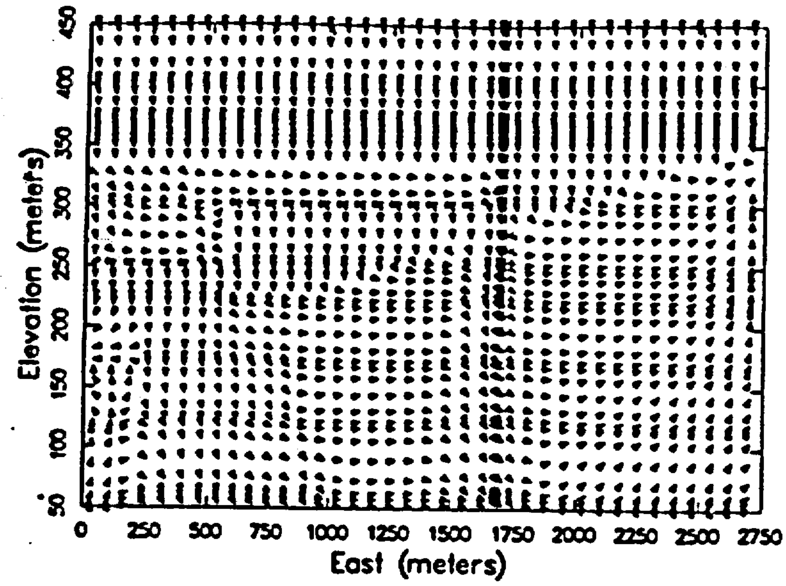

Fig. 8. Steady-state velocity vectors at a constant recharge of 0.1 mm/yr, east-west cross section (North 3450 m).

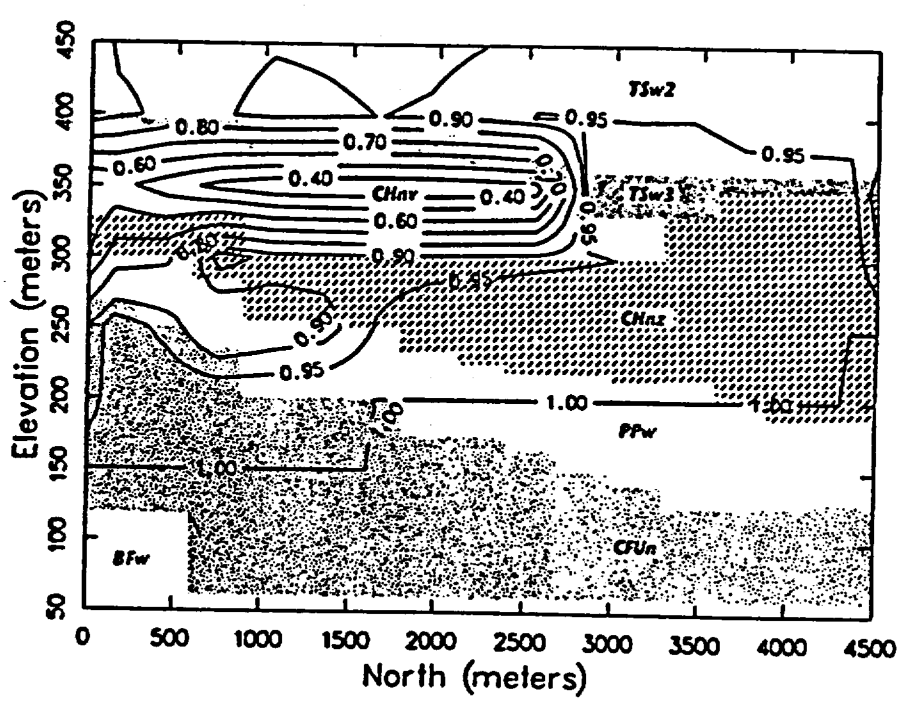

Fig. 9. Steady-state saturation contours at a constant recharge of 0.1 mm/yr, north-south cross section (East 1692 m).

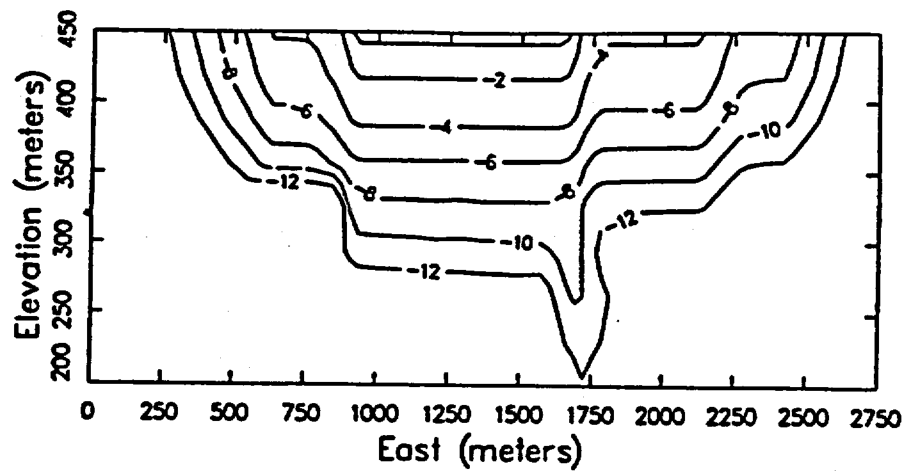

Fig. 10. Log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* = 0.0, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

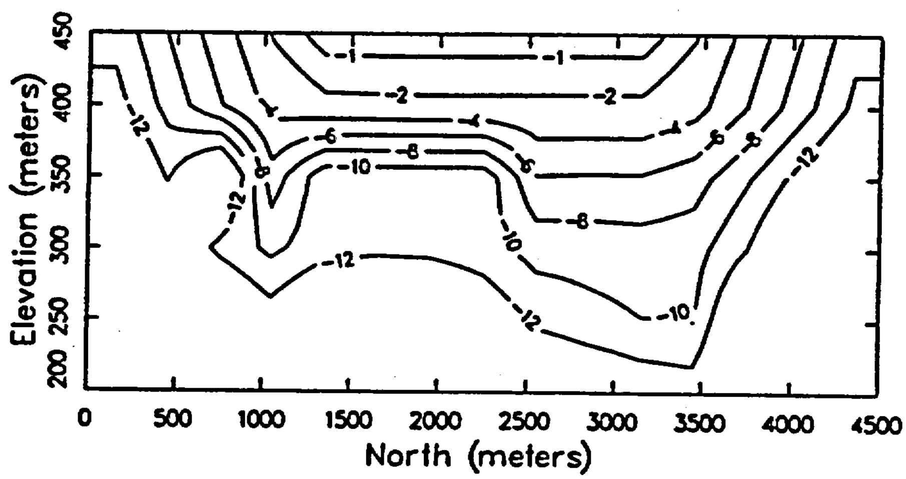

Fig. 11. Log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* = 0.0, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

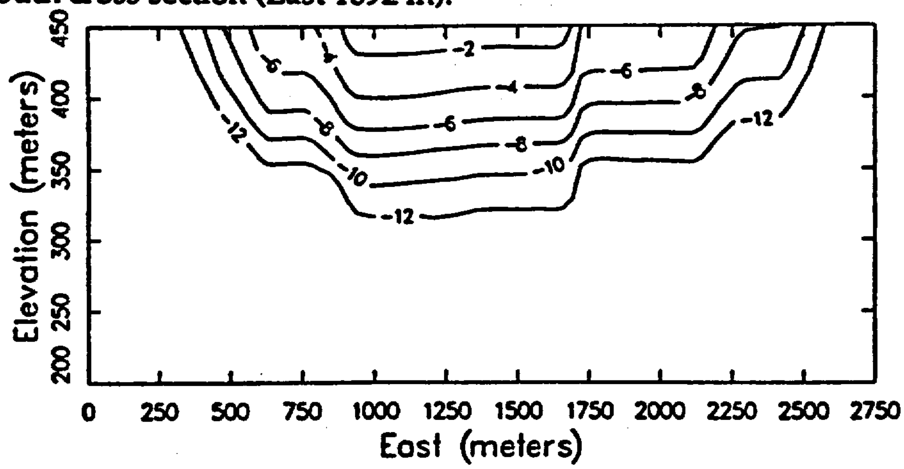

Fig. 12. Log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* realization No. 1, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

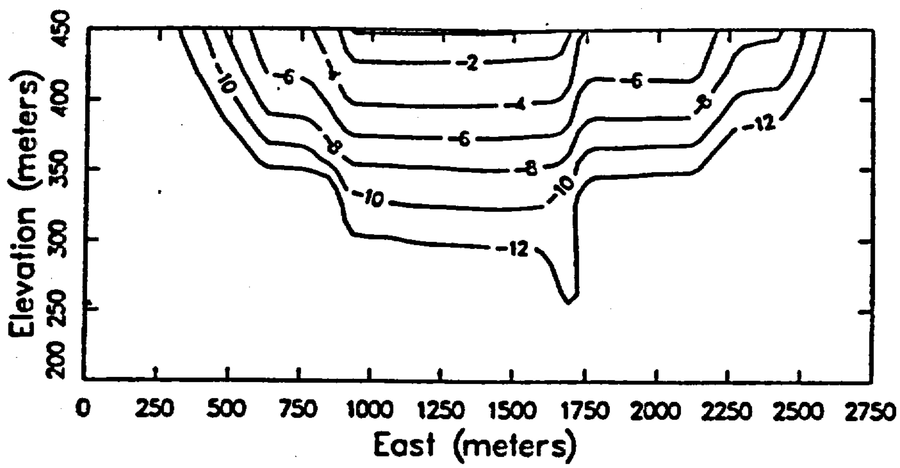

Fig. 13. Log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* realization No. 6, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

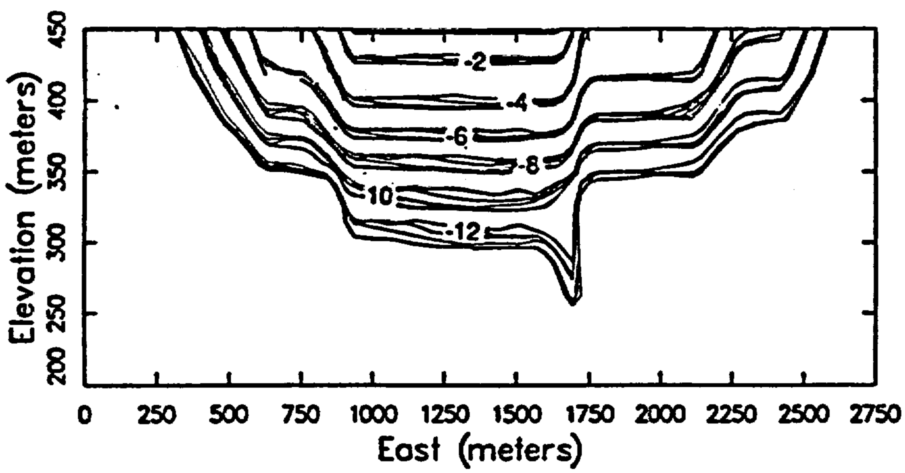

Fig. 14. Overlays of log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* realization Nos. 2 through 6, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

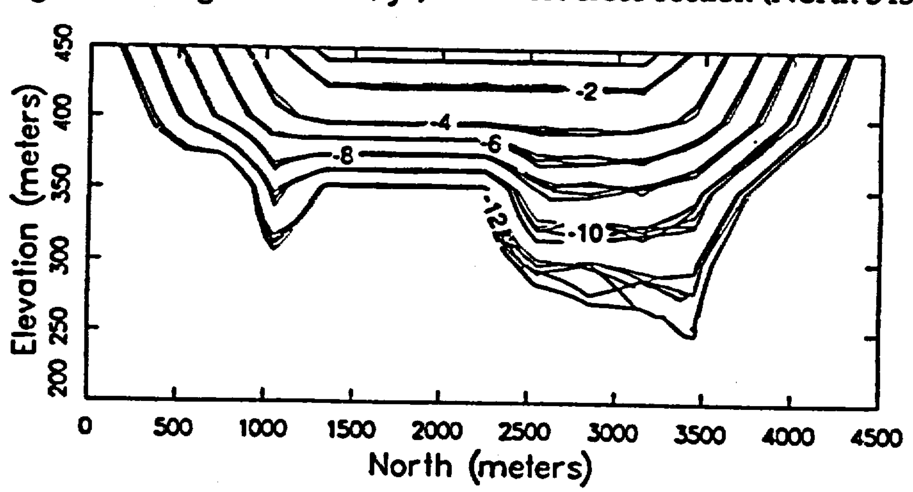

Fig. 15. Overlays of log-scale concentration profiles for ^{99}Tc at 5,070 yrs, *Kd* realization Nos. 2 through 6, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

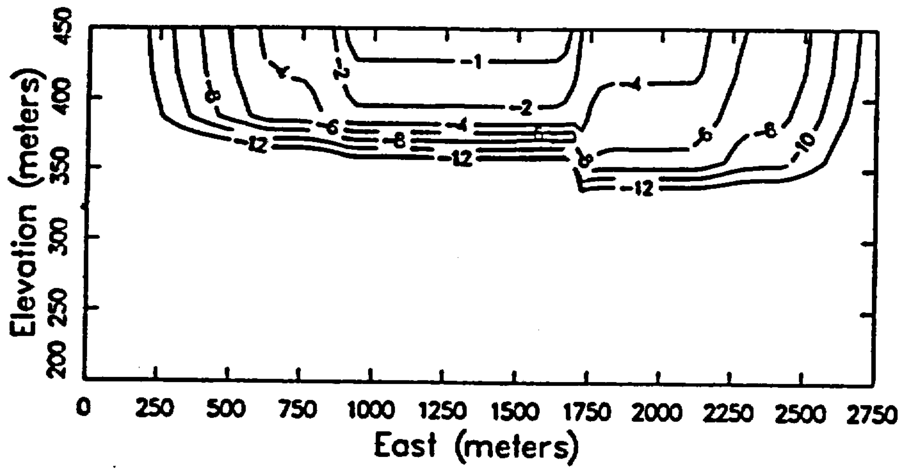

Fig. 16. Overlays of log-scale concentration profiles for ^{135}Cs at 10,000 yrs, *Kd* realization Nos. 1 through 6, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

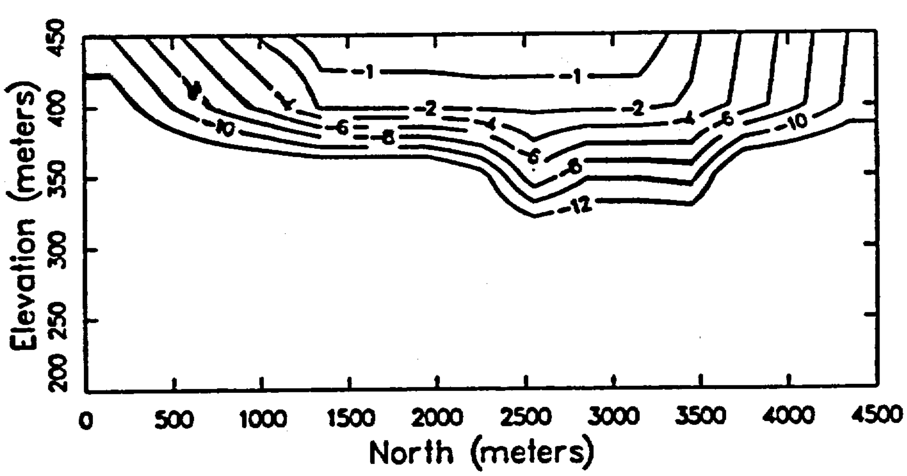

Fig. 17. Overlays of log-scale concentration profiles for ^{135}Cs at 10,000 yrs, *Kd* realization Nos. 1 through 6, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

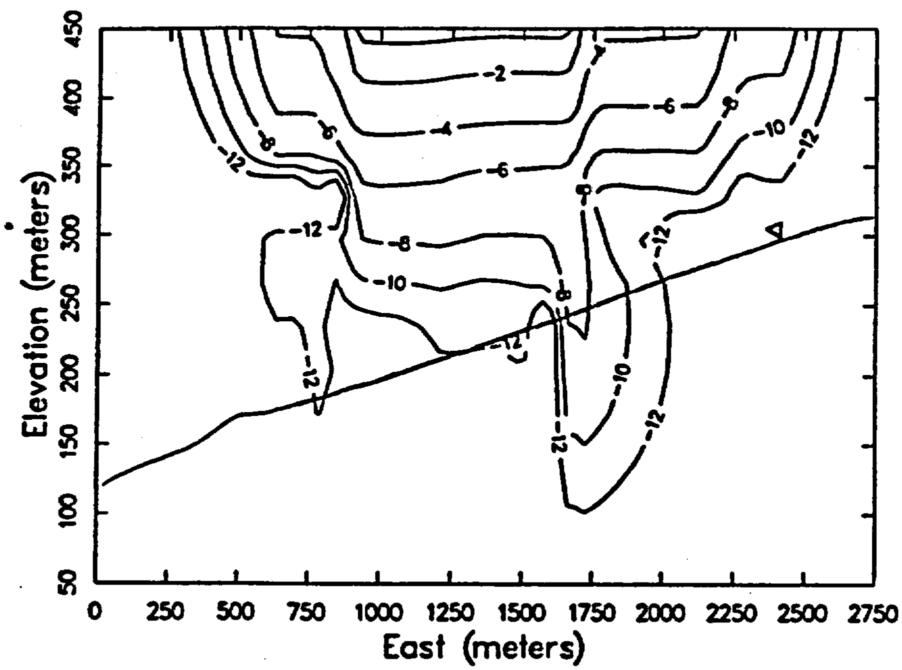

Fig. 18. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

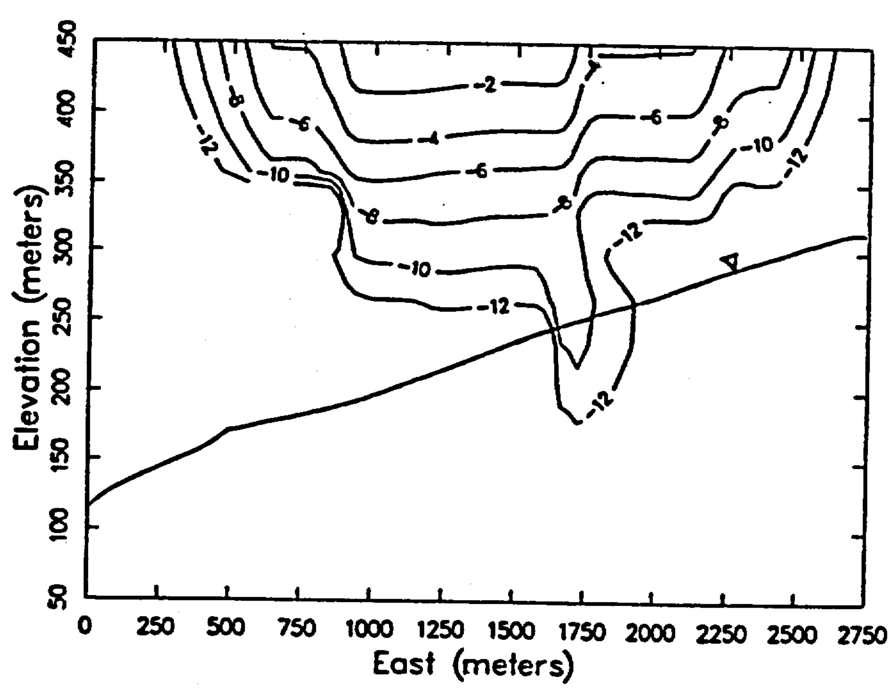

Fig. 19. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, low dispersivity case, *Kd* realization No. 1, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

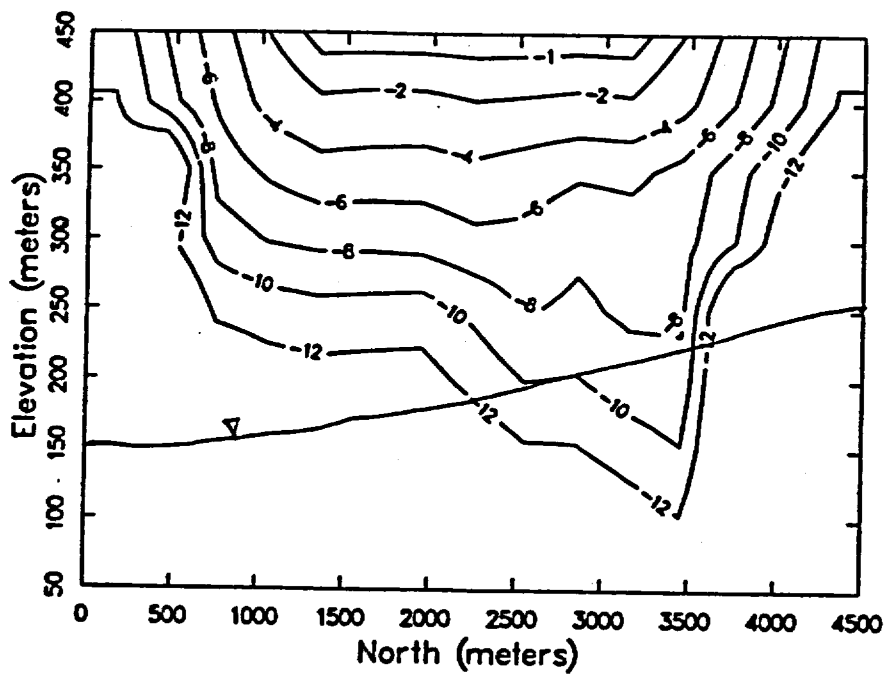

Fig. 20. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

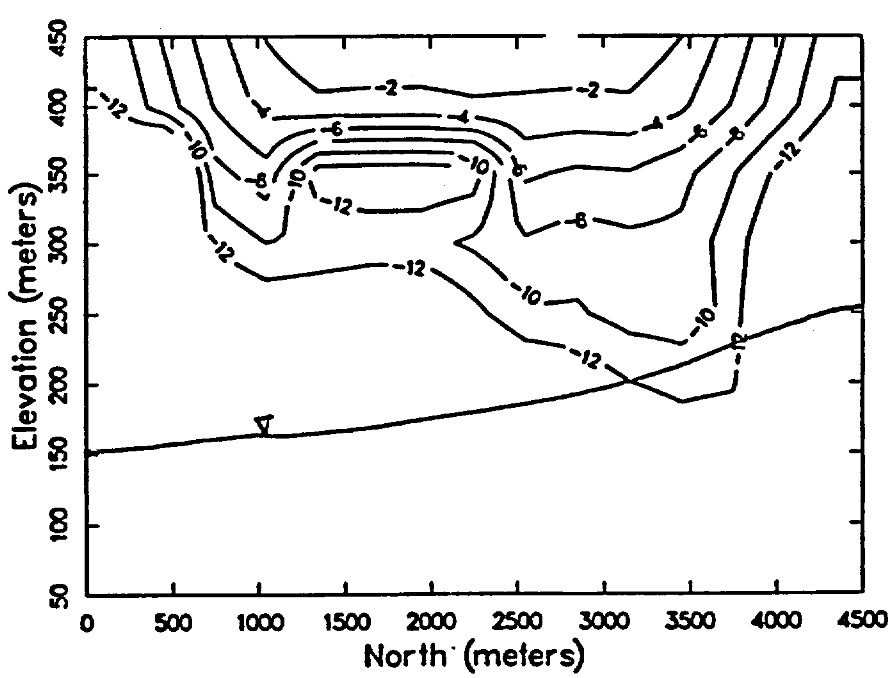

Fig. 21. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, low dispersivity case, *Kd* realization No. 1, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

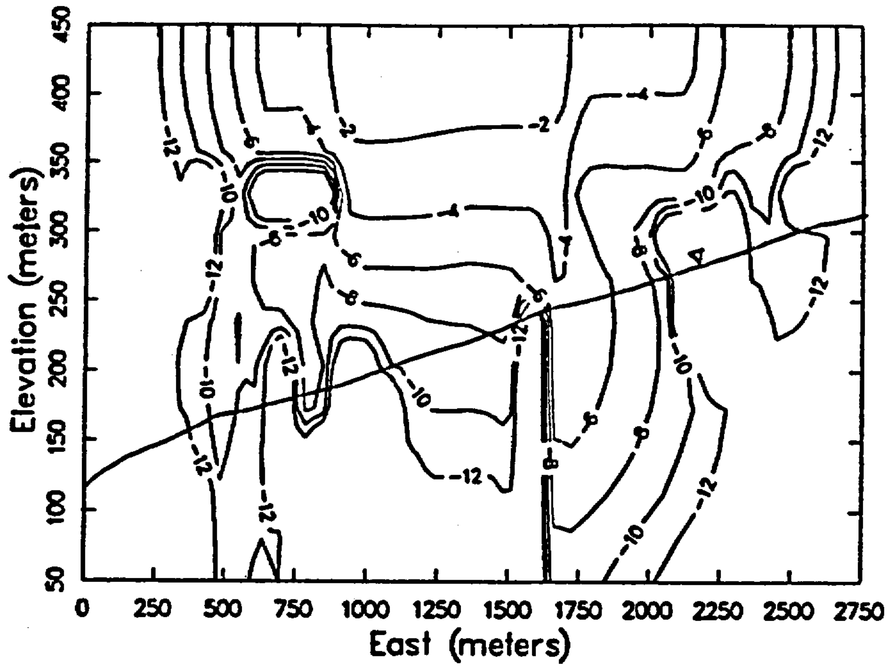

Fig. 22. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, east-west cross section (North 3450 m).

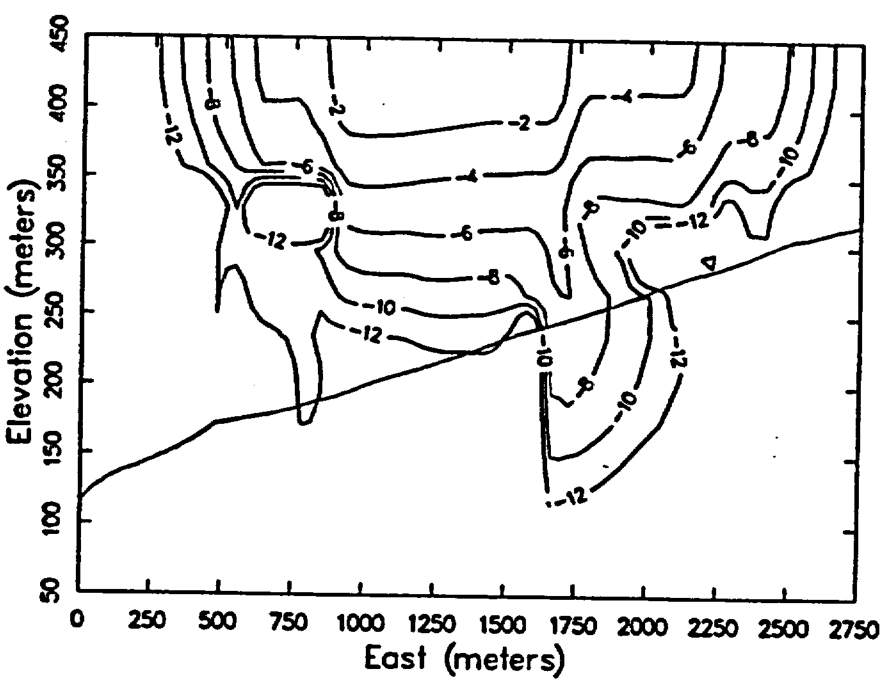

Fig. 23. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, low dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, east-west cross section (North 3450 m).

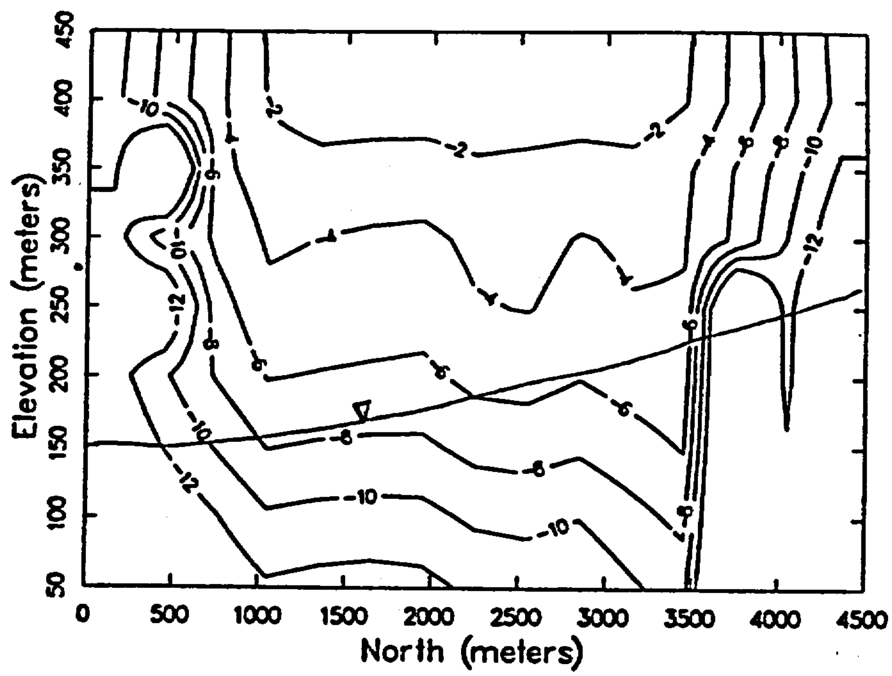

Fig. 24. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

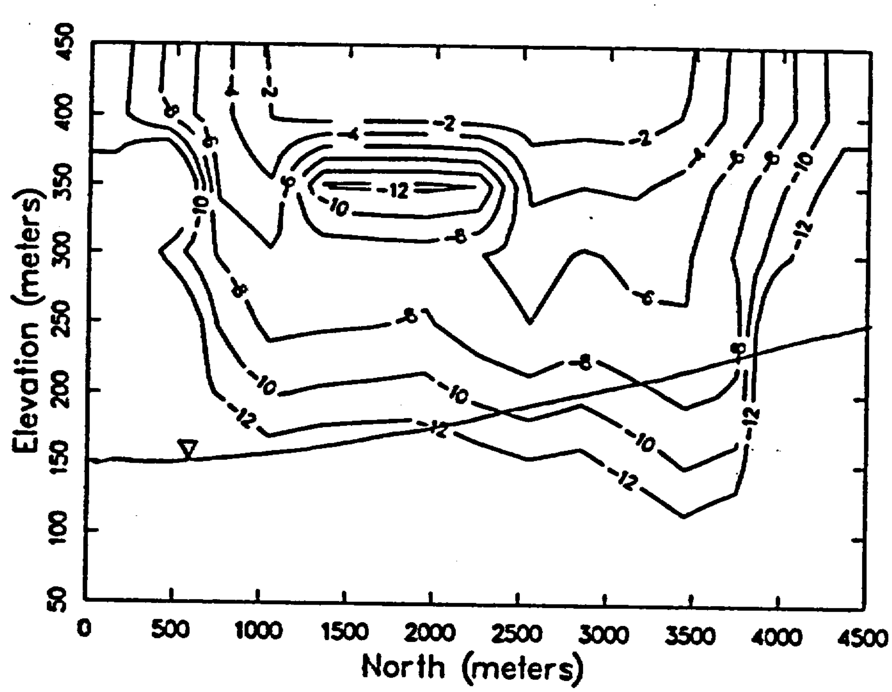

Fig. 25. Log-scale concentration profiles for ^{99}Tc at 10,000 yrs, low dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

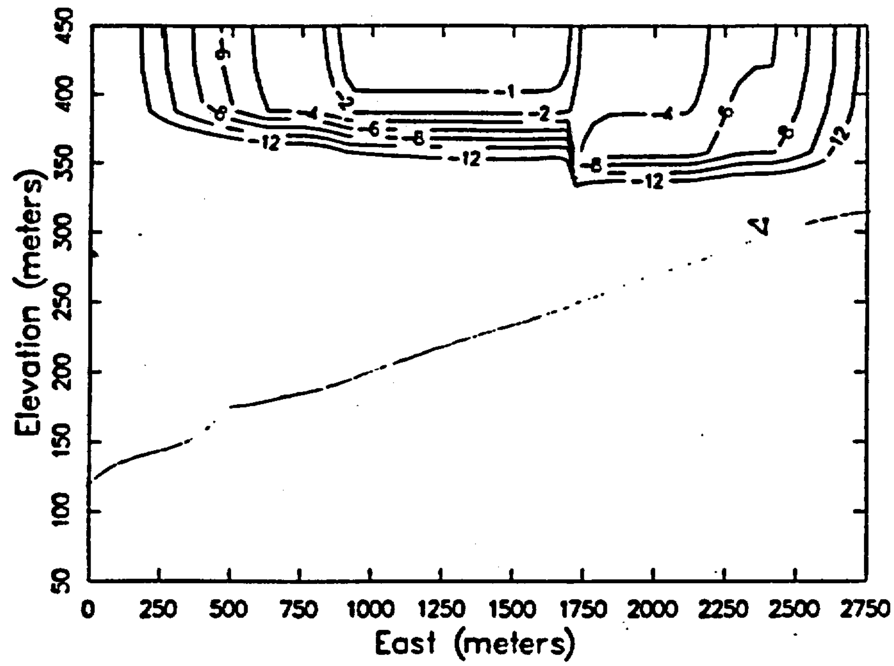

Fig. 26. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, east-west cross section (North 3450 m).

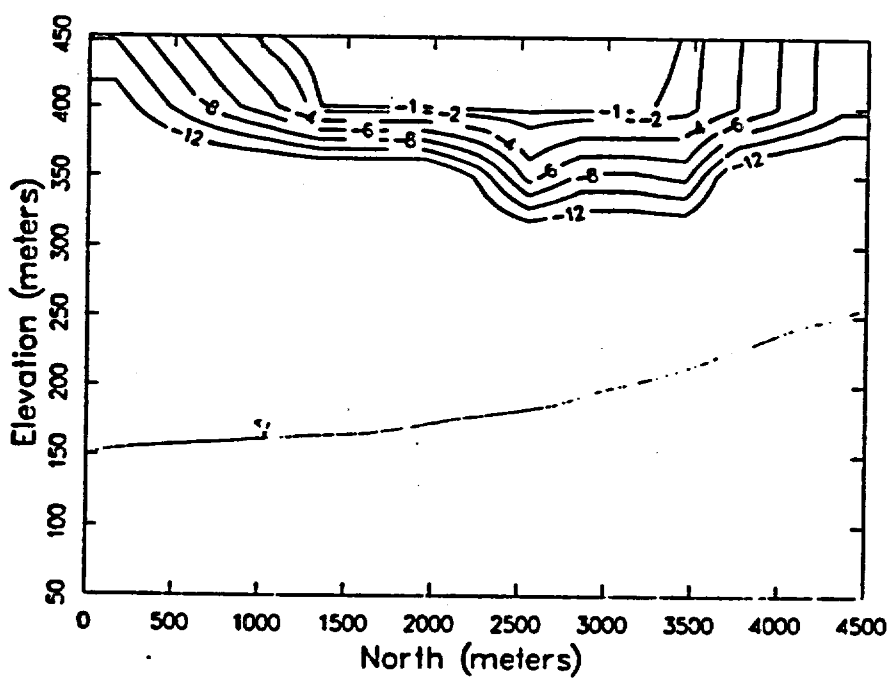

Fig. 27. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

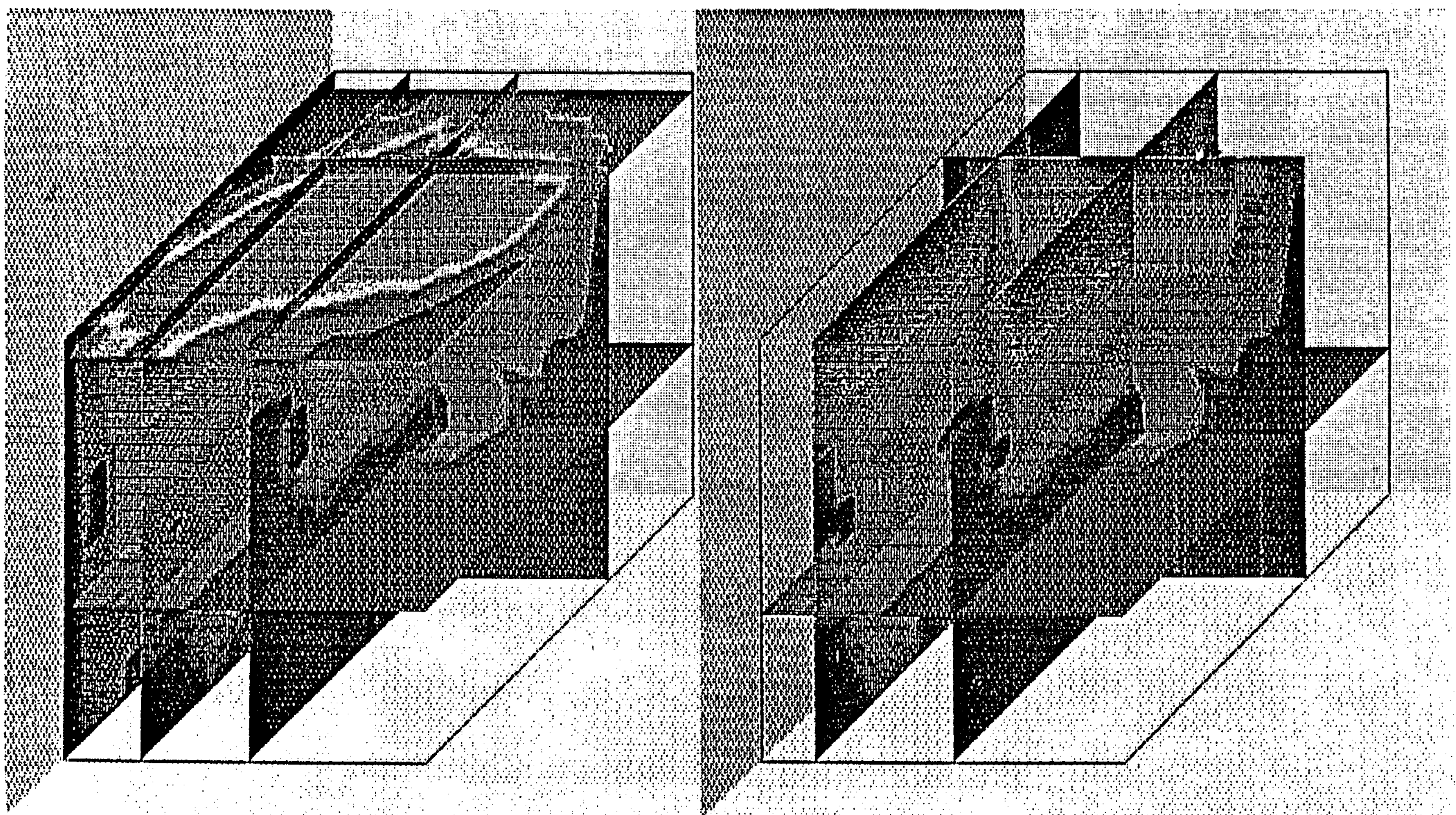

Fig. 28. Three-dimensional visualizations of ^{99}Tc plume at 10,000 yrs, low dispersivity case, *Kd* realization No. 1, recharge = 0.1 mm/yr, constant source.

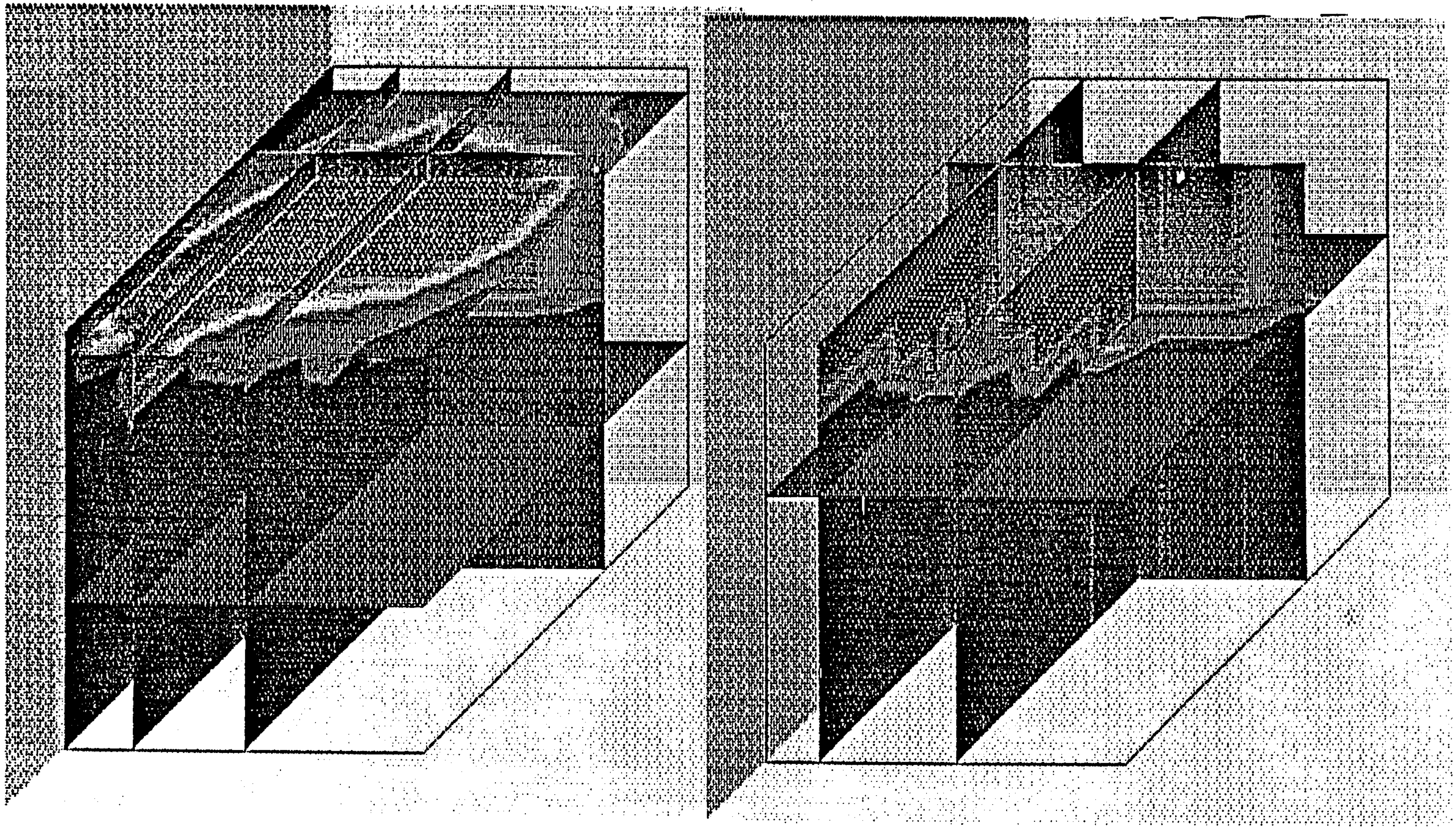

Fig. 29. Three-dimensional visualizations of ^{135}Cs plume at 20,000 yrs, high dispersivity case, *Kd* realization No. 1, recharge = 0.5 mm/yr, constant source.

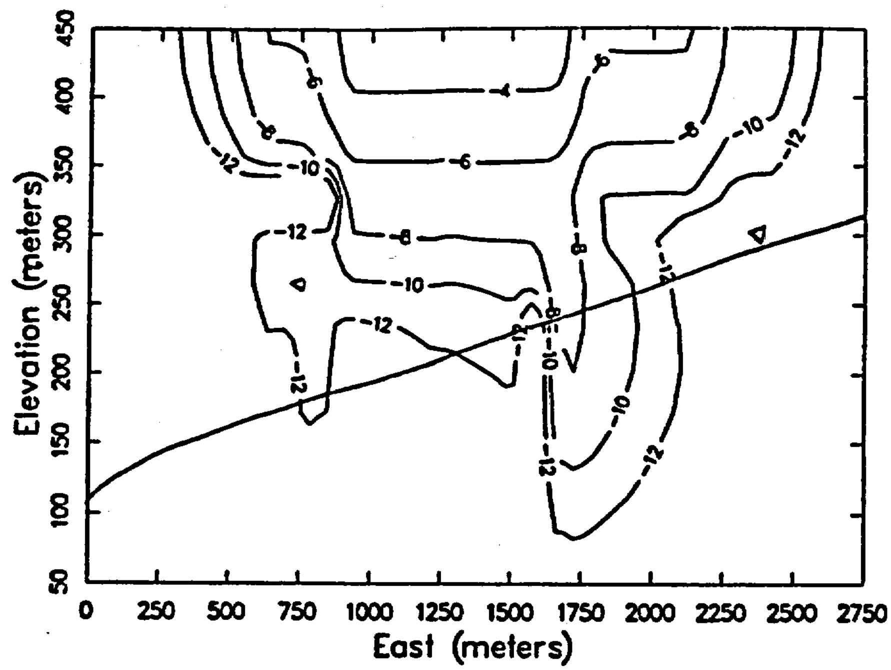

Fig. 30. Log-scale concentration profiles for ^{129}I at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

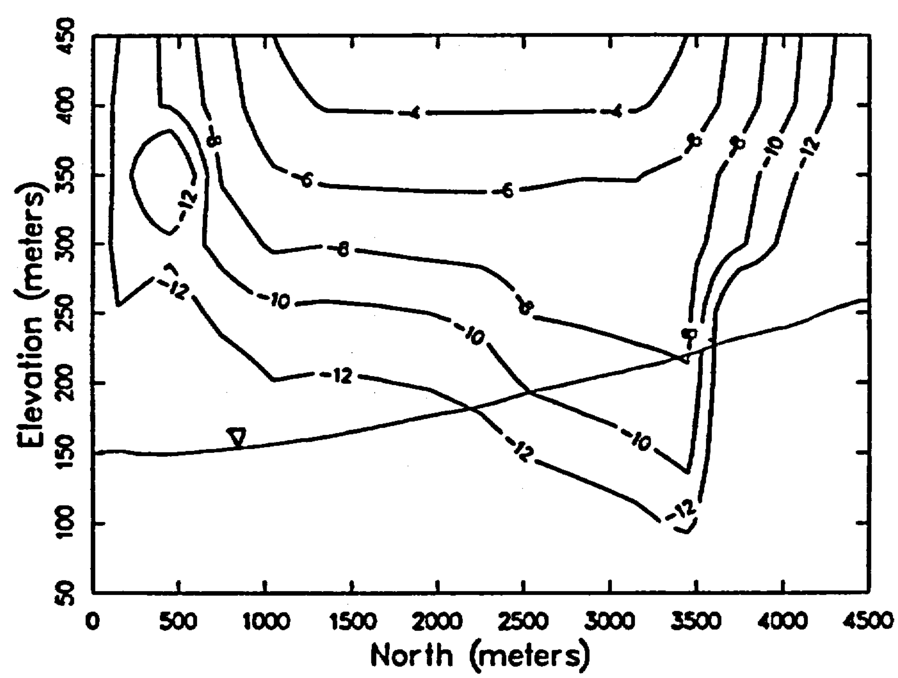

Fig. 31. Log-scale concentration profiles for ^{129}I at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

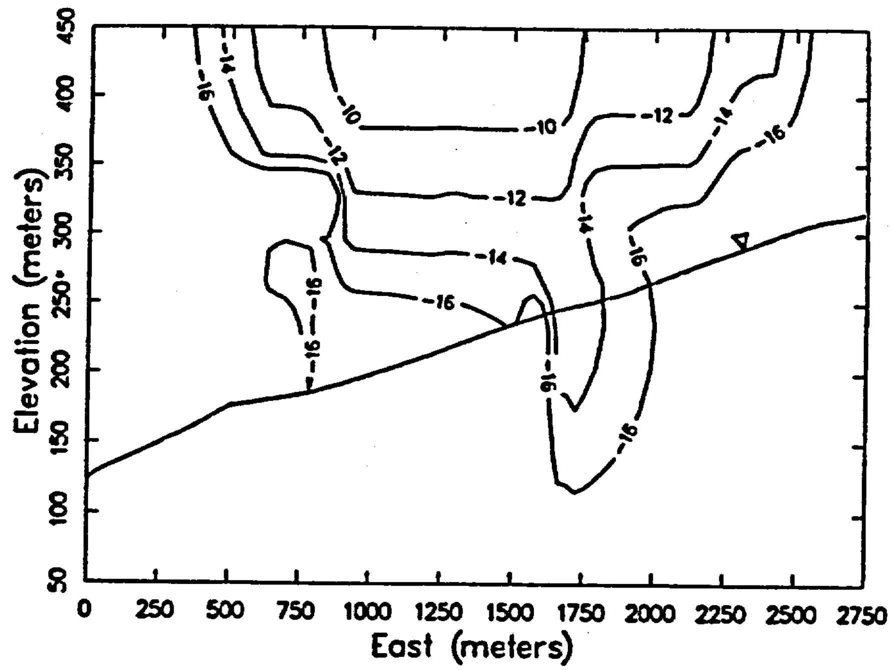

Fig. 32. Log-scale concentration profiles for ^{129}I at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.1 mm/yr, east-west cross section (North 3450 m).

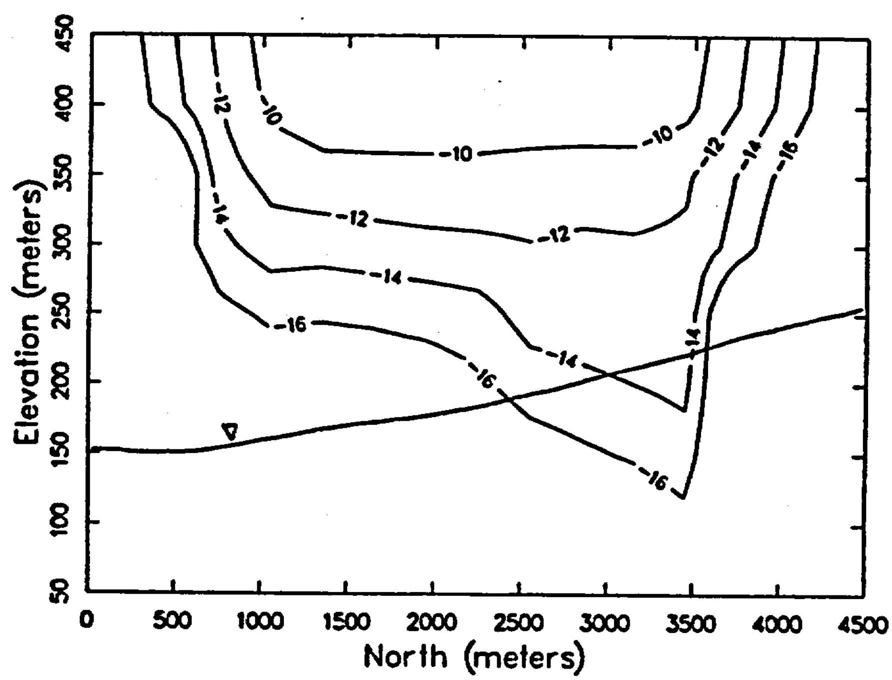

Fig. 33. Log-scale concentration profiles for ^{129}I at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

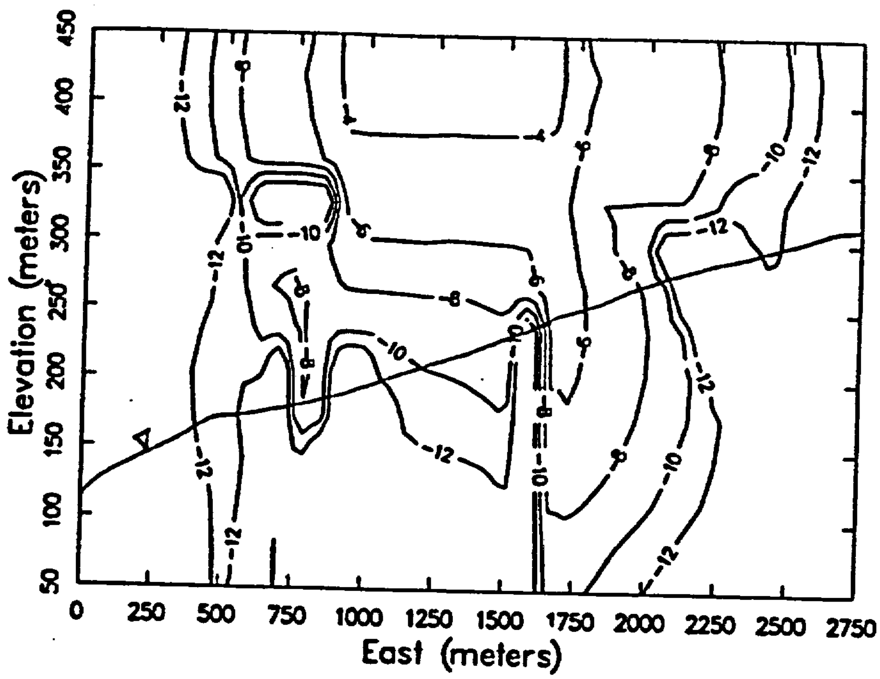

Fig. 34. Log-scale concentration profiles for ^{129}I at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.5 mm/yr, east-west cross section (North 3450 m).

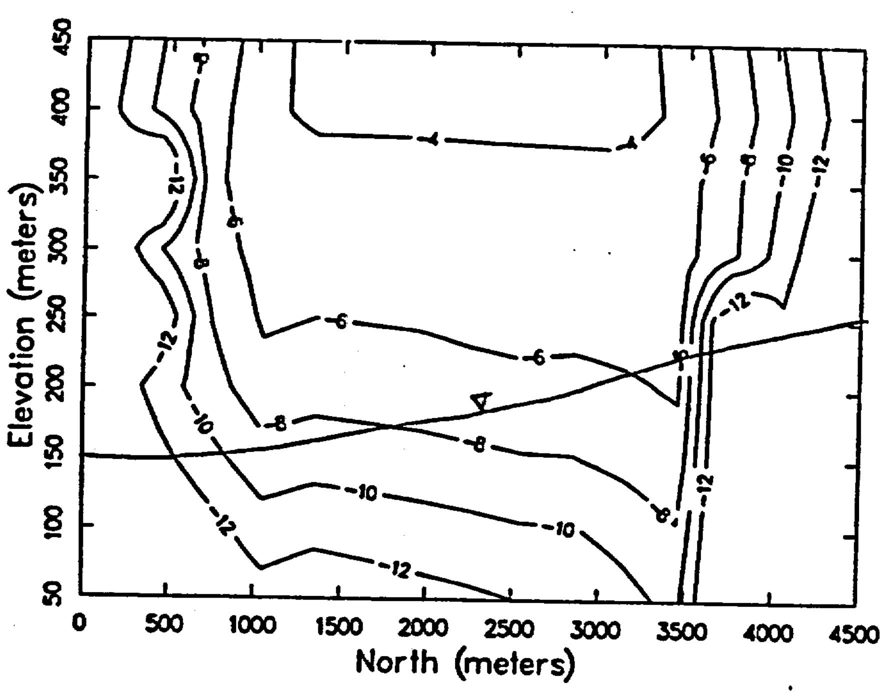

Fig. 35. Log-scale concentration profiles for ^{129}I at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

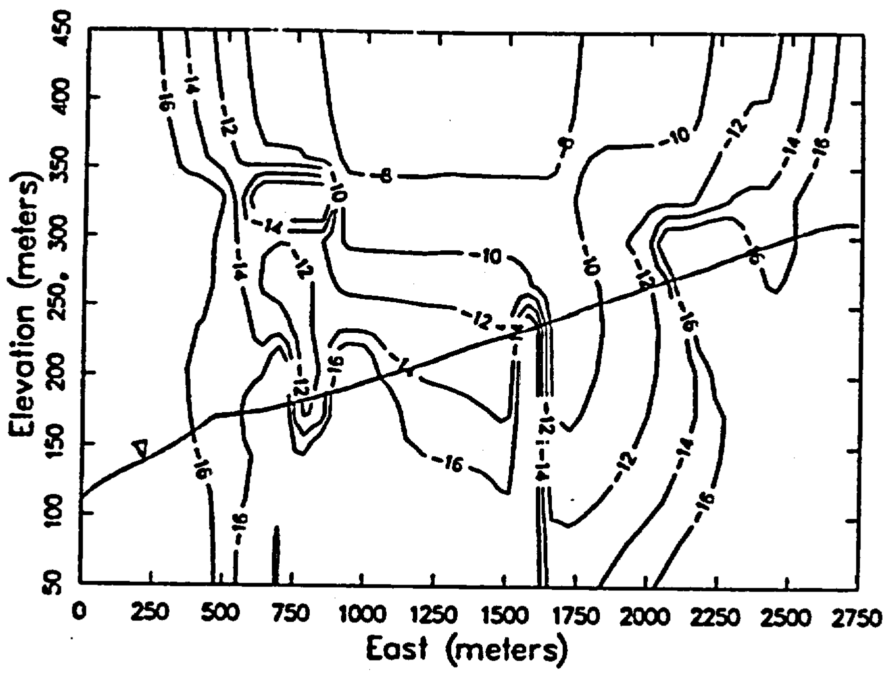

Fig. 36. Log-scale concentration profiles for ^{129}I at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.5 mm/yr, east-west cross section (North 3450 m).

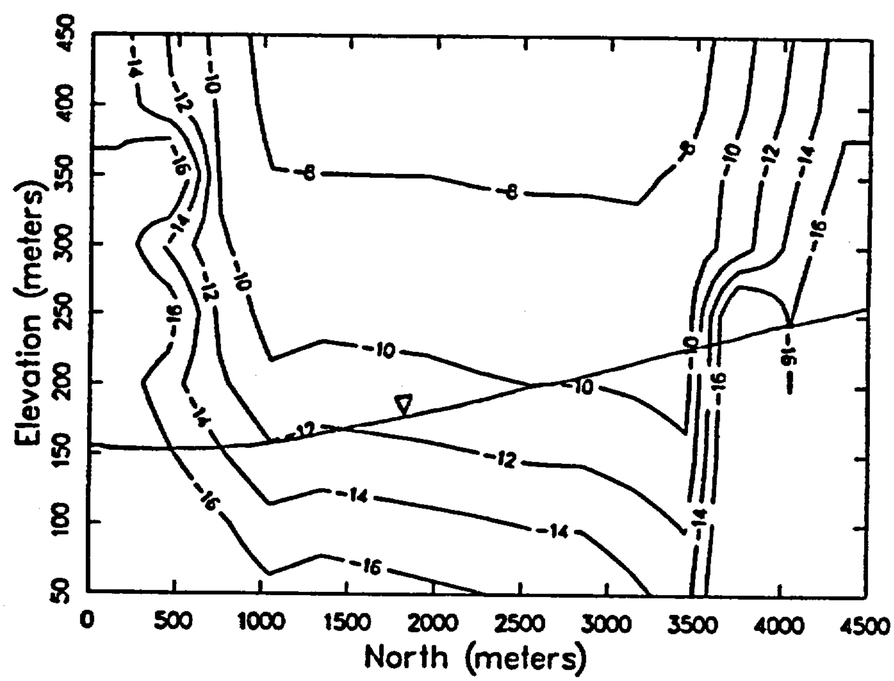

Fig. 37. Log-scale concentration profiles for ^{129}I at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

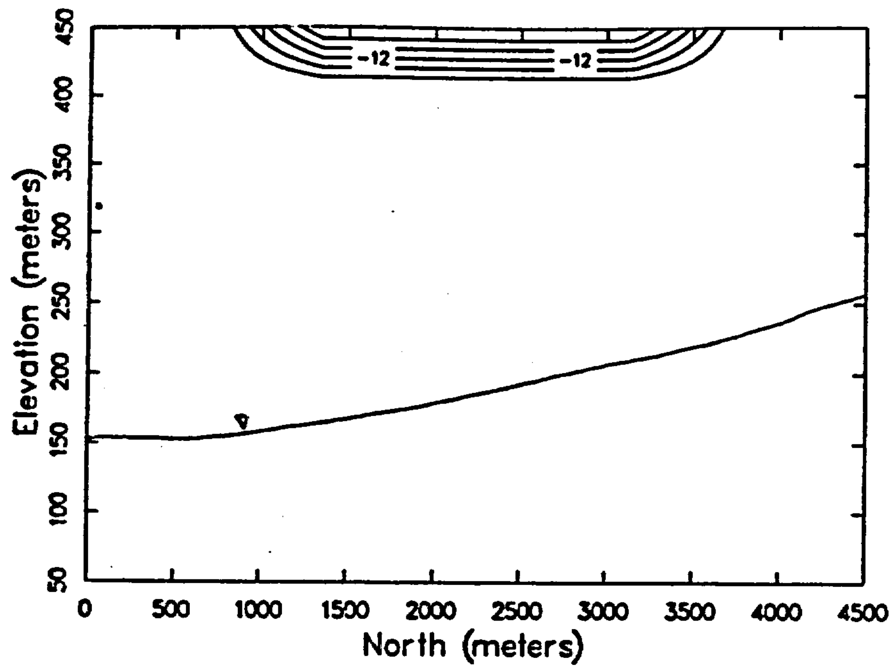

Fig. 38. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

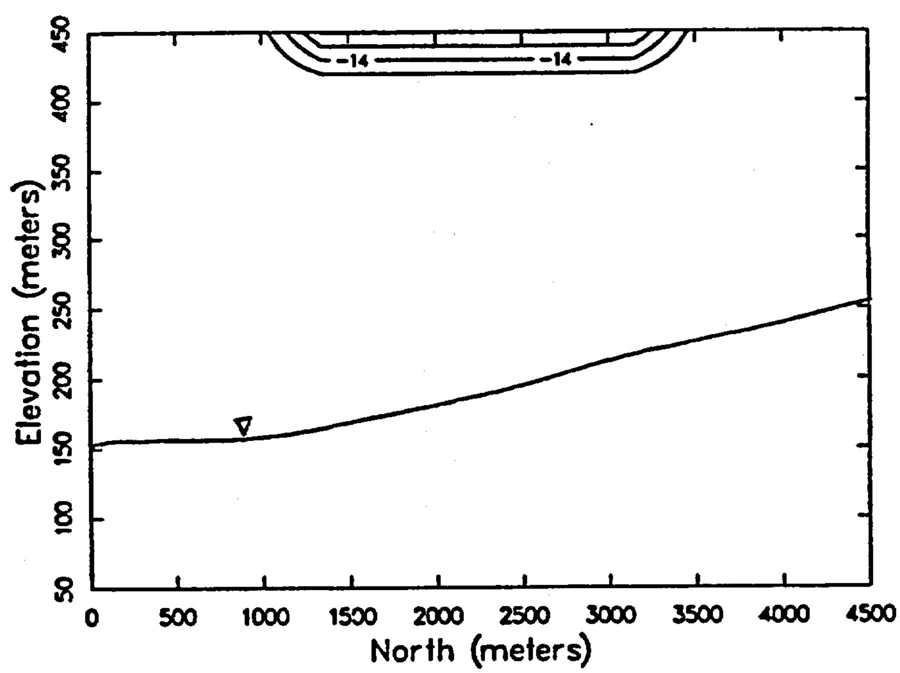

Fig. 39. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.1 mm/yr, north-south cross section (East 1692 m).

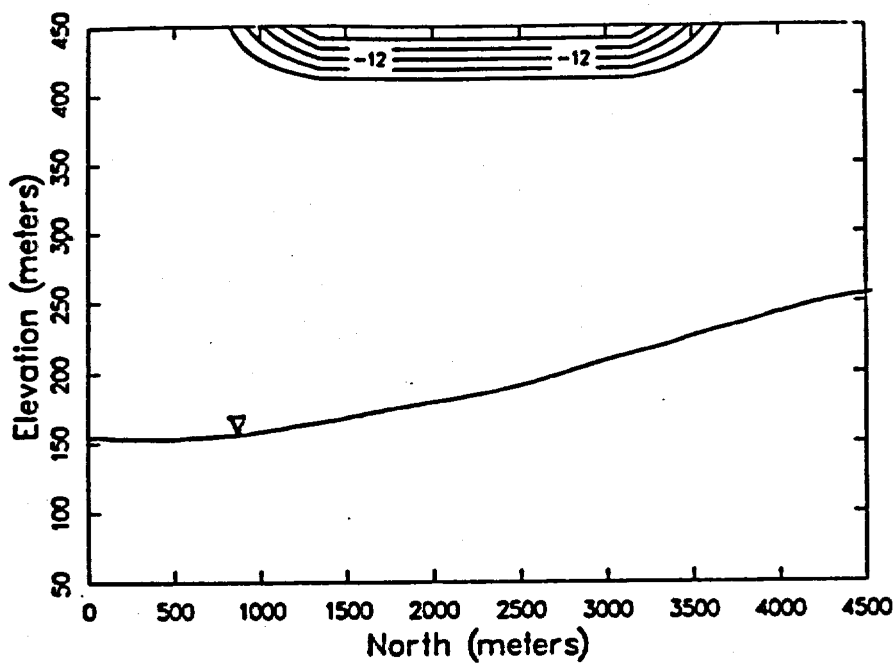

Fig. 40. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, moist-continuous source, high dispersivity value, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

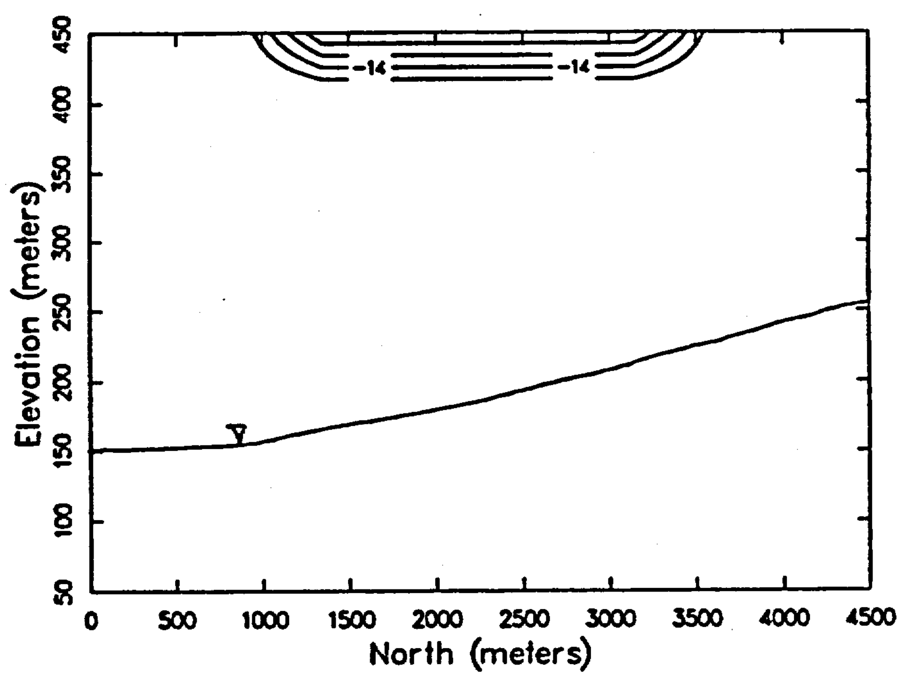

Fig. 41. Log-scale concentration profiles for ^{135}Cs at 10,000 yrs, flow-through source, high dispersivity value, recharge = 0.5 mm/yr, north-south cross section (East 1692 m).

TUESDAY	WEDNESDAY	THURSDAY
9am Entrance Meeting (at LATA) 5/6 S. Bates Mike Clevenger 17 J. Martin Lynn Sanders P. Cloke/N. Cox SP 831341/3 Pam Rogers/ Terry Morgan (QAL) A. Simmons/J. Heaney SP 831342 Larry Hersman/ Donna Williams (QAL)	5/6 S. Bates Donna Williams or Mike Clevenger 17 J. Martin Lynn Sanders P. Cloke/N. Cox SP 8313711/2/3 Kay Birdsell/ Lynn McDonald or Carol LaDelfe (QAL) A. Simmons/J. Heaney SP 831351/2 Dave Morris/ Terry Morgan (QAL)	5/6 S. Bates Donna Williams or Mike Clevenger 17 J. Martin Lynn Sanders A. Simmons/J. Heaney SP 831361/2 Ines Triay/ Terry Morgan (QAL)
LUNCH	LUNCH	LUNCH
5/6 S. Bates Mike Clevenger 17 J. Martin Lynn Sanders P. Cloke/N. Cox SP 831341/3 Pam Rogers/ Terry Morgan (QAL) A. Simmons/J. Heaney SP 831351/2 Dave Morris/ Terry Morgan (QAL)	5/6 S. Bates Donna Williams 17 J. Martin Lynn Sanders P. Cloke/N. Cox SP 8313711.2.3 Kay Birdsell/ Lynn McDonald or Carol LaDelfe (QAL) A. Simmons/J. Heaney SP 831361/2 Ines Triay/ Terry Morgan (QAL)	SQA N. Cox Gary Cort Address any open issues. Exit will be held at 9 am at LATA, Friday morning.

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		Neil D. Cox			
3-01	LANL YMP QAPP, R5 Para. 3.4	3.4 TECHNICAL REVIEWS Technical reviews shall be performed in accordance with a QP that defines the following: o the criteria for selection of the technical reviewers, o the procedure for technical reviews, and o the method of review documentation.			
	TWS-QAS-QP-03.2, R0 Para. 7.0	7.0 QUALITY ASSURANCE REQUIREMENTS Records The following records will be generated through implementation of this procedure: (copies of all document versions; document review forms; Att. 1, 3, and 5; Att. 2 if reviewer is not YMP certified; transmittal cover letters.)			

9 AUDITOR SIGNATURE

10 DATE

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3-01 con't		1. Verify that records include original draft submitted for technical review.			
		2. Verify that records include version approved by YMPO.			
		3. Verify that records include published TIP if published.			
		4. Verify that records include document review forms and comment resolutions correctly prepared. (Att. 4)			
		5. Verify that records include a Publications Traveler (Att. 1) with all 24 lines signed and dated.			
		6. Verify that records include a signed and dated Review Criteria form signed and dated. (Att. 3)			
		7. Verify that records include a completed Policy Review Form, signed and dated. (Att. 5)			
		8. Verify that records include transmittal cover letters.			

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3-01, con't		9. If any reviewer is not YMP certified, verify each is covered by Att. 2, Reviewer Qualifications.			
		(NOTE: Jot down the identities of such reviewers.)			
		10. Verify that all referenced final reports have an accession number.			
		11. All LANL reports published must have an accession number before publication. VERIFY.			
		12. If Computer Software has been used to generate data, verify that software is fully documented OR that a disclaimer is included about not meeting SQA requirements.			
		13. If new data are reported, verify that the QA Level of the data producing activity is reported.			
		(NOTE: Identify and enumerate any such reports.)			

9 AUDITOR SIGNATURE

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	LANL YMP QAPP, R 5 Para. 3.1.3	The organization that develops a scientific investigation planning document shall conduct a technical review of it.... The scientific investigatio planning document shall be reviewed per LANL procedures.			
3-2	TWS-QAS-QP-03.3, R0 Para. 6.2.1	REVIEW AND APPROVAL OF STUDY PLANS TECHNICAL REVIEW The author ensures that the study plan is reviewed technically according to QP-03.2.... The technical review is performed by any qualified Project or LANL participant other that the person who developed the original document. Verify that each SCP Study Plan audited underwent a technical review under procedure QP-03.2 by one or more qualified participants. NOTE: This also includes any major changes to a study plan. Use QP-03.2 for audit.			
3-3	Para. 6.1	Verify that each study plan audited has an appendix that includes QA level assignments as well as specific details of the specific controls that will be applied.... (per Att. 2).			

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3-4	Para. 6.2.2	Verify that a QA Review was performed on each study plan audited (Signed and Dated Att. 3).			
3-5	Para. 7.1	Verify that each QA Records package is complete with the most recent version of the study plan, the QP-3.2 travelers, all review comments, and the LANL Study Plan QA Review Form.			
3-6	LANL YMP QAPP, R 5 Para. 3.1.6	DOCUMENTING SCIENTIFIC INVESTIGATIONS There are two kinds of documentation that can be used for the QA documentation and control of scientific work: the scientific notebook and the detailed technical procedure (DP).... Bound notebooks, logbooks, or appropriate forms shall be used to document the performance of DPs and the control over all other aspects of the work. Documentation of scientific work, i.e., experiments and research, shall be performed to provide a written record of the experiment or research.			

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3-6	TWS-QAS-QP-03.5, R0 Para. 6.1	Identification - The Resident File Custodian (RFC) assigns a unique group identification number, such as a TWS number. The following information is recorded inside the front of each notebook and logbook: - unique identification number - assignee's name or instrument(s) or activity covered by the book, and - starting date for the books use. When loose leaf pages are used, the pages must be consecutively numbered. Verify that "books" are uniquely identified, have the above required information inside, and have consecutively numbered pages.			
3-7	Para. 6.2	The experimenter signs and dates each entry. Verify signed and dated entries.			

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3-8	Para. 6.3	Entries shall be in a photocopiable ink with no open spaces for later entries, and with pages firmly affixed. Verify the above requirements in each "book" examined.			
3-9	Para. 6.6.2	If any deviation from a DP occurs, any data that could be compromised by a malfunction or failure must be evaluated for acceptance or rejection by the PI. The PI writes and signs a statement regarding acceptance or rejection in the notebook or logbook. In case of a DP deviation, verify the above action. (NOTE: any such occurrence in the margin.)			
3-10	Para. 6.6.3	Research and Development in-process entries shall be signed and dated on the day the entries are made. Verify the above required action.			

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3-11	Para. 6.6.5	If researcher creates files of data, these shall be referenced in the notebooks by a unique identification number and storage location. The researcher must consecutively number the loose pages of the file. Verify the above required action. (NOTE: the occurrence in the margin.)			
3-12	Para. 6.7	When final results have been obtained for the experiment and research, the PI documents in a project report a summary of the outcome.... The report becomes a Project QA Record. Verify the above action for any concluded experiment or research. (NOTE: such cases in the margin.)			
3-13	Para. 6.8	Any necessary corrections may be made by the individual or PI who made the original entry USING a SINGLE LINE STROKE through the incorrect entry. Verify that any corrections are made this way.			

9 AUDITOR SIGNATURE ____________ 10 DATE ____________

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3-14	Para. 6.9	At a minimum, all notebooks and logbooks must be independently reviewed when they are completed or when the activity is terminated.... The reviewer states that the notebook or logbook has been reviewed and understood and signs and dates the final entry reviewed. Interim technical reviews are suggested. Verify the above action for all completed or terminated experiments (or interim reviews).			
3-15	Para. 6.9	THE LOGBOOK RECEIVES A QA REVIEW, RATHER THAN A TECHNICAL REVIEW FOR CLARITY AND FOR CORRECTION OF OBVIOUS ERRORS. DETERMINE THE MEANING OF THIS STATEMENT in the light of the requirement just above for technical review of a logbook.			

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3-16	LANL YMP QAPP, R 5 Para. 3.5	PEER REVIEWS When applicable, LANL shall institute a peer review process to provide adequate confidence in the work being reviewed. A peer review QP shall meet the requirements of NUREG-1297 and Appendix J of this QAPP.			
	TWS-QAS-QP-03.7, R0 Para. 6.1	The initiation of a Peer Review is documented in a memo or letter from the TPO to the Principal Investigator (PI) or design manager in charge of the work to be peer reviewed. The memo or letter also documents the justification for the review. Verify that such a letter was written to initiate all peer reviews.			
3-17	Para.6.2	The selection of the Peer Review Group (PRG) and the designation of the chairperson (by the TPO) are documented in the peer review report. Verify this selection procedure.			

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3-18	Para. 6.3	The technical qualifications and relationship of each peer reviewer to the work being reviewed are documented in the final report of the PRG.... The final report also includes the YMP resume for each member of the PRG.... Any reviewer not working on the YMP must formally become part of the YMP by receiving training in the use of the QAPP and this QP, and their qualifications must be documented in accordance with QP-02.1. Verify such action in the case of a non-YMP reviewer. (Note any such instances in the margin.)			
3-19	Para. 6.4.1	The TPO, or his designee, prepares a peer review plan that contains a description of the work to be reviewed, the size of the PRG, the technical fields to be represented by the members of the PRG, and a suggested schedule for the review.... The plan identifies the criteria against which the work will be reviewed and includes,at a minimum, the criteria listed in QAPP Appendix J, Section J.5. Verify that the peer review plan contains the above information.			
3-20	Para. 6.4.2	The chairperson...prepares written documentation of the results of all meetings, deliberations, or other activities of the PRG. This documentation is included in the PRG's final report. Verify that this documentation is within any final peer review report.			

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OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
3-21	Para. 6.4.3	The written report is signed by each member of the PRG. Verify the required signatures.			
3-22	Para. 6.5	The PI or design manager prepares responses to the peer review comments if responses are required and these responses are reviewed by the TPO or his designee. If the PI is required, verify that written responses were prepared and reviewed.			
3-23	Para. 6.6	IF there are unresolved issues and IF the PI is unable to concur with the objections of the PRG, the matter may be referred to successively higher levels of management.... Any remaining unresolved concerns of the PRG are documented in the final report of the work reviewed. Verify that this process was used if appropriate. (NOTE: The occurrence of any such cases in the margin.)			

9 AUDITOR SIGNATURE

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OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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		Jerry Heaney			
3H-01	TWS-QAS-QP-03.2, Rev. 0, Para. 6.1.1, "Procedure for Preparation and Technical and Policy Review of Technical Information Products"	Verify that Technical Information Products provide references for data that is used or presented.			
3H-02	Para. 6.1.1	Verify specific laboratory notebook pages are called out as well as notebook numbers where data is extracted from notebooks.			
3H-03	Para. 6.1.2	Verify a disclaimer is included in the report when software used has not been developed in accordance with QA requirements.			
3H-04	Para. 6.1.3	Verify that the quality level of the activity that produced data is reported.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
3H-05	Para. 6.1.4	Verify assession numbers are included for references.			
3H-06	Para. 6.2.1	Verify at least one independent technically qualified reviewer is selected to review the TIP. TECHNICAL INFORMATION PRODUCT. JS 3/18/92			
3H-07	Para. 6.2.1	Verify that reviewer qualifications for non-Project reviewers are available.			
3H-08	Para. 6.2.3, CR No. 160	Verify appropriate review criteria has been specified and added criteria contains a justification.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-09	Para. 6.2.4	Verify comment resolutions are handled in accordance with this paragraph.			
3H-10	Para. 6.3.1.2	Verify the TPO performs a policy review.			
3H-11	Para. 6.3.1.9	Verify the Project Office approves TIPs prior to publication.			
3H-12	Para. 7.1	Verify records include the Project Office approved version of the TIP.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

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3H-13	TWS-QAS-QP-03.3, Rev. 0, Paras. 5.1, 6.0 and 6.2.1, "Procedure for Preparation and Review of SCP Study Plan"	Verify study plan authors and technical reviewers are certified per QP-02.1.			
3H-14	Para. 6.1	Verify study plan appendices include current QA controls.			
3H-15	Para. 6.2.2	Verify policy reviews per QP-03.2 are conducted for study plans.			
3H-16	Para. 6.2.6	Verify major technical changes to study plans are reviewed per procedure requirements.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-17	Para. 7.1	Verify study plan record packages contain records required by this paragraph.			
3H-18	TWS-QAS-QP-03.5, Rev. 0, Para. 6.1, "Procedure for Documenting Scientific Investigations"	Verify notebooks and logbooks have a unique ID number, assignee's name, instrument or activity covered by the book, and a book start date.			
3H-19	Para. 6.1	Verify pages in looseleaf binders are consecutively numbered.			
3H-20	Para. 6.2	Verify field notebooks contain, as appropriate: - Activity title - Activity objective - Field location - Sample ID			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-21	Para. 6.3	Verify entries in notebooks and logbooks are in accordance with paragraph requirements.			
3H-22	Para. 6.4	Verify logbook entries are signed or initialed and dated.			
3H-23	Para. 6.5.1	Verify notebooks contain initial information required by the specific DP.			
3H-24	Para. 6.5.2	Verify research and development notebooks document the items in this paragraph.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-25	Para. 6.6.1	Verify data and other information required by a DP are entered.			
3H-26	Para. 6.6.2	Verify a statement about acceptance of data is entered in the logbook when a DP is deviated from.			
3H-27	Para. 6.6.3	Verify in-process entries for research and development are recorded as required by this paragraph.			
3H-28	Para. 6.6.4	Verify changes in experiments are approved from PI or Project Leader.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-29	Para. 6.6.5	Verify data files are referenced in notebooks by number and location.			
3H-30	Para. 6.8	Verify corrections in notebooks are initialed and dated.			
3H-31	Para. 6.9.1	Verify notebooks and logbooks receive a technical review and are signed and dated. A statement as to if the notebook or logbook was reviewed and understood is required.			
3H-32	TWS-QAS-QP-03.7, Rev. 0, Para. 6.1, "Peer Review"	The initiation of a Peer Review is documented in a memo or letter from the TPO to the PI. Verify that such a letter was written to initiate all peer reviews.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-33	Para. 6.2	The selection of the Peer Review Group (PRG) and the designation of the chairperson (by the TPO) are documented in the peer review report. Verify this selection procedure.			
3H-34	Para. 6.3	...The technical qualifications and relationship of each peer reviewer to the work being reviewed are documented in the final report of the PRG. ...final report also includes the YMP resume for each member of the PRG. ...Any reviewer not working on the YMP must formally become part of the YMP by receiving training in the use of the QAPP and this QP, and their qualifications must be documented in accordance with QP-02.1. Verify such action in the case of a non-YMP reviewer. (Note any such instances in the margin.)			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-35	Para. 6.4.1	The TPO, or his designee, prepares a Peer Review Plan that contains a description of the work to be the reviewed, size of the PRG, the technical fields report be represented by the members of the PRG, and suggested schedule for the review.... The plan identifies the criteria against which the work will be reviewed and includes, at a minimum, the criteria listed in QAPP Appendix J, Section J.5. Verify that the Peer Review Plan contains the above information.			
3H-36	Para. 6.4.2	The chairperson...prepares written documentation of the results of all meetings, deliberations or other activities of the PRG. This documentation is included in the PRG's final report. Verify that this documentation is within any final Peer Review Report.			
3H-37	Para. 6.4.3	The written report is signed by each member of the PRG. Verify the required signatures.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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3H-38	Para. 6.5	... The PI or design manager prepares responses to the peer review comments if responses are required and these responses are reviewed by the TPO or his designee. If the PI is required, verify that written responses were prepared and reviewed.			
3H-39	Para. 6.6	If there are unresolved issues and if the PI is unable to concur with the objections of the PRG, the matter may be referred to successively higher levels of management. ...Any remaining unresolved concerns of the PRG are documented on the final report of the work reviewed. Verify that this process was used if appropriate. (Note the occurrence of any such cases in the margin.)			

9 AUDITOR SIGNATURE

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		Sandra Bates			
6-1	LANL-YMP-QAPP, Revision 5, Section 5.2	Verify that instructions, procedures, and plans specify appropriate quantitative or qualitative criteria for determining satisfactory work performance and QA compliance.			
6-2		Verify that documents specify checkpoints in the work process at which compliance with the criteria shall be determined and verified.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-3	LANL-YMP-QAPP, Revision 5, Section 5.2	Verify that means for identifying approved or rejected products or services is provided.			
6-4	LANL-YMP-QAPP, Revision 5, Section 5.3	Verify that QPs require reviewers of instructions, plans, procedures, and drawings to consider whether activities described o are repeatable, o will affect waste isolation capabilities, o will interfere with other site characterization activities.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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6-5	LANL-YMP-QP-06.1, Revision 3, Section 6.3.2	Verify that to issue a controlled document or update, the QAS Resident File Custodian performs the following:			
	Subsection 6.3.2.4	o Identifies the document(s) as "Controlled."			
	Subsection 6.3.2.5	o Assigns a date by which the Controlled Document Acknowledgment is to be returned, if not provided as described in Section 6.1.			
	Subsection 6.3.2.6	o Prepares a Controlled Document Acknowledgment (Att. 1) with complete instructions.			
	Subsection 6.3.2.7	o Distributed the document(s) to the recipient.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-6	LANL-YMP-QP-06.1, Revision 3, Subsection 6.3.3.2	Verify that the recipient signs and returns the Controlled Document Acknowledgment by the date indicated.			
6-7	LANL-YMP-QP-06.1, Revision 3, Subsection 6.3.4	Verify that when all signed Controlled Document Acknowledgments are received from recipients, the QAS Resident File Custodian forwards the appropriate records to the RPC according to TWS-QAS-QP-17.3.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-8	LANL-YMP-QP-06.1, Revision 3, Section 6.4.3	Verify that when controlled documents are returned or withdrawn, the QAS Resident File Custodian modifies the applicable Master Controlled Document List to reflect changes.			
6-9	LANL-YMP-QP-06.1, Revision 3, Section 6.5	Verify that the QAS Resident File Custodian maintains a reference copy of all controlled documents that are either withdrawn or superseded by a later revision.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-10		Verify that withdrawn controlled documents are stamped "Obsolete" and that superseded controlled documents are stamped "Superseded" and copies are forwarded to the RPC according to TWS-QAS-QP-17.3.			
6-11	LANL-YMP-QP-06.2, Revision 1 Section 6.2.2	Verify that a draft of the QP is prepared in accordance with Attachment 3 requirements (see attachment).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

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6-12		Verify that the QP has "DRAFT" stamped on the cover page.			
6-13	LANL-YMP-QP-06.2, Revision 1 Subsection 6.2.2.1	Verify that QPs contain a cover page as page 1 (See Att. 4) that documents approval of the procedure.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

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6-14	Subsection 6.2.2.2	Verify that QPs contain a History of Revisions (Att. 5) as page 2 that documents all revisions to the procedure and contains information on superseded procedures.			
6-15	Subsection 6.2.2.3	Verify that for revisions to QPs, revised text is indicated by a vertical bar in the margin next to changes, as applicable.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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6-16	LANL-YMP-QP-06.2, Revision 1 Section 6.2.4	Verify that the QAPL forwards the QP to supervisors of organizations affected and to quality reviewers for review.			
6-17	LANL-YMP-QP-06.2, Revision 1 Section 6.2.5	Verify that reviewers conduct a review of the draft QP and complete the QA Review Checklist (Att. 2).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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6-18	LANL-YMP-QP-06.2, Revision 1 Section 6.2.7	Verify that the QAPL signs and dates the cover page and designates training required in Section III of the QP Action Request.			
6-19	Section 6.2.8	Verify that the TPO signs and dates the cover page.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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6-20	LANL-YMP-QP-06.2, Revision 1 Subsection 6.2.10.1	Verify that the DCC enters the effective date on the cover page and on the History of Revisions.			
6-21	Subsection 6.2.10.2	Verify that the DCC updates the QA Manual (QAM) and issues the QP in accordance with QP-06.1.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

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6-22	LANL-YMP-QP-06.2, Revision 1 Section 6.3.1 Subsection 6.3.1.1	Verify that for QP deletions the QAPL continues processing the QP Action Request prepared in Section 6.1 by marking "N/A" in Section III.			
6-23	Subsection 6.3.1.2	Verify that supervisors of affected organizations are notified of the deletion.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-24	LANL-YMP-QP-06.2, Revision 1, Section 6.3.3	Verify that the DCC updates the QA Manual regarding deletions according to QP-06.1.			
6-25	LANL-YMP-QP-06.2, Revision 1, Section 7.1	Verify that the following records are maintained for new or revised QPs and that they are filed as record packages in accordance with QP-17.3: o QP Action Requests o Draft QP o Review Sheets o Quality Assurance Review Checklist o Final approved QP o Correspondence related to these documents			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-26	LANL-YMP-QP-06.3, Revision 0 Subsection 6.2.2.1	Verify that Detailed Technical Procedures (DPs) contain a cover page as page 1 that documents preparation, review, and approval of the procedure (See Att. 3).			
6-27	Subsection 6.2.2.2	Verify that Page 2 of DPs is a History of Revisions (See Att. 4) that documents all revisions to the procedure.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-28	LANL-YMP-QP-06.3, Revision 0 Subsection 6.2.2.3	(continued) Verify that revised text is indicated by a vertical bar in the margin.			
6-29	Subsection 6.2.2.4	Verify that Attachments are listed in Section 10.0 of the DP and are paginated as specified in Att. 2.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-30	LANL-YMP-QP-06.3, Revision 1 Subsection 6.2.3.1	Verify that technical reviewers are selected pursuant to TWS-QAS-QP-03.2, Section 6.2.1, as follows: o For all reviewers not certified YMP participants, Att. 2 to TWS-QAS-QP-03.2, is filled out.			
6-31	LANL-YMP-QP-06.3, Revision 1	Verify that the QA reviewer completes the LANL YMP Review Sheet (Att. 4 to Subsection 6.2.4.1 TWO-QAS-QP-03.2).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-32	Subsection 6.2.4.1	Verify that the QA reviewer completed the QA Review Checklist (Att. 2 to LANL-YMP-QP-06.2).			
6-33	LANL-YMP-QP-06.3, Revision 1 Subsection 6.2.4.2	Verify that the technical reviewer completed the LANL YMP Review Sheet (Att. 4 in TWS-QAS-QP-03.2).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-34	LANL-YMP-QP-06.3, Revision 1 Subsection 6.2.10.1	Verify that the Records Coordinator enters the effective date on the DP cover page and on the History of Revisions.			
6-35	LANL-YMP-QP-06.3, Revision 1 Subsection 6.2.10.2	(continued) Verify that the Records Coordinator updates the QAM by listing the DP and its level of training (as indicated on the DP Action Request) in the Table of Contents. Verify that the DP is inserted in the QAM.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-36	Subsection 6.2.10.3	Verify that the Records Coordinator notifies LANL YMP personnel of training requirements for new DPs and of revisions or deletions of existing DPs in accordance with TWS-QAS-QP-02.7.			
6-37	LANL-YMP-QP-06.3, Revision 1 Subsection 6.2.11.1	Verify that the DP preparer files copies of the following in the group resident file in accordance with TWS-QAS-QP-17.3: o DP Action Request o original draft DP o All LANL YMP Review Sheets o QA Review Checklist o related correspondence			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-38	Subsection 6.2.11.2	Verify that the DP preparer sends two copies of the records package to the Records Coordinator.			
6-39	LANL-YMP-QP-06.3, Revision 1 Subsection 6.3.2.1	Verify that the Records Coordinator updates the QAM by entering "deleted" for the revision number of the DP in the Table of Contents and removes the procedure from the QAM. (If the DP was superseded, the RC enters "superseded by".)			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
6-40	Subsection 6.3.2.2	Verify that the Records Coordinator notifies of DP deletions according to TWS-QAS-QP-06.1.			
6-41	Subsection 6.3.2.3	Verify that the Records Coordinator files a copy of the DP Action Request and related correspondence as a records package in the QAS Resident File and forwards two copies to the RPC in accordance with TWS-QAS-QP-17.3.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		John Martin			
17-1	LANL-YMP-QP-17.3, Rev. 1, Para. 5.1	Verify that the Administrative and Control Project Leader generates and signs an access list for personnel who oversee the daily operation of the RPC and who are authorized to forward records to the CRF. In addition, verify through review of records and visual observation that personnel on the access list are in fact the people who have access and transmit records.			
17-2	LANL-YMP-QP-17.3, Rev. 1, Paras. 6.1.1, 6.1.1.1, 6.1.1.2, 6.1.1.3, and 6.1.1.4	Verify that a unique identification system is established and maintained in accordance with procedural prerequisites.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-3	LANL-YMP-QP-17.3, Rev. 1, Para. 6.2.1	Verify that a TWS Log indicates date of document, the author, the recipient, status of the record and the title or subject, as applicable.			
17-4	LANL-YMP-QP-17.3, Rev. 1, Para. 6.2.3	Verify that a copy of the TWS Log is transmitted to the RPC no later than 15 days after the end of a month.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-5	LANL-YMP-QP-17.3, Rev. 1, Para. 6.2.5	Verify that the RPC staff submits TWS Logs to the CRF after the end of each calendar year.			
17-6	LANL-YMP-QP-17.3, Rev. 1, Paras. 6.3.1 and 6.3.2	Verify that records have had the WBS element assigned and designated either "QA" or "QA N/A."			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-7	LANL-YMP-QP-17.3, Rev. 1, Paras. 6.3.3 through 6.3.6	Verify that the records submitted by the originator to the RPC meet the following: - Record date - Record title or subject - The recipient's name/organization - The originator's name - The record must be easy to read, clear and distinct - Colored paper should not be used - Record should no be torn - Photo copies properly aligned - Black ink - No information obliterated - Corrections properly performed - Record complete			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-8	LANL-YMP-QP-17.3, Rev. 1, Para. 6.4.1	Review the Record Package Traveler (Attachment 2) for completion of the following: - Date of Record Package completion - WBS number - TWS number - QA designation - Title or subject - Total number of pages - Table of contents - Signature			
17-9	LANL-YMP-QP-17.3, Rev. 1, Para. 6.5	Verify that records are authenticated properly: - Individual Records - By initialing or signing the dated document. - Record Packages - Sign and date the Record Package Traveler.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-10	LANL-YMP-QP-17.3, Rev. 1, Paras. 6.6.3, 6.6.3.1, 6.6.3.2, 6.6.3.3, and 6.6.3.4	Assure that completed records or Record Packages are submitted to the RPC within 10 working days subsequent to completion.			
17-11	LANL-YMP-QP-17.3, Rev. 1, Paras. 6.7.1, 6.7.2, and 6.7.3	Upon receipt of a record by the RPC, verify that the following attributes are met: - Stamps "RPC Received" and initials and dates the first page of the record. - Performs review in accordance of 6.3 through 6.5. - Completes record rejection form, if required.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-12	LANL-YMP-QAPP, Rev. 5, Para. 17.5	Verify that LANL maintains a list that contains the signature and initials of persons authorized to authenticate records. In addition, verify by review of records submitted and authenticated.			
17-13	LANL-YMP-QP-17.3, Rev. 1, Para. 6.8	Verify that storage of records is consistent with QP requirements for dual storage and storage of "one-of-a-kind" records.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17-14	LANL-YMP-QP-17.3, Rev. 1, Para. 9.0	Assure that all LANL personnel are trained to QP-17.3.			
17-15	LANL-YMP-QP-17.3, Rev. 1, Para. 6.13	Verify retrievability of records from the RPC.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		Neil Cox			
19-1	LANL-YMP SQAP R0, paras. 7.0 and 7.3.5	LANL YMP Software Configuration Management activities shall be predicated upon the principle of baseline management. As such, the purview of the SCM effort shall be restricted to the software and computational baselines defined in TWS-QAS-QP-03.19.... The CSA effort shall maintain sufficient information in the Computer Program Library to identify differences between successive versions of a certified software application and to recreate any previously certified version.... Through the mechanism of formal CSA reports, the CSA effort shall provide the capability the current configuration of any certified baseline and to track changes throughout the system of certified software.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-1 con't	TWS-QAS-QP-3.20 R0 Paras. 6.3.1.1.2, 6.3.1.1.3, 6.2.8.1, and 6.2.8.1.4	CSA RECORDS COLLECTION Archiving. Ensure that the information provided on the supplemental information form is recorded in the CSA data base. Updating the CSA Active File. When a supplemental documentation form is closed, place a copy of the form in the CSA Active File pending its incorporation into a records package for transfer to the LANL YMP Records Processing Center. BASELINE SANCTIONING - If the Technical and Policy Review requires changes to any of the reviewed documents, initiate Software Change Requests or Software Incident Reports as appropriate to effect the modifications. Suspend the process until the required changes have been processed through the life cycle and approved by the CCB. Notification of Registered Users. Upon sanctioning a new version of a previously sanctioned software-application, notify the registered users of the application by transmitting a copy of the corres-ponding Engineering Change Notice to each.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-1 con't		1. Verify the existence of a configuration status record with unique configuration identifiers. (CSA Data Base)			
		2. Verify that the Configuration Item Active File exists.			
		3. Verify that periodic reports of CSA efforts are produced.			
		4. Verify that any existing actions were accomplished under configuration change control by the CCB.			
		5. Verify that all user's were notified of any actions taken by means of CSA reports or some other means.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-2	LANL-YMP SQAP R0,Paras. 6.2 and 7.3.5	A closed baseline shall be subject to the formal change-control policies and procedures specified in TWS-QAS-QP-3.20,.... Modification of a closed baseline shall require a formal change-processing cycle initiated by a Software Change Request or Software Incident Report. ...CSA reports shall be established.... A summary listing of the users to whom sanctioned software or data have been distributed for use in technical calculations.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-2 con't	TWS-QAS-QP-3.20, R0 Paras. 6.2.8.1.1, and 6.2.8.1.4	For a software baseline, subject the following baseline components to review: Models and Methods Summary, Users Manual Document, and Version Description Document. For a computational baseline, subject the Data Set Description to review. Notification of Registered Users. Transmit a copy of the corresponding Engineering Change Notice to each. 6. Verify that any changes to software were assessed for impact, evaluated, coordinated, and baseline updated. (Examine the CSA summary listing of the status of proposed changes Para. 7.3.5). 7. Verify that affected users were notified in accordance with procedure (?).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-3	LANL-YMP SQAP R0, Para. 6.0 and 11.0	Formal reviews shall be performed to assess the technical content of each proposed baseline and to ensure compliance with this SQAP at each stage of the life cycle. Reviews shall be performed under the auspices of the CCB.... During a formal review, the CCB shall assess issues raised by reviewers and decide which issues have merit. Issues with merit shall be documented and an issue resolution plan and schedule shall be developed.... Implementation of a strategy for recovery from catastrophic failures of the primary media. A documented program of backups shall be sufficient to satisfy this requirement.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-3 con't	TWS-QAS-QP-3.20, R0 paras. 6.2.8.1 and 6.4	Subsequent to certifying an implementation or computational baseline, sanction the baseline through technical and policy review and CCB approval. Functional Configuration Audit... Evaluate the functional characteristics of the baseline.			
		8. Verify existence of technical/peer reviews for each phase in the CSA data base and CSA active file.			
		9. Verify the existence of Functional and Physical Configuration Audits. (Objective evidence?) (NOTE: What procedure is used for a physical audit?)			
		10. Verify the location of the CSA active file and the Computer Program Library. (Any duplicate media necessary? Para. 11.0)			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-4	LANL-YMP SQAP R0, Para. 5.3 and 5.3.7.1	Verification and validation shall be performed on all software prior to its use in performing technical calculations or, if this is not possible, a written justification shall be prepared and maintained with the software, and the software shall be identified and controlled accordingly. In all cases, verification and validation of any software application shall be completed prior to submittal of a license application to the extent that the software is used to support the license application. The designer shall produce three levels of V & V documentation: a formal V&V plan, V&V procedures, test results, V&V report.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-4 con't	TWS-QAS-QP-03.22 R0 Paras. 6.1 and 6.2	VERIFICATION of SOFTWARE - The developer demonstrates the traceability of requirements into the software design.			
		MODEL VALIDATION - For each model incorporated into the application, perform validation steps.			
		11. Verify that life cycle documentation contains V&V plan , V&V procedures, test results, and V&V report.			
19-5	LANL-YMP SQAP R0,Para. 5.3	Verification and validation shall be performed on all software prior to its use in performing technical calculations or, if this is not possible, a written justification shall be prepared and maintained with the software, and the software shall be identified and controlled accordingly. In all cases, verification and validation of any software application shall be completed prior to submittal of a license application to the extent that the software is used to support the license application.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-5 con't	TWS-QAS-QP-03.22, R0 paras. 6.1 and 6.2	Update the V&V Report - Include the results of the verification testing effort in the V&V Report and interpret the results to develop a recommendation regarding whether the results are adequate to support verifying the software.			
		Perform the Validation Analysis - Implement the validation plan to determine whether the model can be validated.			
		Update the V&V Report - Include the results of the validation analysis in the V&V Report and interpret the results to develop a recommendation regarding whether the results are adequate to support validating the model.			
		12. Verify existence of software verification reports.			
		13. Verify existence of model validation reports.			
		14. Verify existence of technical and peer review reports, each with a software review plan.			
		15. Verify action taken to resolve any defects and/or deficiencies.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-6	LANL-YMP SQAP R0, Paras. 5.3.1.1 and 5.3.1.2.1	The V&V effort shall demonstrate traceability of the software requirements into subsequent software baselines throughout all phases of the life cycle.... The tester shall ensure that the formal testing is adequate to demonstrate correct operation of the software and is appropriate to the intended use, complexity, and development heritage of the software under test.			
	TWS-QAS-QP-03.22, R0 paras. 6.1.2, 6.3.1.1 and 6.3.2.1	Formal Testing - Develop the test plan. If sufficient resources are available, develop the test plan concurrently with the detailed design. Execute plan and update the V&V Report. 16. Verify that there has apparently been sufficient exercise of software to detect unintended functions.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-7	LANL-YMP SQAP R0, Para. 5.2.5.1.2	Pre-existing Development Software - (For this type), the CCB shall specify a lifecycle that is adequate to establish and/or develop life-cycle documentation to the degree possible and to qualify the software for use. The CCB shall specify the required life-cycle phases and associated documentation components according to the requirements of the subject software class.			
	TWS-QAS-QP-3.21, R0 paras. 6.1.1 and 6.3.3.2	The Software change Request form provides a means for proposing enhancements to existing software, for requesting authorization to develop new software, or for requesting authorization to convert pre-existing software to comply with the provisions of the LANL SQAP. Life-Cycle Specification.... Initiate a life-cycle specification process by preparing a Life-cycle Specification form.			
		17. Verify that the lifecycle documentation is reconstructed per 5.2.5.1.2.			
		18. Verify verification and validation activities from code assessment and support documentation.			
		19. Verify review and approval by the CCB prior to application.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-8	LANL-YMP SQAP Rev. 0 para. 5.2.2.2	The CCB shall specify the life-cycle phases that must be traversed to complete a software task. As a minimum, the CCB shall require those phases specified in Table 1 for the corresponding software class.			
	TWS-QAS-QP-3.19,R0 Appendices A thru M	(Prepare baseline component documentation in accordance with the Appendices.)			
		20. Verify that documentation includes mathematical derivations, physical models, etc. (MMS)			
		21. Verify that documentation includes SDD documentation.			
		22. Verify that documentation includes SRS listings.			
		23. Verify that documentation includes TR instruction to permit replication by an independent user.			
		24. Verify that the documentation includes UM, VVD, VVP, and VVR.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-9	LANL-YMP SQAP R0,Paras.7.3.3 and 13.0	Records in the CSA Active File shall be retained until such time as they are transmitted to the RPC, at which time they shall be purged from the file. Records collection, retention, and maintenance shall be the responsibility of the SCM Configuration Status Accounting effort.			
	TWS-QAS-QP-3.19 R0 Section 7.0	After certification by the SCM Organization, each baseline is incorporated into a certified-baseline records-package.			
		25. Verify that documentation in the CSA active file has been received by the Records Processing Center.			
		26. Verify that contents of packages (folders) contain the above information as a minimum. (CSA) For finished products, the packages should include Software Product Summaries (SPS).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-10	LANL-YMP SQAP R0, Para. 5.2.4.1	During this phase (REQUIREMENTS-PHASE), the developer shall compile the Requirements Baseline (see Section 4.3.2.1 and TWS-QAS-QP-03.19). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and QP-03.22) and shall submit the baseline to all reviews required by the CCB.... The SCM organization shall audit the Requirements baseline prior to scheduling and initiating a formal review.			
	TWS-QAS-QP-3.19,R0 Appendix H	The Software Requirements Specification documents the functional and performance requirements of the application and describes external interfaces and design constraints. 27. Verify the completion of a software requirements specifications document and the baseline of same as a permanent record.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-11	LANL-YMP SQAP R0, Para. 5.2.4.2	DESIGN-PHASE - During this phase, the developer shall compile all of the baselines that are specified for the Design Phase by the CCB (see Section 4.3.2 and QP-03.19). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and QP-03.22) and shall submit the baseline(s) to all reviews required by the CCB.... The SCM Organization shall audit Design-Phase baseline(s) prior to scheduling and initiating a formal review by the CCB.			
	TWS-QAS-QP-3.19, R0 Appendix G	The Software Design Document is a development document that describes the top-level design of a software application. 28. Verify the completion of a software design description and baseline of same.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-12	LANL-YMP SQAP R0, Para.5.2.4.3	IMPLEMENTATION-PHASE - During this phase the developer shall compile all the baselines that are specified for the Implementation Phase by the CCB (see Section 4.3.2 and QP-03.19). The developer shall perform all V&V activities that are specified for this phase (see Section 5.3 and QP-03.22) and shall submit the baseline(s) to all reviews required by the CCB.... (SCM shall audit prior to reviews.)			
	TWS-QAS-QP-3.19, R0 Appendix F	The Source-Code Listings document is an evidential-documentation component that provides a compendium of listings of all of the source code that is delivered with the software application. The Source-Code Listings document shall comply with the requirements of Section E(6) of NUREG-0856. 29. Verify that the Source-Code Listing is within the records.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-13	LANL-YMP SQAP R0, Paras. 5.3.1.2 and 5.3.1.2.1	Verification and validation shall be performed on all software prior to its use in performing technical calculations or, if this is not possible, a written justification shall be prepared and maintained with the software, and the software shall be identified and controlled accordingly. The tester shall ensure that the formal testing is adequate to demonstrate correct operation of the software and is appropriate to the intended use, complexity and developmental heritage of the software under test.... The CCB shall be the judge of the adequacy of the testing effort via reviews.			
	TWS-QAS-QP-3.19, R0 Appendices L & M	The V&V PLAN and PROCEDURES document is development documentation that encapsulates the V&V plan and the V&V procedures that are derived from the plan. The V&V Report presents a critical analysis of the Test Results with respect to the expected results specified in the V&V Plan and Procedures. 30. Verify the completion of a software test and Verification Plan/Report (VVP/VVR). 31. Verify that the VVP/VVR is under a Configuration Management Baseline. 32. Verify that the VVP/VVR describes the results of V&V tests.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-14	LANL-YMP SQAP R0, Para. 5.2.4.3	(SOFTWARE PRODUCT COMPLETION) - At the conclusion of any Implementation-Phase in-process review and after all associated review-issues have been resolved, the SCM Organization shall transfer a copy,of the approved baseline to the CPL (code media or papers?). After the completion of the SOFTWARE ACCEPTANCE REVIEW and after all associated review-issues have been resolved, the SCM Organization shall certify and sanction the Implementation baseline.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-14 con't	TWS-QAS-QP-3.19, R0 Appendix E and TWS-QAS-QP-3.21, R0 para. 5.3 and TWS-QAS-QP-3.20, R0 para. 6.3.2	The Software Assessment and Support Documentation (SAD) is evidential documentation that is provided to comply with the requirements of Section D of NUREG-0856. The CCB responsibilities include: assessing the baselines produced by the development organization through a program of formal reviews of the baseline documents. CSA Records Maintenance and Storage. - Updated supplemental documentation is recorded in the CSA data base. A copy of a closed form is entered in the CSA Active File. Only closed CSA records are employed in a records package. 33. Verify that a Software Product Summary (SPS) has been submitted to the SQM upon completion of the software product. 34. Verify the technical review of software. (Timely) (Para. 6.9.1) 35. Verify that the software has been baselined (CM). Examine the CSA active file. 36. Verify that the CSA active file lists all the requirements, their resolution, and copies of supplemental documentation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-15	LANL-YMP SQAP R0, Para. 8.0	The LANL YMP shall provide a formal mechanism for reporting problems that are discovered in a certified baseline, requesting changes or enhancements to a certified baseline, or initiating a new software-development effort. Formal documentation shall be provided for each of the above events.			
	TWS-QAS-QP-3.21, R0 paras. 6.1.1 and 6.1.2	The SOFTWARE CHANGE REQUEST is the mechanism for initiating perfective or adaptive maintenance operations on the latest version of an existing application. The Software Incident Report form provides a means for reporting discrepancies or problems in existing software or computational data. It is the mechanism for initiating corrective maintenance operations on the latest version of an existing software application or computational data set. 37. Verify that a formal discrepancy procedure exists. (QP-15.2?) 38. Verify that the maintenance phase has been implemented (Examine the CSA active file for signs of activity.) 39. (Duplicate deleted)			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-16	LANL-YMP SQAP, Rev. 0, para. 7.2.4	Releases shall be performed in support of the modification or enhancement of certified baselines, to disseminate certified hardware and computational data to the user community, and to make PRERELEASE versions of applications available to the user community. Releases shall be authorized by the CCB and administered by the Software Configuration Manager. Engineering Release Assessment Release Sanctioned Baseline Probation			
	TWS-QAS-QP-3.21, R0 para.6.5.1	If the associated Engineering Change Directive authorizes work on existing software, initiate an engineering release by preparing a CPL Transmittal Request form. 40. Examine the documentation on the execution of any release and verify that it was authorized by the CCB.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-17	LANL-YMP SQAP R0, para. 5.2.5.1	For PRE-EXISTING development software, the CCB shall specify a life cycle that is adequate to establish and/or develop life-cycle documentation to the degree possible and to qualify the software for use. The CCB shall; specify the required life-cycle phases and associated documentation components according to the requirements for the subject software class.			
	TWS-QAS-QP-3.19, R0 para. 1.0 and Appendices C thru M	This QP provides the procedures for documenting the process and products of all LANL YMP software-and computational-data-development activities. Furthermore, it provides detailed descriptions of the components of all LANL YMP software and computational-data baselines that are generated at each stage of the development process. 41. Verify that the documentation conforms to NUREG-0856 checklist. 42. Verify inclusion of mathematical theory and manipulations. 43. Verify that summaries, reports, and reviews are included. 44. Verify that user instructions are sufficient for independent replication.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-18	LANL-YMP SQAP R0,Para. 5.3.2	All mathematical models embodied in (LANL) software shall be subject to validation to ensure that they accurately represent physical reality within the domain of the application. The validation strategy for each model shall be described in detail in the software documentation documentation. (The CCB shall be the judge of adequacy.)			
	TWS-QAS-QP-03.22, R0 Paras. 6.4.1 and 6.4.2	VALIDATION OF COMPUTATIONAL DATA - Evaluate the veracity of the computational data set.... Document the data validation effort in the V&V Report. CCB evaluates the computational data evaluation effort as documented in the V&V Report. 45. Verify that validation documentation is stored in the software's permanent file. 46. Verify the methods used for validation are consistent with this SQAP.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-19	LANL-YMP SQAP R0, Para. 7.2	The Configuration Control effort shall establish organizational and administrative controls on changes to all baselines. - Procedures, enforcement, releases, certification and sanctions and controlling code, data and the acquisition thereof.			
	TWS-QAS-QP-3.17, R0 para. 5.3 TWS-QAS-QP-3.20, R0 para. 6.2.8.1.4	The responsibilities of the CCB are: provide a forum for all formal YMP baseline reviews and approve, approve conditionally, or reject any proposed baseline. Notification of Registered Users. ...transmit a copy of the corresponding Engineering Change Notice. 47. Verify that change approval is at the same level as the original. 48. Verify that changes are listed in the CSA data base. 49. Verify that Registered Users are notified of error correction or change status. (NOTE: Ask if there is immediate notification of a fault.) 50. Verify that lists of open and closed ERs and CRs are kept.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-20	LANL-YMP SQAP R0, Paras. 7.3.1 and 7.3.5	CSA records shall comprise all certified baselines, all supplemental-documentation documentation forms, and all formal CSA reports. ... A Baseline shall enter the CSA domain when it is certified. ... A formal CSA report shall enter the CSA domain when it is generated by the CSA effort. ... A supplemental-documentation form shall enter the CSA domain when it is closed.			
	TWS-QAS-QP-3.20, R0 para. 6.3.1	CSA Records Collection includes: Marking (ID),Archiving, Updating the CSA Active File, and CSA Reports. 51. Verify the existence of a CSA data base and examine CSA reports. (SELECTED FEW) 52. Verify the existence of(something like) a directory of users. (See Item 19-19 of this checklist. 53. Verify method of notifying users of planned or implemented changes.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-21	LANL-YMP SQAP R0, Para. 10.0	All certified code shall be maintained within a secure database (the CPL) under the administrative control of the SCM Organization. (See QP-03.-20)			
	TWS-QAS-QP-3.18, R0 paras. 5.3 and 6.3.1.1	The SCM Organization ensures that all data submitted for storage in the CPL is checked for quality and is safely and securely stored and protected against loss or damage. Also SCM shall archive each certified computational data base in the CPL in accordance with QP-03.20. 54. Verify two separate media storage locations, free of stray fields (one local one remote), for each backup copy). 55. Verify that Backup Log contains: date, storage media, medium number, file identification, and the physical location of the copies. NOTE: Ascertain the number of copies of user documentation and their location.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-22	LANL-YMP SQAP R0, Paras. 7.2.4.3 and 7.2.5	The release of a sanctioned baseline shall be performed to make the primary products of a sanctioned baseline available to the user community. The SCM Organization shall implement procedures to sanction a certified implementation or computational-data baseline. .... Completion and documentation of the sanctioning process constitutes a formal approval to use the sanctioned baseline.			
	TWS-QAS-QP-3.20, R0 para. 6.2.9	Interface Control -- To obtain the latest version of a LANL YMP sanctioned software application or certified data-set, complete a Software/Data Dissemination Request and submit to the SCM. 56. Verify procedure exists. 57. Verify implementation of the above procedure with approvals of the CCB. 58. Verify that any interim results are identified in order to qualify their use and limitations.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		NOTE: THE REMAINING ITEMS DEAL WITH ACQUIRED, EXISTING, OR COMMERCIAL SOFTWARE			
19-A24	LANL-YMP SQAP R0, para. 5.2.5.2.3	The CCB shall specify the required life-cycle phases and the associated documentation components according to the requirements for the associated software class. All documentation components and reviews required by this SQAP for new development software of the same software class shall be obtained or developed for ACQUIRED NONCOMMERCIAL SOFTWARE during the appropriate life-cycle phase or, if this is not possible, the reasons shall be documented and maintained with the software.			
	Procedure Unknown	59. Verify that a procedure is in place to request all available documentation .			
		60. Verify that all available documentation was obtained for all such codes. (100 % sample)			
		61. Verify that all such codes have a unique version identification, revision number(s) and user-related documentation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-A10	LANL-YMP SQAP R0, Para. 5.2.5.2.3	Same as Item 19-A-24 of this checklist.			
	Procedure Unknown	62. Verify that orders for acquired software specify requirements.			
		63. Verify that a review of the specifications of the received software was used to see that that the software conforms to the requirements or that the acquired code was marked as deficient.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-A12	LANL-YMP SQAP R0, Para. 5.2.5.2.4	Whenever ACQUIRED SOFTWARE enters the change-processing cycle for enhancement or repair, the affected modules shall be subject to a formal, software development life-cycle as specified by the CCB and shall be treated in every respect as new development software. Affected modules shall conform to QP-03-19.			
	TWS-QAS-QP-3.21, R0 para. 6.3.3.2.4	If the Requirements, Design, and/or Implementation baselines are specified by the life-cycle specification form, the corresponding baseline closure reviews shall be conducted (SRR,CDR, and SAR).			
		64. Verify the submittal of Software Acceptance Review and Software Product Summary Forms (SPS) or equivalent to the SCM.			
		65. Verify that the SPS lists all items associated with the product and the location of all documentation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-01

1 ORGANIZATION Los Alamos

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19-A15	LANL-YMP SQAP R0,Para. 5.2.5.2.3	.....One of the strategies described in Section 5.2.5.1.2 shall be used to produce the appropriate documentation and to qualify the subject software.			
	TWS-QAS-QP-3.20, R0 para. 6.2.7.1.2 and 6.2.8.1.2	Document the baseline certification process on a Baseline Certification Notice. Document the baseline sanctioning process on an Engineering Change Notice.			
		66. Verify that the CCB has reviewed and approved the acquired software. Examine the CSA active file.			
		67. Verify that software technical/peer reviews, if any, conform.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		WBS Nos. 1.2.3.4.1.2.1 and 1.2.3.4.1.2.3			
		Study Plans 8.3.1.3.4.1, Rev. 0 and 8.3.1.3.4.3, Rev. 0			
1		Under what grading report is work under WBS Nos. 1.2.3.4.1.2.1 and 1.2.3.4.1.2.3 being performed. Examine this grading report.			
2		Does this grading report impose controls on on-going scientific investigations for sorption? If so, what are these controls? Confirm by examining grading report.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
3		Do investigations of sorption involve software? If so, where in the lifecycle is the relevant software development now? Examine documentation to confirm.			
4		Has the recently proposed strategy for use of sorption data, the minimum Kd approach, been incorporated into Study Plans 8.3.1.3.4.1 and 8.3.1.3.4.3? Examine revised draft, if available.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
5	SPs 3.4.1/.3 Sec. 2.1, Page 3	Where does LANL's study of sorption stand with respect to completion of the baseline data set? Examine available evidence.			
6	SPs 3.4.1/.3 Sec. 2.1, Page 3	Where does LANLs study of sorption stand with respect to augmenting the baseline data set for variables such as groundwater composition, radionuclide concentration, pH? Examine available evidence.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
7	SPs 3.4.1/.3, Sec. 2.3.2, Page 5	Do the experiments conducted during the last year at Stanford University on the sorption of Np provide data on sorption kinetics? Are reports available?			
8	SPs 3.4.1/.3, Sec. 2.3.2, Page 5	Do the most recent experiments on sorption of Cs and Sr show that they are rapidly sorbed? Are reports available?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
9	SPs 3.4.1/.3, Sec. 2.3.2, Page 5	For what single minerals and elements has LANL determined sorption ratios? Examine available evidence.			
10	SPs 3.4.1/.3, Sec. 2.3.2, Pages 5 and 6	Has the interference of one trace actinide with the sorption of another, e.g, interference with Np sorption, or a single mineral been investigated? Examine available documentation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
11	SPs 3.4.1/.3, Page 6	Has the recent work at Stanford permitted the identification of surface complexes of Np? - On silica phases? If so, which phases? - On feldspar? If so, which phases?			
12	SPs 3.4.1/.3, Page 6	What is the effect of CO2 on the sorption of Np on quartz? On feldspar? Examine available documentation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
13	SPs 3.4.1/.3, Page 6	Has it yet been determined which minerals dominate the sorption of Np in tuff? If so, examine available documentation.			
14	SPs 3.4.1/.3, Sec. 2.5.2, Page 7	What accuracy (detection limit) is now achievable in the analysis of aqueous concentrations of actinides? How does this compare to expected solubilities.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
15	SPs 3.4.1/.3, Sec. 2.5.3, Pages 7 and 8	Recent work has provided preliminary data on the effect of crushing on the sorption of actinides. What will be the next steps?			
16	SPs 3.4.1/.3, Sec. 2.5.4., Page 8	What progress has been made on the use of EXAFS for characterization of surface species?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17	SPs 3.4.1/.3,	Will EXAFS and the atomic force/scanning tunneling microscope both be used? If so, what are relative advantages of each?			
18	SP 3.4.3, Sec. 3.0, Page 9	What is the status of the sorption modeling activity (SCP Study 8.3.1.3.4.3)?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
19		What is the theoretical nature (e.g., curve shape) of the relationship between sorption ratio and water/rock ratio? How well does this compare to observations? Examine any available plots of data.			
20	SP 3.4.3, Sec. 3.1.4, Pages 11 and 12	Of the minimum 120 tests anticipated in the study plan, about how many have been done? How many are now anticipated? Get specifics, if possible.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
21	SP 3.4.3, Sec. 3.1.5.1, Page 11	What advantages and disadvantages would there be in calculating the sorption ratio as: (activity on the solid phase/sq. cm. of surface area of the solid phase)/(activity in solution/ml. of solution)?			
22		What procedure is used to determine the Sorption/Desorption ratio by a batch method? Confirm implementation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
23		What procedure is used to crush rocks for sorption work? Confirm implementation.			
24		What procedure is used for isotope dilution mass spectrometry? Has it been implemented?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
25		Have procedures been written for the use of the scanning tunneling/atomic force microscope?			
26		What procedure is used to control CO2 partial pressure? Confirm implementation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
27		Does the Stanford group use the same procedures as LANL?			
28		What procedures are used in analyzing aqueous solutions? Confirm implementation.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL | 2 Page 15 of 23

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
		WBS No. 1.2.3.4.1.5.1			
1		Under what grading report is work under WBS No. 1.2.3.4.1.5.1 being performed? Examine this grading report.			
2		What controls does this grading report impose on on-going scientific investigations as developments for retardation sensitivity?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
3		Where is CTCN in the software lifecycle? Confirm by examining records. Also, confirm how the corresponding baselines were established and that this is an agreement with the specifications established by the configuration control board.			
4		What is the heritage of CTCN? Confirm by examining records.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
5		What is the class of CTCN? Confirm by examining records			
6		Have any modifications been made to CTCN? If so, what were they? Confirm that proper procedures, such as filing and approval of a software change request, review procedures, verification and validation, etc., were followed.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
7		Where is NCSA in the software lifecycle? Confirm by examining records. Also confirm how the corresponding baselines were established and that this is in agreement with the specifications established by the configuration control board.			
8		What is the heritage of NCSA? Confirm by examining records.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
9		What is the class of NCSA? Confirm by examining recor			
10		Have any modifications been made to NCSA? If so, what were they? Confirm that proper procedures, such as filing and approval of a software change request, review procedures, verification and validation, etc., were followed.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
11		Where is TRACRN in the software lifecycle? Confirm by examining records. Also confirm how the corresponding baselines were established and that this is in agreement with the specifications established by the configuration control board.			
12		What is the heritage of TRACRN? Confirm by examining records.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
13		What is the class of TRACRN? Confirm by examining records.			
14		Have any modifications been made to TRACRN? If so, what were they? Confirm that proper procedures, such as filing and approval of a software change request, review procedures, verification and validation, etc., were followed. Also examine the code to confirm that they have been, or are in the process of being, properly implemented.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
15		What requirements have been placed on TRACRN? Confirm by examining the Software Requirements Specification. Also examine the code to confirm that they have been, or are in the process of being, implemented.			
16		Has the Models and Methods Summary for TRACRN been completed? Examine the summary, if so, to confirm that proper procedures and approvals were followed.			

9 AUDITOR SIGNATURE 10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-02

1 ORGANIZATION LANL

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
17		Has the Software Design document for TRACRN been completed? Examine the document, if so, to confirm that proper procedures and approval were followed.			
18		Has any verification or validation for TRACRN been performed? Examine the "V&V Plan and Procedures," "V&V Report," and "Verification and Validation" document, if so, to confirm that proper procedures and approvals were followed.			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
T-1	WBS 1.2.3.4.1.2.2 SP 8.3.1.3.4.2	Biological Sorption and Transport How are the standard and accepted microbiological techniques listed on p.10 and 14 brought into compliance with the QA program?			
T-2	SP 8.3.1.3.4.2	Is the Chelex 100 ion exchange resin a commercial product? If so, verify standardization of its composition. If not, how is standardization achieved?			
T-3	SP 8.3.1.3.4.2	If, as stated on p. 13, much of the work is dependent on the ESF (Exploratory Studies Facility), from what source have samples been obtained to date?			
T-4	SP 8.3.1.3.4.2	Related to study plan revisions: a) What is the current status of the study plan? b) Verify that the study plan is being revised in accordance with AP1.10Q, current rev. c) Has the study plan been modified to indicate correctly that ESF access will be via ramps as opposed to shafts? d) How, if at all, will "c" above affect sampling plan?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION				2 Page 2 of 1	
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.2.2	Biological Sorption and Transport			
T	SP 8.3.1.3.4.2	" " "			
T-5	SP 8.3.1.3.4.2	What steps will be taken to assure that samples will not be contaminated between the time they are collected and the time they are analyzed?			
T-6	SP 8.3.1.3.4.2	In the study plan, it is stated that some procedures are standard and some will be developed. a) What technical procedures are currently being worked to? b) What additional procedures have been worked to in the past year? c) Verify this through laboratory notebook record. (Note: see procedures on p.16-17, AODC + chelation).			
T-7	SP 8.3.1.3.4.2	Is a grading report in effect for the work described on p.19? If not, what is the status of the work and of the grading report?			
T-8	SP 8.3.1.3.4.2	a) Is a grading report in effect for work described on p.19 for sorption? b) What, if any, data have been supplied to the sorption study (8.3.1.3.4.1) to date? c) Are these data of a quality-affecting nature?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.2.2	Biological Sorption and Transport			
T-9	SP 8.3.1.3.4.2	What is the status of development of a procedure to assess sorption of actinides by microorganisms? [ACTINIDES]			
T-10	SP 8.3.1.3.4.2	p.21 - Have any procedures been developed for the colloidal agglomeration studies?			
T-11	SP 8.3.1.3.4.2	What has caused the postponement of milestones 3176, 3177, 3080, and 3092?			
T-12	SP 8.3.1.3.4.2	Can the publication "Preliminary Evidence of Siderophore/Plutonium Complexation" be traced to a laboratory notebook?			
T-13	SP 8.3.1.3.4.2	Is the milestone "production + purification of siderophore" a quality-affecting activity? What about ms 3176, "determination of formation constants"? Is it quality-affecting?			
T-14	SP. 8.3.1.3.4.2	A) What software is currently used in this study? B) What software is planned to be used?			
T-15	SP 8.3.1.3.4.2	Are the plutonium Kd experiments quality-affecting work? What is their status? ~~SOW~~			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION					2 Page ~~1~~ 4 of 1
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.3	Radionuclide Retardation by Precipitation Processes			
	SP 8.3.1.3.5.1/2	Dissolved Species Concentration Limits and Colloid Behavior			
T-16	SP 8.3.1.3.5.1/2	How are the PAS, PDS, and LIF systems calibrated?			
T-17	SP 8.3.1.3.5.1/2	Does a laboratory notebook demonstrate compliance with TWS-INC-DP-35, pH measurements?			
T-18	SP 8.3.1.3.5.1/2	p.17- With respect to flow paths, how will the speciation studies focus on fastest transport pathways as opposed to speciation along all paths?			
T-19	SP 8.3.1.3.5.1/2	p.20- a) Discuss the necessity for the elaborate colloid studies that are planned and the duration of the tests (i.e., what is the rationale as opposed to assessing how far a colloid may travel?) b) how is the S.P. review comment on this topic being addressed in revision of the study plan?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-0~~2~~3

1 ORGANIZATION				2 Page ~~1~~5 of 1	
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.3	Radronuclide Retardation by Precipitation Processes			
	SP 8.3.1.3.5.1/2	Dissolved Species Concentration Limits and Colloid Behavior			
T-20	SP 8.3.1.3.5.1/2	Explain the problem caused by using teflon pH cells? How has this been solved?			
T-21	SP 8.3.1.3.5.1/2	Where are the NIST-certified buffer solutions kept and recorded? (Note: this may be N/A if at LBL).			
T-22	SP 8.3.1.3.5.1/2	What progress, if any, has been made in determining the better methods of assessing bulk charge of colloids (p.23)?			
T-23	SP 8.3.1.3.5.1/2	What progress, if any has been made in assessing better methods of determining chemical reactivity of colloids? Can the list of methods be more focused at this time?			
T-24	SP 8.3.1.3.5.1/2	Explain what ongoing work is considered scoping and what is quality-affecting. Examine notebook for a quality activity (PAS?)			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-0~~2~~3

1 ORGANIZATION				2 Page ~~2~~6 of 1	
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.3	Radionuclide Retardation by Precipitation Processes			
	SP.8.3.1.3.5.1/2	Dissolved Species Concentration Limits + Colloid Behavior			
T-25	SP 8.3.1.3.5.1/2	Has LANL used TWS-INC-DP-78 (Prep. of Pure Oxidation State Solns?) for this study? If so, examine notebk.			
T-26	SP 8.3.1.3.5.1/2	List the sequence of tests needed to complete a colloid characterization. How long (under normal circumstances) would it take to complete this?			
T-27	SP 8.3.1.3.5.1/2	a) What data will this study provide to the project thermodynamic database (GEMBOCHS)? b) If any has been provided so far, what is it? c) What type of record transmittal occurs?			
T-28	SP 8.3.1.3.5.1/2	What, if any procedures, are used by both LBL and LANL for this study?			
T-29	SP 8.3.1.3.5.1/2	a) What software is used on this study? b) Was any work delayed due to software qualification process? c) Demonstrate compliance with SQAP. (Note: particularly interested in instrument control software for PAS system).			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION					2 Page 17 of 1
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.3	Radionuclide Retardation by Precipitation Processes			
	SP 8.3.1.3.5.1/2	Dissolved Species Concentration Limits + Colloid Behavior			
T-30	SP 8.3.1.3.5.1/2	a) With regard to MS 309 (Report on measured Solubilities of Pu, Am, + Np in J-13 groundwater from oversaturated conditions), what is the difference between MS 309 + MS 3010? b) What form did the 3010 report take (report?) - stated complete in 7/91 monthly. c) Can data be traced to LANL notebk?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-0~~7~~3

1 ORGANIZATION

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.4	Radionuclide Retardation by ~~Diff~~ Dispersive, Diffusive, and Advective Processes			
~~SP~~	SP 8.3.1.3.6.1	Dynamic Transport Column Experiments			
T-31	SP 8.3.1.3.6.1	What procedure was used to prepare core samples and well samples for the tests? Can this be traced to a notebook?			
T-32	SP 8.3.1.3.6.1	p.14 - Were the equations tested and if so, how?			
T-33	SP 8.3.1.3.6.1	For stylus profilometry, what type of instrument/equipment is used and what type of printout is produced?			
T-34	SP 8.3.1.3.6.1	Why does the grading report for this study show it as scoping work + non-quality-affecting?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-0~~2~~3

1 ORGANIZATION

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.4	Radionuclide Retardation by Dispersive, Diffusive, and Advective Processes			
	SP 8.3.1.3.6.2	Diffusion			
✓ T-35	SP 8.3.1.3.6.2	To what extent will the results reported in 3/91 monthly be used for licensing? Trace to notebook. Also 4/91 monthly.			
✓ T-36	SP 8.3.1.3.6.2	How is a tuff beaker prepared? How is it qualified? (so as not to leave behind contaminants for actinides to sorb to).			
✓ T-37	SP 8.3.1.3.6.2	Will this study rely on scaling factors determined by SP 8.3.1.3.7.2? If not, how will scaling factors be addressed?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-07

1 ORGANIZATION

3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.4	Radionuclide Retardation by Dispersive, Diffusive, and Advective Processes			
	SP 8.3.1.3.6.1	Dynamic Transport Column Experiments			
T-38	SP 8.3.1.3.6.1	p.9 - Where is ~~it recorded~~ the accuracy ams 4/8/92 and precision considered normal for analytical chemical measurements recorded?			
T-39	SP 8.3.1.3.6.1	Is TWS-INC-DP-45 (... Ion Chromatography) used by this study? (It's listed in SP but not on list of technical procedures).			
T-40	SP 8.3.1.3.6.1	Verify that samples used in the mass transfer kinetics test have been prepared in accordance with TWS-INC-DP-63. (Notebook).			
T-41	SP 8.3.1.3.6.1	Verify that crushed tuff column studies followed TWS-INC-DP-15.			
T-42	SP 8.3.1.3.6.1	p.20 A) Explain how a fracture is encapsulated for the fractured tuff column experiments. B) Have any of the fracture column experiments been done? C) If so, was qualified core used for samples?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION				2 Page 11 of 12	
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.4	Radionuclide Retardation by Dispersive, Diffusive and Advective Processes			
	SP 8.3.1.3.6.1	Dynamic Transport Column Experiments			
T-43	SP 8.3.1.3.6.1	Can milestone 3119 be traced to lab notebook? (Examine Migration '89 paper for traceability to milestone and to notebook also).			
T-44	SP 8.3.1.3.6.1	6/91 + 7/91 monthly reports tell of unstable solutions of Pu + Np in J-13 water, perhaps due to precipitation, or for Pu, interaction w/ teflon or stainless steel. How has this condition been corrected?			

9 AUDITOR SIGNATURE

10 DATE

OCRWM AUDIT CHECKLIST NO. YMP-92-12-03

1 ORGANIZATION				2 Page 12 of 12	
3 AUDIT ITEM NO.	4 QUALITY REQUIREMENT REFERENCE(S)	5 QUALITY REQUIREMENT/GUIDELINE	6 RESULTS S,X,N/A	7 SUMMARY OF INVESTIGATION	8 PERSON CONTACTED
	WBS 1.2.3.4.1.4	Radionuclide Retardation by Dispersive, Diffusive and Advective Processes			
	SP 8.3.1.3.6.2	Diffusion			
T-45	SP 8.3.1.3.6.2	How will heterogeneities in porosity be accounted for in the tests?			
T-46	SP 8.3.1.3.6.2	Is DP-81 (Unsaturated Tuff Diffusion Experiments) in existence? (Listed for use in SP but not on list of DPs).			
T-47	SP 8.3.1.3.6.2	What software is used for Autocorrelation Photon Spectroscopy? Has it been qualified?			

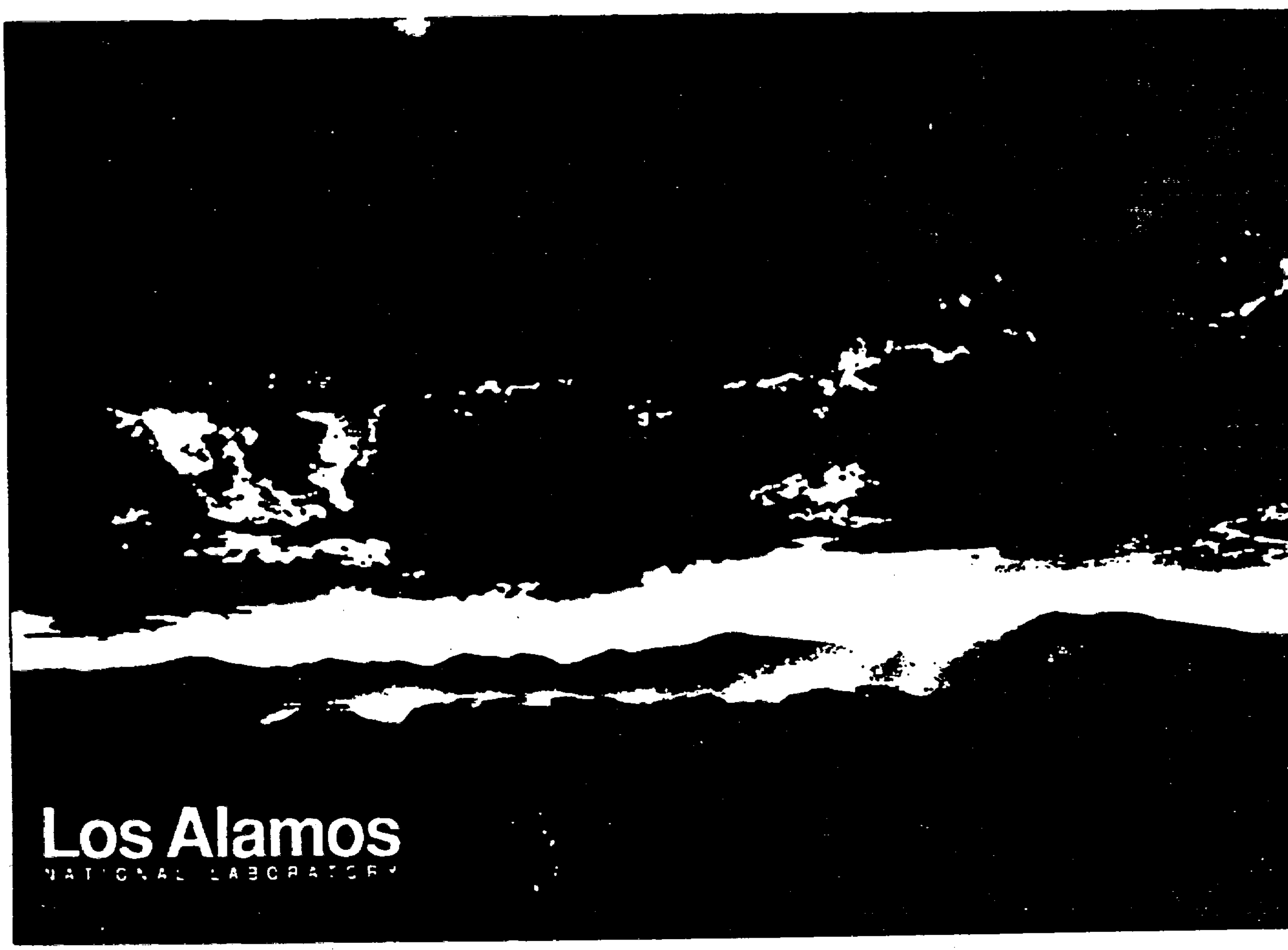
9 AUDITOR SIGNATURE

10 DATE

Yucca Mountain
Site Characterization Project

Monthly Activity Report

November 1991



Attachment to TWS-EES-13-12-91-043

This document has not received formal technical or policy review by Los Alamos National Laboratory or by the Yucca Mountain Site Characterization Project. Data presented in this report represent work progress and are not intended for release from the US Department of Energy.

This work was supported by the Yucca Mountain Site Characterization Project Office as part of the Civilian Radioactive Waste Management Program. This Project is managed by the US Department of Energy, Yucca Mountain Site Characterization Project.

CONTENTS

LOS ALAMOS NATIONAL LABORATORY
YUCCA MOU TAIN SITE CHARACTERI ATION PROJECT

Monthly Activity Report
November 1991

3 >,

WBS 1.2.1
SYSTEMS

The objective of this task is to integrate systems with the Geologic Repository Program, to describe the Yucca Mountain Site Characterization Project Mined Geologic Disposal System, and to evaluate the performance of the natura engineered barrier, and total systems for meeting regulatory standards.

TECHNICAL DATA (WBS 1.2.1.3.5)

ACTIVITIES AND ACCOMPLISHMENTS

Work continued on preparing the draft technical data procedure and on accessing the Automated Data Tracking (ATDT) system.

PLANNED ACTIVITIES

Attend a training class for the ATDT system on 19 December at Sandia National Laboratories. Submit *Preliminary Geologic Map of the Sleeping Butte Volcanic Centers*, by B. Crowe, to Genesis and the RIB.

CAISSON EXPERIMENT (WBS 1.2.1.4.6)

ACTIVITIES AND ACCOMPLISHMENTS

A meeting was held on 7 November at Sandia National Laboratories (SNL) to discuss design of the caisson experiment. The meeting was attended by M. Siegel, B. Glass, P. Hopkins, and D. Ward of SNL and K. Birdsell, N. Rosenberg, and E. Springer of Los Alamos. The porous material to be used was the first issue discussed. A Wedro silica sand was selected because it is easy to pack, has a narrow particle-size distribution that is still in the range found naturally, and works well with laboratory techniques developed by SNL to characterize flow. Initial calculations conducted by SNL have shown breakthrough in 4 days at a saturation of 53%. It was estimated that 75 tons of this material will be required.

The composition of the sorbing layer was the next issue. It was found that a zeolite would migrate through the san under flowing conditions. An option to prevent this is to lay a filter paper or geotextile layer beneath the zeolite to reduce the movement. Although possible, this was not deemed an acceptable solution to the problem. The second choi was limonite to replace a given particle-size range of the sand in the sorbing layer. If sufficient limonite can be found, this will be used.

The tracers to be used in the experiment are nickel, boron, lithium, and bromide. Batch sorption experiments conducted by SNL indicated that the K_d for nickel in the silica sand was high and that an extended experimental duratio would be required in order to complete the experiment. Boron was not expected to be highly sorbing in the sand, but it will be retained by the iron oxides in the sorbing layer. The lithium and bromide are expected to exhibit minimal retardation. An alternative approach may be to change the solution chemistry by lowering its pH to mobilize the boron and nickel.

The bottom boundary condition was considered during the 7 November meeting. This boundary is very important because it will provide total system behavior, in contrast to solution samplers located inside the caisson that will give point measurements. Previous caisson experiments conducted at Los Alamos used a free-draining lower boundary through the outlet, which is unsatisfactory. A lower boundary using suction candles to apply a pressure was the initial design for the current experiment. There may be a need to have further control by either sealing the boundary and placing suction candles above the seal or by installing a large porous plate with the suction candles located to maintain a pressure head and sample discrete intervals. A final decision was not made on the nature of the lower boundary.

A meeting was held with B. Glass (SNL) on 12 November. Issues discussed were the relation between laboratory studies conducted at SNL and how they can help in the caisson experiment and support questions on scaling of parameters. Also, issues relative to filling the caisson and the bottom boundary condition were discussed.

E. Springer attended the Total System Performance Assessment meeting in Las Vegas on 18–20 November.

An FY91 report was received for the caisson analysis using stochastic methods from Drs. Dagan and Rubin. The report is still being reviewed, and the results will be presented in a future monthly progress report.

PLANNED ACTIVITIES

Finalize porous media selection and order the material. Conduct batch experiments with lithium bromide using silica sand and limonite.

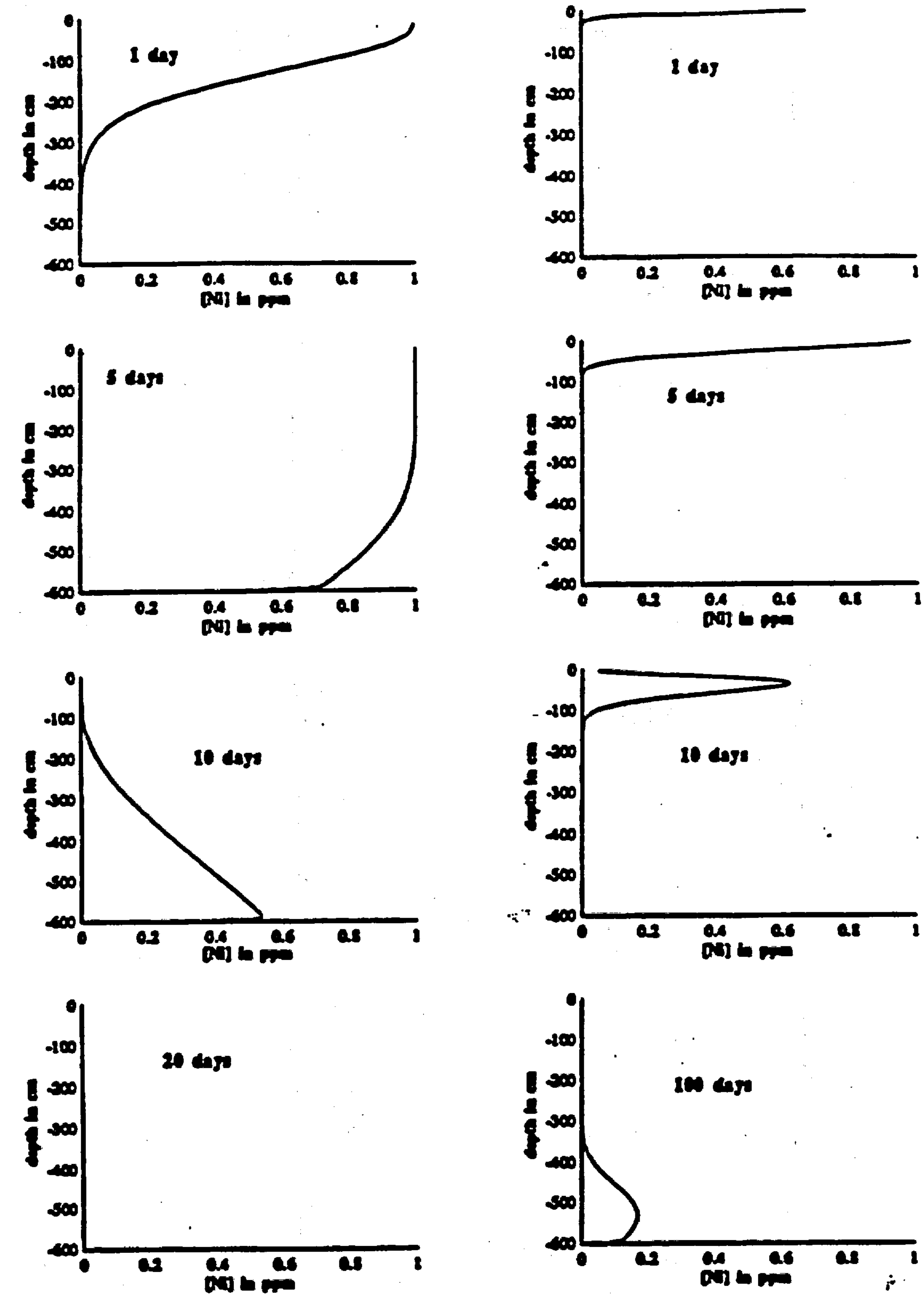
PUBLICATIONS

E.P. Springer and M. D. Siegel
An Integrated Intermediate-Scale Caisson Experiment to Validate Models of Fluid Flow and Contaminant Transport in the Unsaturated Zone
Journal article, Special issue of *Radioactive Waste Management and the Nuclear Fuel Cycle on the Yucca Mountain Project*
In preparation.

PERFORMANCE ASSESSMENT CALCULATIONAL SUPPORT (WBS 1.2.1.4.7)

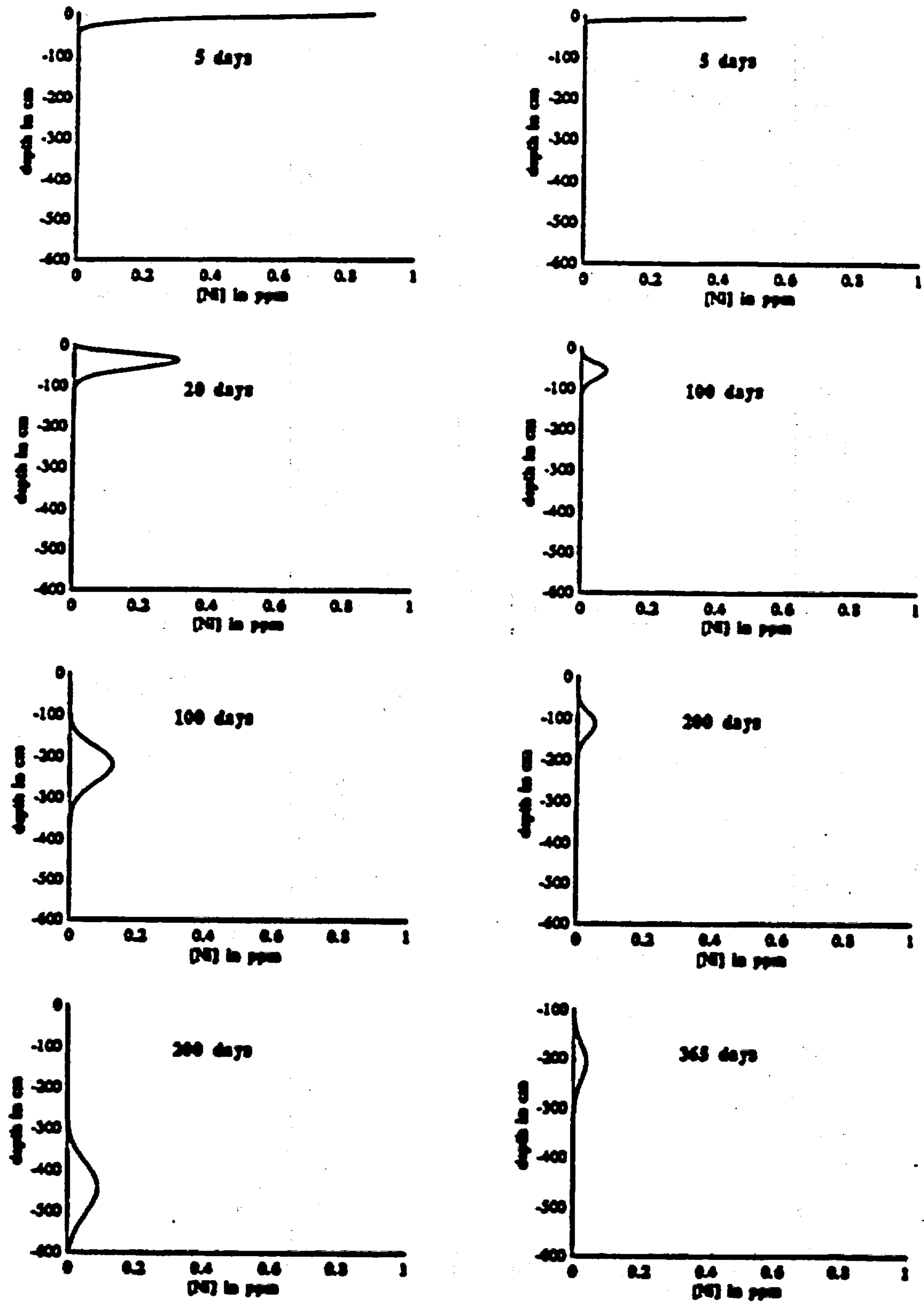
N. Rosenberg and K. Birdsell, along with E. Springer, attended a meeting at Sandia National Laboratories (SNL) on 7 November to discuss the design of the caisson experiment.

N. Rosenberg performed 1-d calculations to estimate Ni transport using a range of K_ds from 0.0 to 70 ml/g (see Figs. 1-3). The results suggest that careful attention to the effect of K_d values on tracer transport is critical to the design of the tracer sampling program. For example, for a K_d of 70, no Ni would be detected below about 1 m from the top even a year after the experiment began. (The length of the caisson is 6 m.) Even with a K_d of 5, transport is significantly retarded—the solute front reaches about 3 m from the top after 100 days. With a K_d of 0.0, the tracer is flushed through the system after only 20 days.



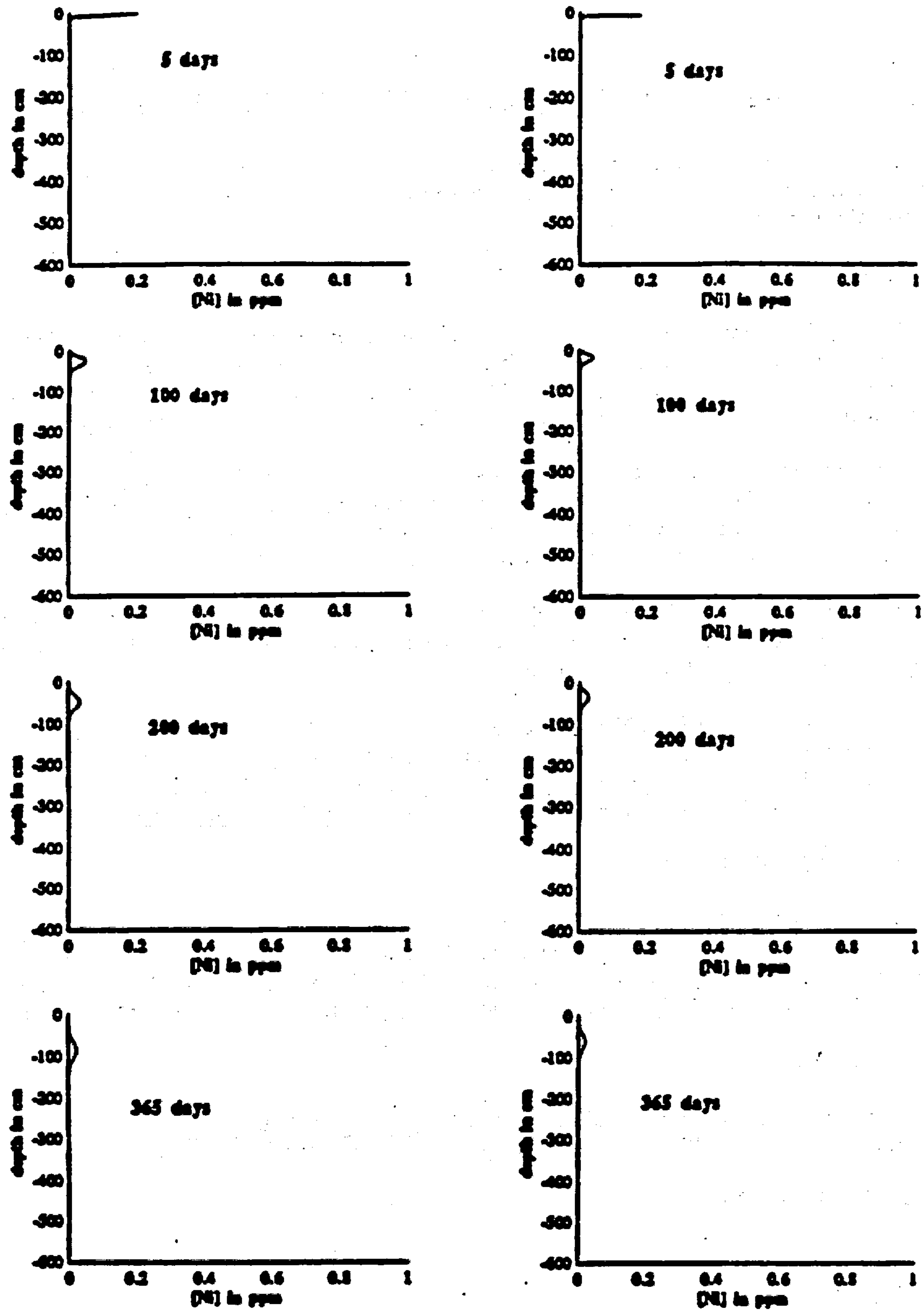
$K_d=0$ $K_d=2$

[Ni] versus depth profiles 1-100 days after the tracer pulse begins



K_d=5 **K_d=20**

[Ni] versus depth profiles 1-365 days after the tracer pulse begins



K_d=50 K_d=70

[Ni] versus depth profiles 1-365 days after the tracer pulse begins

WBS 1.2.3.2.1.1.1
MINERALOGY, PETROLOGY, AND ROCK CHEMISTRY OF TRANSPORT PATHWAYS

The purpose of this activity is to define the important mineralogic and geochemical variables along transport pathways at Yucca Mountain in support of performance assessment and to evaluate the impact of repository construction on natural waste-transport barriers.

ACTIVITIES AND ACCOMPLISHMENTS

Twenty-eight samples from USW G-4 were obtained to investigate possible stratigraphic variation within the rhyolitic portion of the Topopah Spring Member. This part of the Topopah Spring Member is quite homogeneous in major- and trace-element composition; these samples will be used to test Sr-isotopic variability. The core sections were drilled out in 1" plugs at Los Alamos, and the plugs were sent to Z. Peterman of the USGS for isotopic analysis.

Thin sections with acetone-soluble mounts were prepared for possible microscopic transmission/infrared analysis. The goal of this exploratory study will be to evaluate this technique for determining the distribution and nature of alteration features that may be poorly crystalline or distributed as thin mineral coatings. Photography and petrography of four of these thin sections were completed during November.

In fracture mineralogy studies, over 20 fracture samples from Crater Flat drill cores (VH-1 and VH-2) were prepared for scanning electron microscopy and x-ray diffraction (XRD) analysis. These samples include Mn-minerals that will be compared with those found at Yucca Mountain.

For studies of calcites from Yucca Mountain tuffs, the cathodoluminescence instrument at Los Alamos was surveyed to ensure compliance with x-ray safety requirements. In software development, considerable progress was made toward development of an approved version of QUANT, the program developed at Los Alamos and used for quantitative mineral determinations from XRD data. It is anticipated that approval will be obtained within a few months.

PLANNED ACTIVITIES

Work planned within the next few months includes the following activities: (1) continue analysis of Mn-oxide fracture fillings in the Crater Flat and Paintbrush tuffs to determine their distribution and factors controlling that distribution; (2) complete paper on Mn-oxides for publication in a refereed journal; (3) continue analysis of calcites to understand transport and precipitation mechanisms; and (4) complete sampling of cuttings from USW H-5.

PROBLEM AREAS

Many studies still require approval of software for quantitative XRD analysis (e.g., milestone 3137). Approval of software for quantitative XRD analysis is anticipated within the next few months.

MILESTONE PROGRESS

3120
29 May 1992
Calcite in the Upper Paintbrush Tuff

3123
2 March 1992
Mn Minerals in the Crater Flat Tuff
Undergoing extensive revision.

3130
17 August 1992
Fracture Mineralogy of the Paintbrush Tuff

3137
30 September 1992
Mineralogy of Calico Hills for Adit Development
Writing 66% complete; will be completed six months after XRD software approval.

PUBLICATIONS

B. Carlos, D. Bish, and S. Chipera
Fracture-Lining Manganese Oxide Minerals in a Silicic Tuff
Journal article, *Chemical Geology*
Undergoing extensive revision.

D. Bish and S. Chipera
Detection of Trace Clays and Clay Minerals Amounts of Erionite Using X-ray Powder Diffraction: Erionite in Tuffs of Yucca Mountain, Nevada, and Central Turkey
Journal article, *Clay and Clay Minerals*
In press.

D. Vaniman, D. Bish, D. Broxton, B. Carlos, S. Chipera, and S. Levy
Mineralogy as a Factor in Radioactive Waste Transport Through Pyroclastic Rocks at Yucca Mountain, Nevada
Journal article, *J. Geophs. Res.*
Draft complete; may be revised for a different journal.

S. Levy
Natural Gels in the Yucca Mountain Area, Nevada, USA
Conference paper, European Materials Research Society Symposium
In preparation.

WBS 1.2.3.2.1.1.2
MINERALOGIC AND GEOCHEMICAL ALTERATION

The objective of this task is to characterize past and present natural alteration processes that have affected the potential geologic repository and to predict future effects of natural and repository-induced alteration.

ACTIVITIES AND ACCOMPLISHMENTS

S. Levy attended the European Materials Research Society (Scientific Basis for Radioactive Waste Management) fall meeting in Strasbourg, France. Levy's paper on natural gels in the Yucca Mountain area was presented during a symposium on clays and hydrosilicate gels. The paper details the genesis of abundant gels and colloids during digenetic and hydrothermal zeolitic alteration of volcanic glass.

A review of QP-16.2, R1, *Trending*, was completed and transmitted to the QA Project Leader. The review checklist for Study Plan 8.3.1.5.1.3, *Climatic Interpretations of Paleocology*, was also completed.

PLANNED ACTIVITIES

Zeolite stability and glass rehydration studies are ongoing. A concerted effort is being made to obtain QA approval for the software used by G. WoldeGabriel for K/Ar analytical work at Case Western Reserve University.

D. Vaniman will present a talk on calcite-sepiolite associations in waters evaporated from carbonate and tuffaceous aquifers of southern Nevada at the 7th International Symposium on Water-Rock Interaction in July 1992. Vaniman's co-authors are M. Ebinger, D. Bish, and S. Chipera.

PROBLEM AREAS

As a result of the last QA audit, we no longer have an approved vendor for calibration of our ovens; the requirements to qualify calibration vendors will be more involved. Impact on past work?

MILESTONE PROGRESS

3138
30 October 1992
Chemical Transport in Zeolitic Alteration

3141
31 March 1992
Laminated Zone in Trench 14

3142
3 April 1992
K/Ar Dating of Clays and Zeolites
Research continuing; new draft in preparation.

3143
30 September 1991
Experimental Dehydration of Volcanic Glasses
Interim draft complete.

PUBLICATIONS

S. Levy and C. Naeser
Bedrock Breccias Along Fault Zones near Yucca Mountain, Nevada
Chapter in USGS Bulletin on Yucca Mountain studies
In USGS editorial review.

D. Vaniman, D. Bish, and S. Chipera
Rehydration of a Tuff Vitrophyre
Journal article, *J. Geophys. Res.*
Interim draft complete.

WBS 1.2.3.2.1.2
STABILITY OF MINERALS AND GLASSES

The objective of this activity is to produce a model for past and future mineral alteration in Yucca Mountain. The model is intended to explain the natural mineral evolution resulting from the transformation of metastable mineral assemblages to more stable assemblages and the effects of a repository emplacement.

ACTIVITIES AND ACCOMPLISHMENTS

This activity has been deferred.

WBS 1.2.3.2.5
POSTCLOSURE TECTONICS

The objective of these volcanism studies is to determine the hazards of future volcanic activities with respect to siti[ng] a high-level radioactive waste repository at Yucca Mountain.

ACTIVITIES AND ACCOMPLISHMENTS

A talk was presented to the ACNW committee in Washington on 19 November. The talk emphasized the variety of dating methods that are being used for the volcanism program, the importance of using multiple methods, and how differences in results of developmental chronology methods are the expected norm in the early stage of studies. We described the scientific process of using multiple working hypotheses to attempt to obtain high levels of confidence in establishing the history of volcanism in the Yucca Mountain region.

Biological and archeological surveys were completed at the Lathrop Wells center in order to continue trenching studies.

A variety of public interactions involving volcanism participants occurred during November. Talks on volcanoes were presented at the Green Valley Library and the Indian Springs elementary school. We attended and participated in the public update meeting in Reno.

Work in Progress

Much of the month was spent preparing four summary papers for the International High-Level Radioactive Waste Conference in Las Vegas in April 1992. The papers describe (1) the geochemistry of basalt sequences and evidence of waning volcanism for the Crater Flat volcanic field; (2) volcanic recurrence rates for the Yucca Mountain region and bounds that can be established for these rates from high-cone density, volcanic fields; (3) status of field and geochronology studies of the Lathrop Wells volcanic field; and (4) results and plans of studies concerned with the effect[s] of magmatic disruption of the repository and modeling of magma dynamics.

The PACS schedules for volcanism were revised.

Responses to State of Nevada comments on Study Plan 8.3.1.8.1.1, *Probability of Magmatic Disruption of the Repository*, were started. They will be finished in December.

A rough draft of the detailed technical procedure for cosmogenic helium isotopic studies has been completed. It is undergoing review.

Several meetings were held with DOE personnel on preparing an Issue Resolution Report for volcanism. We decided to issue the present rough draft of a summary volcanism report by June 1992. A ~~formal~~ Issue Resolution Report will be written, partly from the content of the volcanism report, in FY93.

PLANNED ACTIVITIES

Additional trenching will be conducted at the Lathrop Wells volcanic center on 16–17 December.

MILESTONE PROGRESS

3174
8 January 1992
Effects of Magmatic Disruption on the Repository (study plan, R0)

3108
30 September 1992
Status of Geochronology Studies at the Lathrop Wells Volcanic Center

3129
10 July 1992
Petrology of Lathrop Wells Eruptive Sequences

PUBLICATIONS

B. Crowe et al.
Multiple Eruptive Events at Small Volume Basaltic Centers: Evidence From the Cima and Crater Flat Volcanic Fields
Journal article
In preparation.

F.V. Perry and B.M. Crowe
Geochemical Evidence for Waning Magmetism and Polycyclic Volcanism at Crater Flat, Nevada
Conference paper, International High-Level Radioactive Waste Management Conference, April 1992
In preparation.

G.A. Valentine, B.M. Crowe, and F.V. Perry
Physical Processes and Effects of Magmetism in the Yucca Mountain Region
Conference paper, International High-Level Radioactive Waste Management Conference, April 1992
In preparation.

B.M. Crowe *et al.*
Methods for Assessing the Risk of Volcanism at the Yucca Mountain Site
Conference paper, International High-Level Radioactive Waste Management Conference, April 1992
In preparation.

B.M. Crowe *et al.*
Status of Geochronology Studies of the Lathrop Wells Volcanic Center
Conference paper, International High-Level Radioactive Waste Management Conference, April 1992
In preparation.

WBS 1.2.3.3.1.2.2 (8.3.1.2.2.2)
WATER MOVEMENT TRACER TESTS

The objective of the water movement tracer tests is to obtain measurements of chlorine isotope distributions to help quantify the percolation of precipitation in the unsaturated zone.

ACTIVITIES AND ACCOMPLISHMENTS

An audit report for Hydro Geo Chem's internal audit was received that contained two deficiency reports, which are being addressed.

Signatures are being obtained for the final versions of six detailed technical procedures (DPs). One draft DP was submitted for technical and QA review.

Drilling continued on the second of twelve neutron-access boreholes for the USGS study *Characterization of Unsaturated-Zone Infiltration*, which is providing QA-traceable ream-cutting samples for chlorine-36 analysis. Work began on drafting a criteria letter for cuttings collection from borehole UZ-16, tentatively scheduled to be drilled by the LM-300 rig starting in February 1992.

Hydro Geo Chem and J. Fabryka-Martin participated in the two-day YMP Workshop on Groundwater Travel Time the Saturated Zone.

PLANNED ACTIVITIES

Submit criteria letter and cutting requests for prototype hole UZ-16; revise DPs for processing samples for chlorine-36 analysis; process cuttings samples from neutron-access boreholes; and process USGS water samples.

MILESTONE PROGRESS

3191
Procedure for Chlorine-36 Analysis of Unsaturated Zone Samples

3192
20 December 1991
Water Movement Tracer Test (study plan) SP
Completed.

WBS 1.2.3.3.1.2.5 (8.3.1.2.2.6)
DIFFUSION TESTS IN THE ESF

The objective of this task is to determine *in situ* the extent to which the nonsorbing tracers diffuse into the water-filled pores of the Topopah Spring welded unit.

ACTIVITIES AND ACCOMPLISHMENTS

No significant activity in this study.

MILESTONE PROGRESS

No level II milestones are planned this fiscal year.

WBS 1.2.3.3.1.3.1 (8.3.1. 2.3.1)
SITE SATURATED ZONE GROUND-WATER FLOW SYSTEM

Experiments will be conducted at the C-Well complex (holes UE25c#1, UE25c#2, and UE25c#3) and in other wells near Yucca Mountain. Reactive tracers will be used to characterize retardation and transport properties on a scale larger than that currently used in laboratory experiments.

ACTIVITIES AND ACCOMPLISHMENTS

Software Qualification

The implementation phase (coding, verification, etc.) of the SORBEQ application has been completed and sent to Software Configuration Manageement for review. The software design document for the FRACNET application has been written and submitted as a partial submission of the Detailed Design Baseline; the Model and Methods Summary is being worked on. The Software Requirements Specification for the FEHMN application has been submitted. G. Cort performed a preliminary informal review to advise us on its acceptability, and we are reviewing his suggestions. The implementation baseline for the interface table tools is under review. Finally, certification of the statistical package SAS for X-Windows has been initiated.

LiBr Sorption Studies

An ion chromatography method has been developed that provides good separation between lithium and sodium and also produces ammonia, potassium, magnesium, and calcium measurements in the same run. B. Newman attended a Dionex ion chromatography seminar and discussed the problem of running acidified cation samples on the ion chromatograph with Dionex personnel. As a result of these discussions, we have ideas on how to set up a cation method for acidified samples and believe that our new cation columns should make this task easier.

Boron Sorption Studies

An evaluation was performed, using the report by G. Gainer titled *Boron Sorption on Hematite and Clinoptilolite* (LAUR-90-4051), to assess the usefulness of boron as a sorbing tracer at the C-Wells. We conclude that there is a significant chance that boron will exhibit minimal sorption at natural groundwater conditions. Given the current funding situation and the likelihood that boron would eventually prove to be inappropriate as a sorbing tracer, we have chosen to drop boron from consideration as a tracer in the C-Wells experiments. The schedule and planning documents will be revised to reflect this change in plans.

PLANNED ACTIVITIES

Continue the effort to bring the computer codes FRACNET, FEHMN, and SORBEQ and other software into compliance with the Software Quality Assurance Plan (SQAP). This consists of compiling existing documentation on these codes and writing new material required by the SQAP.

Continue reviewing software submissions as required.

Continue activities necessary for the batch sorption experiments with lithium bromide, including completing the completion of the development of analytical techniques for measuring lithium concentration, compiling error statistics on the measurements, and determining the cation-exchange capacity of the samples.

Continue developing techniques for measuring the concentration of polystyrene microspheres in solution.

MILESTONE PROGRESS

3193
30 November 1991
Batch Sorption Experiments with Boron Using Single Crystals

3188
16 January 1992
Documentation for SORBEQ

3194
1 April 1992
Batch Sorption Experiments with Lithium

T112
22 June 1992
Final Documentation for FEHMN

3196
27 July 1992
FRACNET Documentation

PUBLICATIONS

W.L. Polzer and H.R. Fuentes
The Use of the Modified Estimate Thermodynamic Equilibrium Properties of Ion Exchange Adsorption of Radionuclides on Volcanic Tuff. Part II. Experimental
Journal article, *Environmental Science and Technology*
Submitted to Project Office 7 August 1990; resubmitted 22 March 1991 under AP-1.3.

B.A. Robinson
FRACNET—Fracture Network Model for Water Flow and Solute Transport
LA-series report
In preparation.

B.A. Robinson
SORBEQ—A One-Dimensional Model for Simulating Column Transport Experiments
LA-series report
In preparation.

WBS 1.2.3.4.1.1 (8.3.1.3.1.1)
GROUND-WATER CHEMISTRY MODEL

The goal of this investigation is to provide conceptual and mathematical models of the groundwater chemistry at Yucca Mountain. These models will explain the present groundwater composition in relation to interactions of minerals and groundwater and will be used to predict groundwater compositions as a result of anticipated and unanticipated environments.

ACTIVITIES AND ACCOMPLISHMENTS

An abstract entitled *Water-Rock Interaction and the pH of Yucca Mountain Ground Water* (M. Ebinger) for the 7th International Symposium on Water-Rock Interactions was accepted for presentation at the July 1992 conference.

Modeling evaporation of different Yucca Mountain waters and waters from the surrounding area continued. Water derived from tuffs generally precipitates calcite and sepiolite at relatively low concentration factors (i.e., as low as twice the initial concentration). Water derived from carbonate aquifer and, in some cases shallow soils, shows some calcite precipitation with dolomite and sepiolite competing for available Mg.

The stability of the pH of waters derived from Yucca Mountain tuffs seem well buffered by $CO_{2(g)}$, precipitation of calcite and opal, exchange with clay minerals and zeolites, and dissolution of tuffs. Simulated introduction of acid solutions to Yucca Mountain waters resulted in little, if any, change in the pH of the mixed solution. Dissolution of tuffs was the main result of such simulations.

PLANNED ACTIVITIES

Track Study Plan 8.3.1.3.1.1 during YMPO review. SP

Continue the USGS collaboration. We will arrange to sample and analyze dissolved gases from USGS water samples and sample water in contact with rock in the upper saturated zone. These data will be used to ascertain Eh conditions independently from Pt electrode measurements, to prepare "snapshots" of water-rock interactions, and for refined models of groundwater chemistry.

MILESTONE PROGRESS

3006
31 March 1992
Eh and pH Buffering Capacity

3415
30 September 1992
Letter Report: Most Active Groundwater Chemistry

WBS 1.2.3.4.1.2.1 and 1.2.3.4.1.2.3 (8.3.1.3.4.1)
BATCH SORPTION STUDIES AND SORPTION MODELS

The objective of this task is to provide sorption coefficients for elements of interest to predict radionuclide movements from the repository to the accessible environment.

ACTIVITIES AND ACCOMPLISHMENTS

The experiments designed to evaluate the effects of crushing on the sorption coefficients obtained by batch techniques have been completed. Surface area determinations have been completed on approximately one-half of the samples. Surface area does not seem to be a major determinant of the variations in sorption coefficients observed for Cs, Sr, and Np in these samples.

Results from a series of experiments designed to evaluate the effect of variations in water/rock ratios on sorption coefficients are now available. The problem addressed in these experiments concerns the unexpected increase in adsorption coefficients for Ba, Cs, and Sr with increasing water/rock ratios when zeolitic tuffs were used in the experiments (Wolfsberg *et al.*, 1981). Those experiments, which used devitrified tuffs, showed a decrease in Ba, Cs, a[illegible] Sr sorption coefficients with increasing water/rock ratios as expected theoretically. As noted in the September 1989 report we suspected colloids might be a problem in the experiments with the zeolitic tuffs. A new set of experiments were carried out with the zeolitic tuffs in which the solutions were separated from the solids using filter membranes wi[illegible] pore sizes on the order of 10 or less as opposed to the 50-nm membranes used in the earlier experiments. The results [illegible] Cs are as follows.

Sample No.	Water/Rock Ratio (ml/g)	K_d (ml/g)
G4-1501	5:1	37,000 (± 5,000) 38,800 (± 6,000)
G4-1501	10:1	37,500 (± 4,000) 46,700 (± 5,000)
G4-1501	30:1	22,800 (± 1,300) 23,300 (± 1,400)

These results indicate that the sorption coefficient for Cs does decrease with increasing water/rock ratio even for th[illegible] zeolitic tuffs. A logical conclusion would be that zeolitic tuffs generate very-fine-grained colloidal material during the batch experimental procedure, probably during the shaking step.

The construction of a vibration isolation booth for the new atomic-force microscope has begun. We anticipate it w[illegible] be completed in December. This instrument will be used to image substrates before and after sorption reactions involvi[illegible] the important radionuclides.

P. Rogers is near completion on the new contract with J. Leckie at Stanford University. The two-month lapse in th[illegible] contract has temporarily halted the experimental work.

A search was initiated for a new staff member in the sorption task. Several candidates will be interviewed in the next two months.

PLANNED ACTIVITIES

Continue to study radionuclide sorption on pure mineral phases. Revise paper for sorption workshop proceedings after policy review. Complete study plan revisions.

MILESTONE PROGRESS

3216
30 September 1992
Mass Spectrometry as Applied to Americium Sorption
Completed (published in *Radiochimica Acta* 52/53, 141-145, 1991).

3009
20 February 1992
Variation of Water-Rock Ratio Sorption Coefficients on Zeolitic Tuff

3212
30 September 1992
Progress Report on Single Mineral Experiments

PUBLICATIONS

A. Meijer
Sorption Studies Review and Strategy
Conference paper, *Proceedings of the Radionuclide Adsorption Workshop*, Los Alamos, NM, 11–12 September 1990
In preparation.

WBS 1.2.3.4.1.2.2 (8.3.1.3.4.2)
BIOLOGICAL SORPTION AND TRANSPORT

The purpose of this research is to determine whether microbial activity can influence the movement of plutonium in tuff. Because fluids are used extensively in the exploration of locations for a nuclear repository, those microorganisms capable of utilizing drilling fluids as growth substrates are of special interest.

ACTIVITIES AND ACCOMPLISHMENTS

Final purification of siderophore run numbers 185 and 186 was completed. As discussed in October's report, the identify of some amino acids in the siderophore produced by *Pseudomonas* sp. is still unknown. Work has continued on identifying these constituents.

PLANNED ACTIVITIES

Continue plutonium K_d and colloidal agglomeration experiments.

MILESTONE PROGRESS

3080
30 September 1992
Report on Chelation

3092
30 September 1992
Report on Colloidal Agglomeration

3176
30 September 1992
Procedure for Determination of Formation Constants
In progress.

3177
30 September 1992
Procedure for Determination of Effects on Colloidal Agglomeration

PUBLICATIONS

L. R. Hersman, D. E. Hobart, and T. W. Newton
Preliminary Evidence of Siderophore/Plutonium Complexation
Journal article, *Journal of Applied and Environmental Microbiology*
Undergoing revision.

WBS 1.2.3.4.1.3
RADIONUCLIDE RETARDATION BY PRECIPITATION PROCESSES

The objective of the solubility determination task is to determine the solubilities and speciation of important waste elements under conditions characteristic of the repository and along flow paths from the repository into the accessible environment.

ACTIVITIES AND ACCOMPLISHMENTS

P. Palmer attended the 9th YMP Open House Tour on 16 November.

Speciation Studies

A great deal of effort has been devoted to developing of sensitive spectroscopic techniques to study actinide speciation based on the sensitivity of f-f electronic absorption bands to oxidation state and ligation of the actinide ions. These efforts assume that data obtained in such studies will be interpretable in terms of changes in complexation of the metal center. However, our current understanding of 5f electronic structure is based on data from solid-state doped sing crystals. In these studies, the local coordination geometry about the central actinide ion is maintained in an almost perfect high-symmetry environment and will have little relevance for species in solution where deviations from perfect high symmetry tend to be the rule rather than the exception. Accordingly, part of our task has been to establish the unique spectral signatures for actinide species extant under environmentally relevant conditions.

To establish spectroscopic signatures that are applicable to interpretation of actinide solution spectra, we need the ability to fine-tune changes in structure and ligand-field strengths. The most convenient way to achieve this fine-tuning through synthetically tailored actinide complexes. Therefore, we have adopted a model compound approach that exploit the versatility of synthetic actinide chemistry to enable this fine-tuning of structural and electronic effects so that a clear correlation of molecular and electronic structure can be established. Speciation information can then be extracted from subsequent spectral data (e.g., from environmental samples) with greater likelihood of success, perhaps making it possibl to obtain the fundamental molecular-level characterization required to fully understand and model actinide transport and transformation processes.

Experimental activities in this model complex investigation have involved both the refinement of synthetic strategies to make available a wide range of actinide complexes with varying structural and electronic perturbations, and the acquisition and interpretation of electronic spectral data for these synthetically-tailored model complexes. We have synthesized and characterized well over 50 new actinide alkoxide complexes and are confident that our methodology wil be applicable to the preparation of the analogous neptunium and plutonium complexes. By careful control of steric bulk on the supporting alkyl group in the actinide alkoxide, one can control oligomerization in the model complexes as exemplified by the x-ray structures of $An(OR)_4$, $An_2(OR)_8$, and $An_3O(OR)_{10}$, where An = Th, U. Many of the same structural types have been prepared and characterized for both Th(IV) and U(IV), indicating a high likelihood for success in preparation of analogous Np(IV) and Pu(IV) complexes for spectroscopic analysis. Our synthetic studies have established that we can indeed control the local coordination geometry about the central actinide ion, and we have built a fairly extensive database of x-ray structural data. Solution NMR studies have demonstrated that these structural types are maintained in solution, and thus, electronic absorption spectra obtained on pure compounds are indicative of each structural type in solution.

These model complexes have been used to determine how observable electronic transitions are perturbed in response to structural changes in the complex in solution. From the spectra obtained for these model complexes, we have found that the f-f transitions naturally fall into obvious groupings by coordination number and symmetry by which we can now differentiate between monomeric, dimeric, and trimeric actinide species in solution. This represents a significant breakthrough for the use of optical spectroscopic techniques in determination of actinide speciation in dilute solution.

The first phase of carbon-13 NMR characterization of Pu(IV) in aqueous carbonate solution is now complete, and data analysis is also near completion. These studies have demonstrated that solution NMR studies will serve as a unique species-specific tool for unraveling the stoichiometry and structure of actinides in carbonate solution. Preliminary studies have identified some of the same species present for both U(VI) and Am(IV).

Work continues on the development of the qualified version of the photoacoustic spectroscopy (PAS) software. We have also recently reinitiated experiments to determine the identity of the supposed "other" Pu(IV) carbonate species reported by Kim *et al.* in 1 M carbonate solutions in the near-neutral pH range. One possibility is that the other species are colloidal in nature. We will test this by acquiring PAS spectra of Pu(IV) colloid at very low concentrations.

Preparation of the manuscript on the developmental phase of our PAS system continued. We have initiated procurement procedures to acquire a commercial data station and software for our wavelength calibration system for the PAS system. We originally intended to develop the software for the control of this instrument "in house." However, we have since identified a commercial source for this purpose, and we estimate a savings of approximately one man-year of effort in software development and qualification. The purchase request was submitted, and we expect to take delivery in February 1992.

A new set of experiments has been initiated in collaboration with I. Triay to study the solution speciation of Np(V) prior to and following contact (batch or column) with Yucca Mountain tuffs. Preliminary stock solutions of Np(V) (10^{-5}M at pH 8.5) in J-13 water were found to be unstable. This instability is surprising because Np(V) appears to be stable in 10^{-3}M $NaHCO_3$ made from distilled water at the same Np concentration and pH. This phenomenon is being investigated.

Solubility Studies

A no-cost extension of the YMP contract for solubility studies at Lawrence Berkeley Laboratory has been initiated; this will run through 31 December 1991.

Plutonium solubility studies at pH 6, 7, and 8.5 in UE25p#1 at 60° C have been initiated. A Pu(IV) stock solution was prepared by electrolysis and assayed for purity by absorption spectrophotometry. The initial filtration experiments for the plutonium cells were performed one day after their start, and the data, as well as the data for the americium/neodymium filtration experiments, are being worked up. The work-up of the initial filtration experiment for the neptunium experiments has been completed. There is virtually no adsorption of the radionuclide onto the Amicon filter at any of the three pH's. However, the filters will be presaturated with 500 microliters of solution before taking actual assays. Assays are being counted from each of the experiments and approach-to-equilibrium plots for each of the radionuclides are being prepared as the results become available.

The Berkeley group corrected and resubmitted rejected record packages. 17 They continued to work on one new draft and one revised DP. They are awaiting the review of their draft DP for the Mettler H6T balance operating and calibrating procedure.

From 18 October–9 November, H. Nitsche was on travel representing his YMP research at two conferences and several research institutions in Europe. From 20–25 October, he attended the 3rd International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere (Migration 91) in Jerez de la Frontera, Spain.

what benefit to YMP?

During his visit, he attended the executive meeting of the Scientific and Organizing Committee for the conference, chaired Poster Session I, and presented two papers—*Dependence of Actinide Solubility and Speciation on Carbonate Concentration and Ionic Strength in Groundwater* and *Overview of Solubility and Speciation Studies for Risk Assessment of Nuclear Waste Repositories.* He also visited the Institute for Nuclear Waste Technology at the Nuclear Research Center, the Institute of Radiochemistry, and the European Institute for Transuranium Elements, all in Karlsruhe, Germany. The European Institute is part of the Joint Research Centre of the Commission of the European Communities, and while there, Nitsche presented a seminar entitled *Selected Research Topics for the Yucca Mountain Site Characterization Project.*

From 4–8 November, Nitsche attended the symposium Scientific Basis for Nuclear Waste Management XV that wa part of the European Materials Research Society 1991 Fall Meeting in Strasbourg, France. He presented an invited talk titled *The Importance of Transuranium Solids in Solubility Studies for Nuclear Waste Repositories.* On 8 November, Nitsche visited the Institute for Nuclear Chemistry at the Nuclear Chemistry Research Center in Strasbourg-Kronenbou France.

PLANNED ACTIVITIES

H. Nitsche will visit Los Alamos to present a seminar and hold discussions with Project management on 3–4 December. D. Morris will represent the Solubility Task at the Fall 1991 Meeting of the American Geophysical Union, from 9–13 December in San Francisco, and D. Hobart will attend the 10th YMP Open House Tour on 7 December.

MILESTONE PROGRESS

3120
30 September 1991
Progress Report on PAS
In preparation.

3031
30 September 1992
Speciation Measurements

3329
30 September 1992
Report on Neptunium, Plutonium, and Americium Solubility Experiments from Oversaturation

PUBLICATIONS

Report on Measured Solubilities of Pu, Am, and Np in J-13 Groundwater from Oversaturation Conditions
LA-series report
In preparation.

Carbonate Complexation of Pu(IV)
LA-series report
In preparation.

C.D. Tait, D.E. Morris, S.A. Ekberg, P.D. Palmer, and J.M. Berg
Plutonium Carbonate Speciation Changes with pH
Abstract, American Chemical Society National Meeting, San Francisco, California, April 1992
Submitted to YMPO on 25 November 1991.

WBS 1.2.3.4.1.4
RADIONUCLIDE RETARDATION BY DISPERSIVE, DIFFUSIVE, AND ADVECTIVE PROCESSES

The objectives of this task are to determine the rate of radionuclide movement along the potential flow paths to the accessible environment and to examine the effect of diffusion, adsorption, dispersion, anion exclusion, sorption kinetics, and colloid movements in the flow geometries and hydrologic conditions expected to exist along the flow path to the accessible environment in the scenarios used for performance assessment.

ACTIVITIES AND ACCOMPLISHMENTS

We finished analyzing the data from the rock beaker experiments (see February 1989 monthly report for details), which were utilized to study the diffusion of radionuclides through Yucca Mountain tuffs. Many of the experimental details already given in previous monthly reports will be repeated here for completeness.

The experimental technique involved fabricating containers in the form of a beaker (made of tuff). Figure 1 shows a cross section of a rock beaker encapsulated in a plexiglass container. The rock beaker sits on the plexiglass container (surrounded by a layer of J-13 water on the sides). A plexiglass stopper is utilized to prevent evaporation. The beaker has an orifice with a radius of 1.4 cm and length of 2.5 cm. The rock beaker has a length of 5 cm and a radius of 3.1 cm.

Sample Rock Beaker

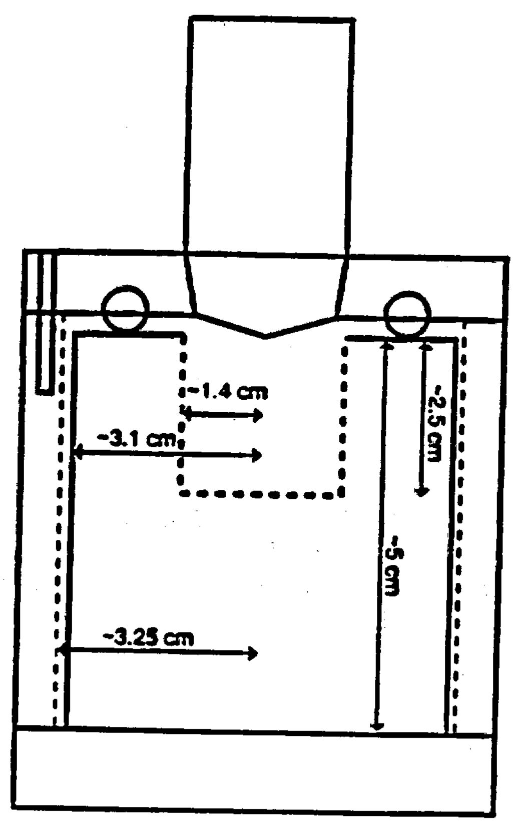


Figure 1.

A solution containing radionuclides of interest was prepared in J-13 water. Actinide solutions were prepared from well-characterized Np(V) and Am(III) acidic solutions. The radionuclides utilized for these experiments were H-3, Tc-95m, Np-237, Am-241, Sr-85, Cs-137, and Ba-133. The J-13 solution containing the radionuclides of interest was placed in the orifice of the rock beakers. Aliquots of the solution containing the radionuclides of interest were taken as a function of time and analyzed for radionuclide concentration. After diffusion is completed, the beakers will be sectioned and the radionuclide concentration will be determined in the tuff. Figure 2 shows the concentration left in the solution in the orifice of the rock beaker (made with tuff G4-737) divided by the initial concentration of the solution placed in the rock beaker as a function of time elapsed after the J-13 solution was placed in the orifice.

The diffusion data were fitted to the diffusion equation given in Fig. 3, utilizing an unqualified version of TRACRN. The sink term Q is zero when the radionuclide is nonreactive. The sink term is given in Fig. 3 for a sorbing radionuclide.

Figure 4 shows the fits obtained utilizing TRACRN for nonsorbing radionuclides (H-3 and Tc-95m) in a beaker made of tuff G4-737. The diffusion coefficients obtained for the nonsorbing radionuclides in all the tuffs studied are given in Table 1. Large anions, such as pertechnetate, are excluded from tuff pores due to their size and charge.

The relationship between F and C (as defined in Fig. 3) describes the sorption mechanism that is observed for the sorbing radionuclides. If sorption is linear, reversible, and instantaneous, then F/C is equal to a sorption coefficient (K_d). To test this assumption, batch sorption experiments were performed utilizing the tuffs studied. The batch sorption procedure consisted of pretreating 1 g of tuff with 20 ml of a J-13 water for two weeks, separating the phases, adding 20 ml of the J-13 solution containing the radionuclides of interest to the pretreated tuff, separating the phases by centrifugation, and determining the amount of radionuclide in both phases. The sorption coefficients (K_d) determined in this manner are given in Table 2.

The diffusion of the sorbing radionuclides could not be fit assuming reversible, instantaneous, and linear sorption. Figure 5 shows the fit that would be obtained assuming the diffusion coefficient determined for tritiated water in tuff G4-737 and the sorption coefficient determined for each sorbing radionuclide in tuff G4-737. Comparison of the fits for the sorbing radionuclides with the actual data obtained (see example in Fig. 6) indicates that conservative transport calculations will result from a batch sorption K_d and the diffusion coefficient obtained for tritiated water.

MILESTONE PROGRESS

3040
30 September 1992
Kinetics of Sorption on Columns of Pure Minerals

PUBLICATIONS

I.R. Triay, A.J. Mitchell, and M.A. Ott
Radionuclide Migration Studies for Validating Sorption Data—Past, Present, and Future
Conference paper, *Proceedings of the Radionuclide Adsorption Workshop*, Los Alamos, NM, 11–12 September 1990
In internal review.

I.R. Triay
Radionuclide Migration in Tuff under Diffusive Conditions
Conference Paper, Migration '91, Jerez de la Frontera, Spain, 14–18 October 1991
In preparation.

G4-737

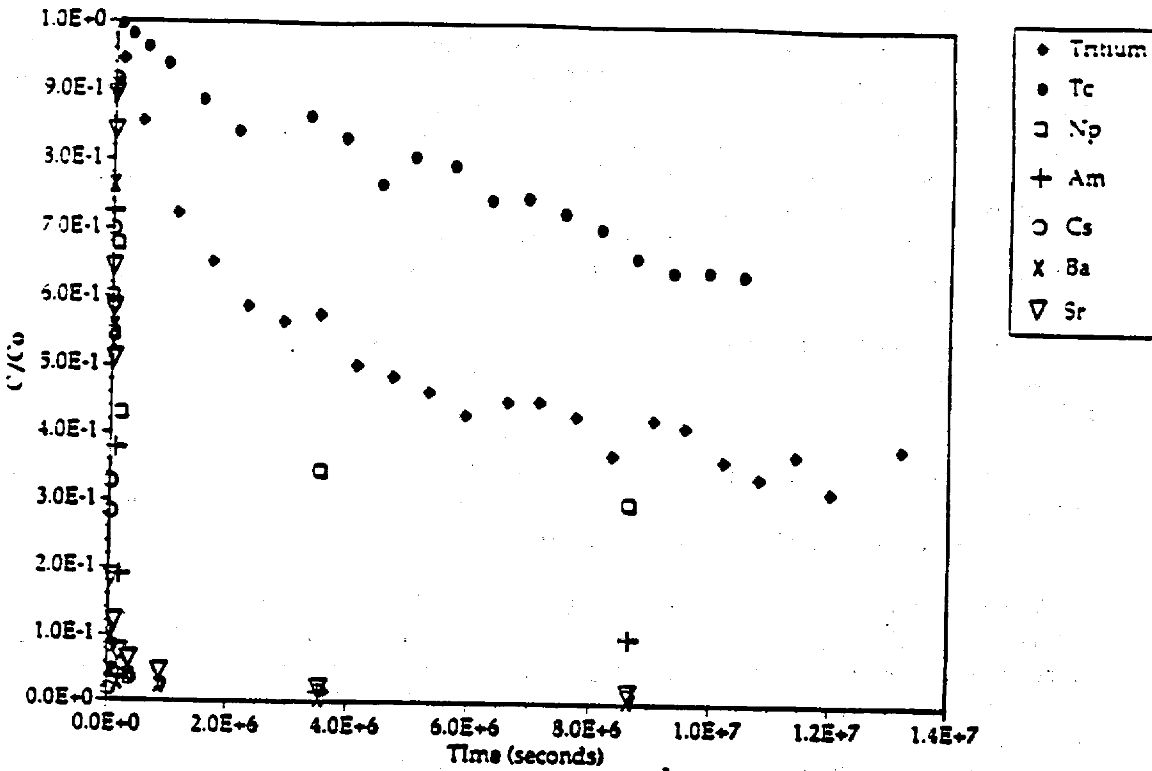


Figure 2.

Diffusion Equation

$$\nabla \cdot (\varepsilon D \nabla C) = \varepsilon \frac{\partial C}{\partial t} + Q$$

$$Q = 0 \text{ (nonreactive)}$$

$$Q = (1 - \varepsilon)\, \rho_s \frac{\partial F}{\partial t} \text{ (sorbing)}$$

D = diffusion coefficient

C = concentration of solute

ε = porosity

t = time

Q = sink or source term

ρ_s = density of the solid particles

$$F = \frac{\text{mass of solute sorbed}}{\text{unit mass of solid}}$$

Figure 3.

Preliminary Data—Do Not Reference

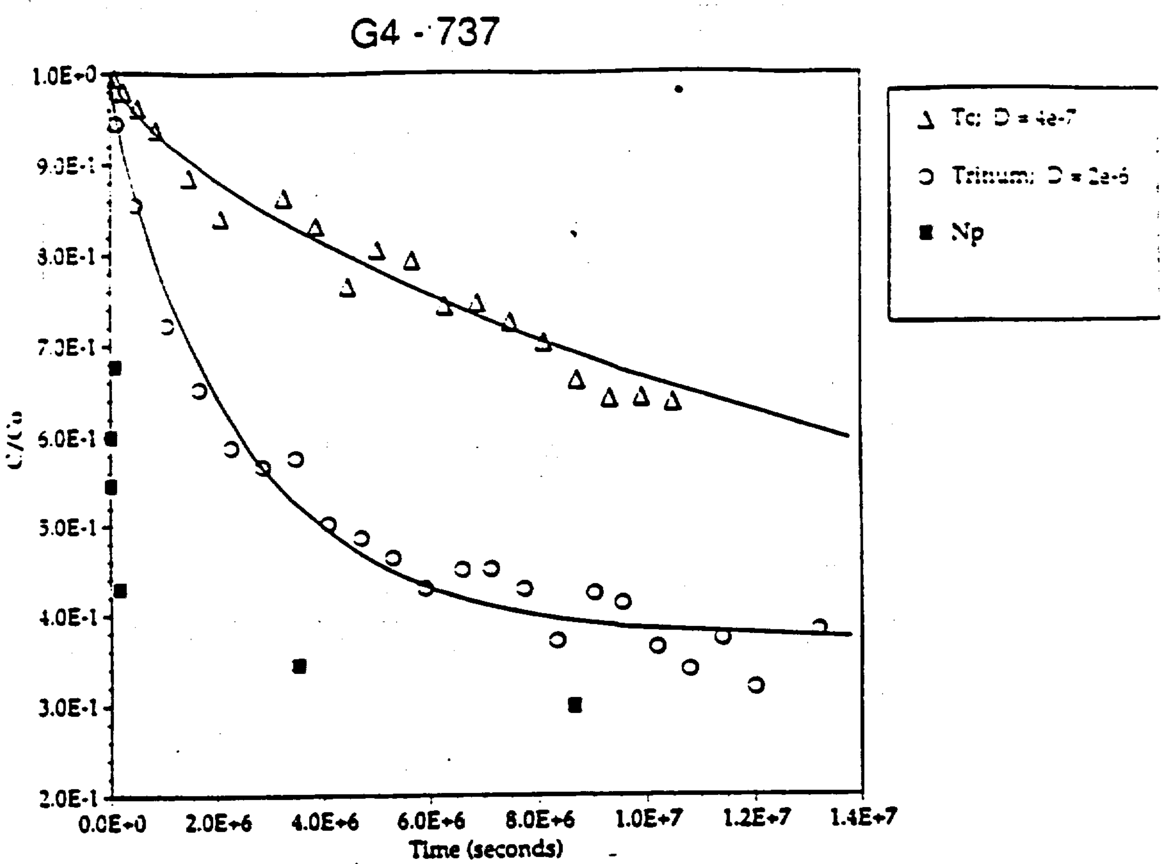


Figure 4.

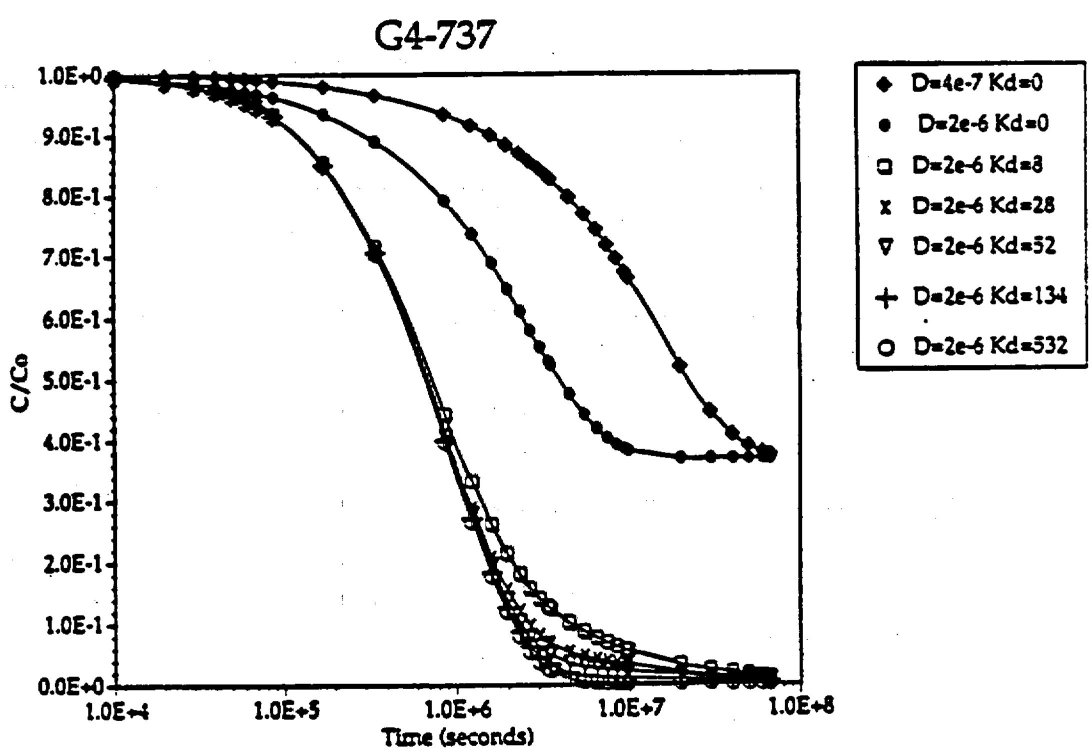


Figure 5.

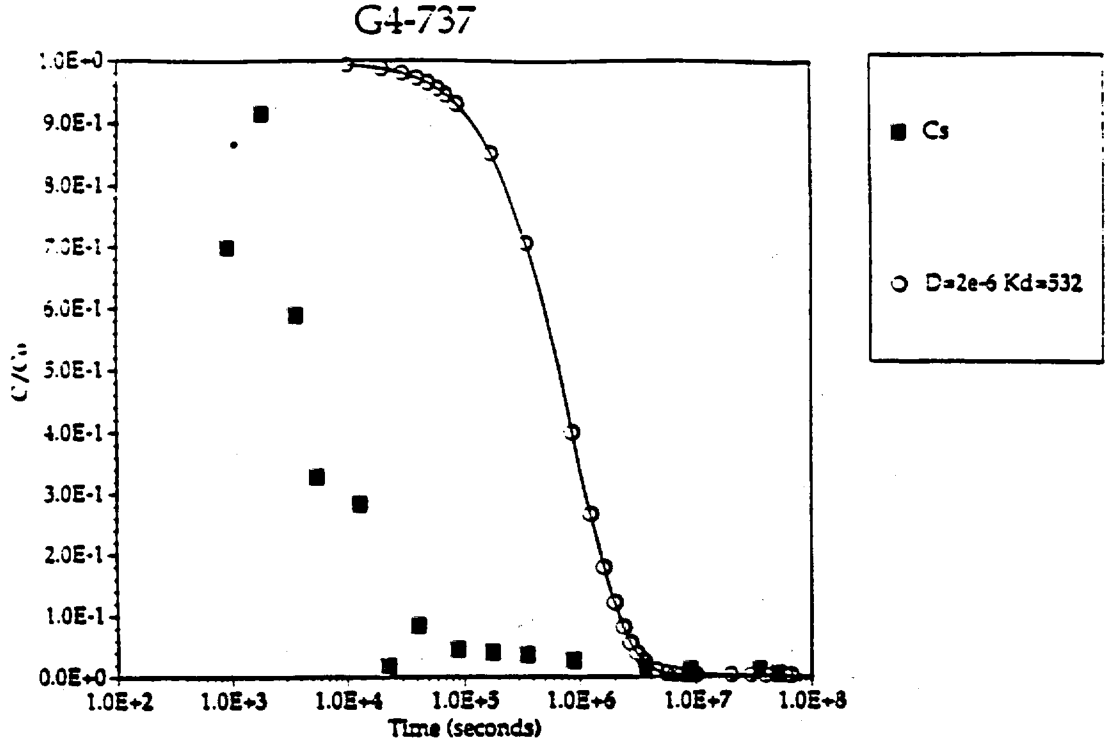


Figure 6.

Diffusion Results

Tuff Sample	Major Minerals, %	Porosity	D (cm^2/s)	
			HTO	TcO_4^-
G4-737	alkali feldspar, 68 cristobalite, 28	0.07	2.2×10^{-6}	3.9×10^{-7}
GU3-304 #1 GU3-304 #2	alkali feldspar, 73 cristobalite, 25	0.06	1.5×10^{-6} 1.6×10^{-6}	3.0×10^{-7} 3.0×10^{-7}
GU3-433	alkali feldspar, 76 cristobalite, 15	0.10	3.5×10^{-6}	
GU3-1119	alkali feldspar, 70 quartz, 19	0.10	2.0×10^{-6}	4.9×10^{-7}
Topopah Outcrop	alkali feldspar, 59 cristobalite, 23 quartz, 12	0.07	1.0×10^{-6}	1.0×10^{-7}

Table 1.

Sorption Results

Tuff Sample	Major Mineral, %	Kd (ml/g)				
		Np	Am	Cs	Sr	Ba
G4-737	alkali feldspar, 68 cristobalite, 28	8	134	532	52	28
GU3-304	alkali feldspar, 75 cristobalite, 25	8		342	18	19
GU3-433	alkali feldspar, 76 cristobalite, 15	9	154	1264	20	61
GU3-1119	alkali feldspar, 70 quartz, 19	8	136	494	42	27
Topopah Outcrop	alkali feldspar, 59 cristobalite, 23 quartz, 12	9		465	20	25

Table 2.

WBS 1.2.3.4.1.5.1 (8.3.1.3.7.1)
RETARDATION SENSITIVITY ANALYSIS

The objectives of this task are to construct a geochemical/geophysical model of Yucca Mountain and to use this model to examine the physical and chemical controls on radionuclide transport along flow paths to the accessible environment.

ACTIVITIES AND ACCOMPLISHMENTS

Analysis of Physical/Chemical Processes

K. Birdsell attended a workshop on Ground-Water Travel Time in the Saturated Zone, 13–14 November, in Tucson. Participants discussed hypotheses for the large hydraulic gradient at Yucca Mountain, modeling of fracture transport in the saturated zone, data collection in the saturated zone, and uncertainty caused by heterogeneity.

QA and Programmatic

Certification of TRACRN continued. Code modifications to incorporate dynamic memory allocation are nearly complete, and modifications to incorporate interface table input/output now completed. The Software Requirements Specification (SRS) document, the Models and Methods Summary (MMS), and the Software Design Document (SDD) are nearly finished. The SRS will be submitted for formal review in early December, and the SDD and MMS will be submitted for informal review at the same time. Calculated results for several verification examples compared favorably with analytic solutions. Work on the user's manual continued.

MILESTONE PROGRESS

3049
27 June 1991
Update Report on Coupled Phenomena
Completed (see Appendix).

3052
30 March 1992
Baseline Documentation for TRACRN

WBS 1.2.3.4.1.5.2 (8.3.1.3.7.2)
DEMONSTRATION OF APPLICABILITY OF LABORATORY DATA

The purpose of this study is to design and conduct experiments to evaluate the applicability of laboratory data and to test models used in the Radionuclide Transport Program to determine far field radionuclide transport. Both intermediate- and field-scale experiments and natural analogs will be assessed for their potential to provide the required data.

ACTIVITIES AND ACCOMPLISHMENTS

E. Springer attended a meeting on 5 November to discuss options for initial north or south excavation of the Exploratory Studies Facility (ESF). E. Springer also attended the workshop on saturated-zone groundwater travel time held in Tucson, Arizona, during 13–14 November. The workshop consisted of prepared presentations and open discussions; this format was effective in allowing issues to be discussed and making information available. One of the fundamental issues from the radionuclide transport aspect is related to stratigraphic control of flow and transport in the unsaturated zone. Is there a single unit or do the geologic units need to be addressed separately? A Hydrology Integration Task Force meeting was held immediately following the workshop.

A talk titled *The Use of Anthropogenic Analogues in Site Characterization of Low-Level Radioactive Waste Sites* was presented at the 13th Annual DOE Low-Level Waste Management Conference, in Atlanta, Georgia, on 19 November.

E. Springer attended a meeting in Las Vegas on 26 November to discuss the scope of the ESF underground test program and the material prepared for TPP 91-5.

PLANNED ACTIVITIES

Continue processing change request and developing study plan. Support the Test Coordination Office in the selection of a north portal for the ESF.

PUBLICATIONS

E.P. Springer
The Use of Anthropogenic Analogues in Site Characterization of Low-Level Radioactive Waste Sites
Conference Paper, Proceedings of the 13th Annual DOE Low-Level Waste Management Conference, Atlanta, Georgia, 19–21 November 1991
In preparation.

WBS 1.2.5
REGULATORY AND INSTITUTIONAL

The purpose of this task is to coordinate the regulatory and institutional Project requirements within the Los Alam programmatic structure. The focus of this coordination effort is on the integration of the technical work within the regulatory and institutional framework.

Study Plans

Water Movement Test, R3 (8.3.1.2.2.2). A revision incorporating NRC and State of Nevada comments was submittec on 16 October 1991.

Diffusion Test in the Exploratory Studies Facility, R0 (8.3.1.2.2.5). A revision incorporating DOE/HQ and Project Office comments was submitted on 11 June 1991.

Testing of the C-Hole Sites With Reactive Tracers, R1 (8.3.1.2.3.1.7). Issued by DOE/HQ as a controlled document and sent to the NRC on 10 April 1990.

Mineralogy, Petrology, and Chemistry of Transport Pathways, R3 (8.3.1.3.2.1). Accepted by the NRC on 4 September 1990. Responses to NRC comments were submitted on 19 August 1991.

History of Mineralogy and Geochemical Alteration at Yucca Mountain, R0 (8.3.1.3.2.2). A revision incorporating SAIC comments was submitted on 13 June 1991.

Kinetics and Thermodynamics of Mineral Evolution and Conceptual Model of Mineral Evolution, R0 (8.3.1.3.3.2 8.3.1.3.3.3). Comment resolution meeting for DOE/HQ and Project Office comments was held on 14–15 March 1990; revision activity has been deferred.

Sorption Studies and Sorption Modeling, R0 (8.3.1.3.4.1; 8.3.1.3.4.3). Comment resolution meeting for DOE/HQ and Project Office comments was held in February 1990; revision is in progress.

Biological Sorption and Transport, R1 (8.3.1.3.4.2). Revision, incorporating DOE/HQ and Project Office comments, was submitted to Project Office on 20 May 1991. Additional revised text was submitted to the Project Office on 28 August 1991.

Dissolved Species Concentration Limits, and Colloid Formation and Stability, R0 (8.3.1.3.5.1; 8.3.1.3.5.2). Submitt to Project Office on 17 August 1990.

Dynamic Transport Column Experiments, R0 (8.3.1.3.6.1). Comment resolution meeting for DOE/HQ and Project Office comments was held on 28–30 August 1990; revision is in progress.

Diffusion, R0 (8.3.1.6.2). Comment resolution meeting for DOE/HQ and Project Office comments was held on 28–30 August 1990.

Probability of Magmatic Disruption of the Repository, R0 (8.3.1.8.1.1). Revision incorporating DOE/HQ and Project Office comments was submitted on 19 June 1990.

Effects of Magmatic Disruption of the Repository, R0 (8.3.1.8.1.2). In preparation.

Characterization of Volcanic Features, R0 (8.3.1.8.5.1). Accepted by NRC on 4 September 1990.

Retardation Sensitivity Analysis, R0 (8.3.1.3.7.1). A revision incorporating DOE/HQ and Project Office comments was submitted on 18 June 1991.

Ground Water Chemistry Modeling, R0 (8.3.1.3.1.1). Submitted to Project Office on 15 March 1991.

WBS 1.2.6
EXPLORATORY STUDIES FACILITY

These exploratory studies (ES) will address the issues and information needs associated with the feasibility of storing high-level nuclear waste in a geologic repository at Yucca Mountain.

ACTIVITIES AND ACCOMPLISHMENTS

Plans for the management and controls of fluids, materials, and tracers were finalized and submitted for YMPO acceptance.

Participated in meetings on management and control of water to be used at the ESF, held an ESF Test Coordination meeting in Las Vegas, participated in Test Integration meetings, and supported YMPO meeting on prioritizing the ESF access construction.

Briefed YMPO on ESF testing and current planning basis for the ESF tests.

PLANNED ACTIVITIES

Evaluate the location of north portals, and develop recommendations for RSN regarding the preferred location.

Meet with M&O on resolving comments on Construction Implementation Plan (CIP) developed by M&O.

Begin the following initiatives: implement concepts proposed in the Fluids, Materials, and Tracers Management Plan; update ESF Test Support Requirements Document; develop interfaces for testing and the ESF design; prepare SCPB changes (Sections 8.3 and 8.4) to incorporate new ESF configuration and tests descriptions as developed through TPP 91-5; prepare Title II Test Planning Packages; and develop new networks for ESF testing. 5, 6,

The following work will continue: meet on management of water used during site characterization, work with M&O in finalizing the CIP, replan the Los Alamos effort for FY92 and FY93.

WBS 1.2.6.8.4
INTEGRATED DATA SYSTEM

1, 5, 6, 17, 19

The integrated data system (IDS) supports the Exploratory Studies Facility (ESF) test program by providing a central facility to automatically measure and control aspects of the ESF tests. The primary purposes of the IDS are to assist the principal investigators (PI's) in acquiring high-quality test data in a uniform, controlled fashion and to transfer those data to the PI's organizations for data management and analysis.

ACTIVITIES AND ACCOMPLISHMENTS

This activity has been deferred.

WBS 1.2.9.1.2.4
TECHNICAL SOFTWARE MANAGEMENT

The purpose of this activity is to manage the development, implementation, and use of all software employed on activities that will support a license application; to manage the configurations of all software and computational data; and to provide tools and procedures that support these activities.

ACTIVITIES AND ACCOMPLISHMENTS

Software Engineering

A total of 51 RIDs (over 120 individual issues) were generated for the INTERFACE_TABLES application during its Software Acceptance Review. Most of these issues have now been addressed, and the application is nearly ready for resubmission to the Change Control Authority for verification of the changes.

NetCDF Version 2.0 became available; netCDF is the underlying software used for interface tables. The software was downloaded from UCAR and built on our local Ultrix and VMS workstations. The INTERFACE_TABLES application was rebuilt under the new version of netCDF, and everything works well.

The software section continued to participate in the review of software—both formal CCB-initiated reviews and informal internal reviews of various baseline components of the applications under development.

The second of our fall series of software engineering seminars, *Object Oriented Design and Its Application in Ada* by Sue Spaven of Sandia National Laboratories, took place on 20 November.

Work proceeded on the following applications:

- COMMAND-LINE PARSER—An application that will give Ada developers a standard method for defining commands and for obtaining information from the command line. Although some prototype design work had been accomplished based on a functional decomposition of the problem, the possibility of pursuing an object-oriented design was investigated. Also, additional requirements were identified for the application.
- PSEUDOCODE FORMATTER—An integral part of the DOCGEN application that will format and syntax-check pseudocode. Because the requirements are well-understood, extensive prototype design and implementation work has proceeded while awaiting CCB approval of the requirements.
- CONDITION NOTIFICATION FACILITY—A reuse component that will provide a common look to all error messages generated by an Ada application. The design baseline was submitted for review.
- EXTENDED STRING UTILITIES—A package of nearly 40 Ada utilities that permits developers to manipulate variable length strings. Work on the design baseline continued.
- EXTENDED COPY UTILITIES—A package of Ada utilities that permits developers to copy from one type of variable length string to another. Work on the design baseline continued.

During the week of 4 November, the operating systems on all three DECstations, the VAXstation, and the VAX 4000 were upgraded. Though necessary, the upgrades incurred a significant interruption of the normal work schedule.

The new Hewlett Packard 730 workstation (running at 75 MIPS) and two HP X-Window terminals were installed. Affected developers are adapting to the new environment.

We received an X-Windows product for the Macintosh called eXodus. This product was installed and configured to run X-Windows applications on DECstation (such as terminal windows, file managers, session managers, and e-mail windows) and to display them on a Macintosh, thus enabling the Macintosh to act as an X-Windows terminal. Because we often have more software developers than we have workstations, this product could prove to be quite useful.

Support of the SCM effort continued, as well as close support for developers needing to incorporate interface tables into their software.

Software Configuration Management (SCM)

During November, the SCM effort processed five baseline submissions: storing the submitted material in the Certification Environment, generating the attendant SCM documentation, performing Physical and Functional Configuration Audits on each, and generating software review packets to support Configuration Control Board review of each. The SCM effort also sanctioned two software applications and updated the Computer Program Library for each.

Two Configuration Control Board (CCB) meetings were held at which one review was approved, five change initiations were accepted, one software implementation notice was discussed, and one SCM variance was authorized.

The Configuration Manager continued work on the Software Requirements Specification for the Configuration Status Accounting Database upgrade. This upgrade will allow Los Alamos participants to interact directly with the database to generate, sign, and submit SCM forms. Concurrently with this task, an upgrade of the Computer Program Library architecture is in progress.

PLANNED ACTIVITIES

SCM will continue to manage submitted baselines and change orders; develop a Software Requirements Specification for the CSA Database upgrade; and develop a Software Requirements Specification for the Computer Program Library upgrade. Software engineering will continue the following activities: specification, design, and implementation of DOCGEN (we expect a working, mostly debugged prototype of the pseudocode formatter) and specification and design of the data dictionary portion; specification and design of the command line parser (in particular, an object-oriented design will be pursued); design and implementation of the condition notification facility; design and implementation of the extended string utilities; design and implementation of the extended copy utilities; and support the schedule-update effort for the Project Control Section. Staff will also resubmit the INTERFACE_TABLES implementation baseline.

WBS 1.2.9.1.4
RECORDS MANAGEMENT

3,6,17

The objective of this task is to manage records and documents related to the licensing of a geologic repository for the disposal of high-level radioactive waste by developing, implementing, and maintaining a comprehensive, automated, and integrated information management system.

ACTIVITIES AND ACCOMPLISHMENTS

Procurement of Commercial-Grade Items and Services, LANL-YMP-QP-04.4, R1, was issued and distributed.

The Records Processing Center rejected 9 records and accepted 64 records in November; however, records will not be transmitted to the Central Records Facility until the stop work order is lifted.

WBS 1.2.9.3
QUALITY ASSURANCE

The Quality Assurance (QA) Program supports Los Alamos Yucca Mountain Site Characterization Project participants and ensures that their efforts provide data and evidence admissible for the repository-licensing process.

ACTIVITIES AND ACCOMPLISHMENTS

Grading

Of the 32 Los Alamos grading packages being prepared, 27 are approved, 3 have been withdrawn, and 2 are in YMPO review. We have also evaluated all approved grading reports.

Document Control

Procurement of Commercial-Grade Items and Services, LANL-YMP-QP-04.4, R1, was issued and distributed.

Training

Training classes for indoctrination and QP-3.5 (scientific investigations) were held. J. March continued efforts to evaluate the Los Alamos training program through a series of interviews. Training to the new orientation class will be available in early January.

Program Development

The following quality administrative procedures (QPs) have been revised: QP-16.3 (reporting concerns), QP-4.4 (commercial-grade procurement), and QP-4.5 (noncommercial-grade procurement). Eight other procedures are in variou stages of the review cycle.

Deficiencies

Responses to corrective action requests (CARs) YMP-92-001, -002, and -003 were submitted for YMPO approval. At YMP's request, an amended response to CAR YMP-92-003 was submitted. Responses to CARs YMP-92-001 and -003 have been orally accepted.

Audits

The audit of LS-2 was completed. Audit reports LANL-AR-91-13 (University of New Mexico), LANL-AR-91-14 (Hydro Geo Chem) and LANL-AR-91-15 (LS-2) were approved and distributed. The audit report for the DOE mini-auc conducted in October (Audit Report YMP-92-01) was received. The Los Alamos audit schedule was revised and distributed.

PLANNED ACTIVITIES

Grading package revisions will continue. Uncompleted audit and survey reports will be completed, and an audit of criterion 18 will be conducted. Revisions to several QPs will continue. There will be a concerted effort to close-out an open CARs this calendar year. S. Bolivar is compiling an annual progress report of all quality-associated activities.

PROBLEM AREAS

The new QA Requirements Document will affect several QPs, and revisions will take time. Revisions to other QPs may be delayed due to personnel issues.

APPENDIX

ATTACHMENTS AND LEVEL III MILESTONE REPORTS

Molecular Models For Actinide Speciation

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Abstract

Much effort has been devoted to the development of sensitive spectroscopic techniques for the study of actinide speciation based on the sensitivity of f-f electronic absorption bands to oxidation state and ligation of the actinide ions. These efforts assume that data obtained in such studies will be interpretable in terms of changes in complexation of the metal center. However, our current understanding of 5f electronic structure is based on data from solid state doped single crystals. In these studies the local coordination geometry about the central actinide ion is maintained in an almost perfect high-symmetry environment, and will have little relevance for species in solution where deviations from perfect high symmetry tend to be the rule rather than the exception. We have developed a vigorous research program in the systematic preparation and spectroscopic characterization of synthetic actinide complexes (Th, U, Np, and Pu) in which we can control nuclearity, oxidation state, and molecular structure. These complexes have been used to determine how observable electronic transitions are perturbed in response to structural changes in the complex in solution. From the spectra obtained for these model complexes, we have found that the f-f transitions naturally fall into obvious groupings by coordination number and symmetry by which we can now differentiate between monomeric, dimeric, and trimerc species in solution.

Glossary

NMR	Nuclear Magnetic Resonance
FTIR	Fourier Transform Infrared
UV	Ultraviolet
NIR	Near Infrared
An	Actinide
OR	Alkoxide
OAr	Aryloxide
THF	Tetrahydrofuran, C_4H_8O
i-Pr	Isopropyl, $CH(CH_3)_2$
t-Bu	Tertiary butyl, $C(CH_3)_3$
Ph	Phenyl, C_6H_5
Me	Methyl, CH_3
R	Alkyl, C_nH_m
Ar	Aryl, C_6H_5
L	Ligand
dmpe	Bis(dimethylphoshino)ethane, $(CH_3)_2PCH_2CH_2P(CH_3)_2$
py	pyridine, C_5H_5N

Introduction

The study of radionuclide speciation is fundamentally important to the determination of radionuclide solubility in the ground water at Yucca Mountain. Radionuclide speciation is strictly defined as (1) the identification of the radionuclide, (2) the determination of oxidation state, and (3) the formula and molecular structure of the ionic and/or solid complex (i.e., the stoichiometry and structure of the metal ion as complexed by ions and/or other ligands). Although direct solubility measurements will provide limits for the concentrations of important radionuclides under certain specific ground water conditions, they cannot possibly provide concentration limits for all foreseeable ground water conditions. Therefore, a basic thermodynamic characterization of radionuclide speciation is needed to bridge any gaps in the data acquired from direct solubility determinations and to provide the fundamental thermodynamic constants needed for modelling solubility under conditions that are not specifically considered in the solubility determination. In the speciation study, we need to identify the important complexes of the radionuclides that may exist under conditions likely to be encountered at the proposed Yucca Mountain Repository, and determine their formation constants.

It is difficult to study many of the complex equilibria in solution directly using conventional methods because, at environmentally-relevant pH values, the concentration of many relevant actinide ions is extremely low. These experimental difficulties can be overcome in several ways. We are currently developing an approach that uses modern, ultrasensitive, laser-based spectroscopic techniques. These techniques include the absorption-based probes known as photoacoustic spectroscopy (PAS), the related method of photothermal deflection spectroscopy (PDS), and the complementary, emission-based probe known as laser-induced fluorescence (LIF) spectroscopy. Because of the extreme sensitivity of these methods, electronic spectral data can be obtained directly for solutions having site-specific characteristics.

These ultrasensitive spectroscopic techniques rely on information contained in the electronic absorption band structure of the radionuclide complexes to characterize speciation. The principal electronic transitions that give rise to these characteristic absorption bands are Laporte-forbidden f-f transitions within the manifold of 5f electronic states of an actinide complex. Although these transitions do not involve bonding electrons, the energies, intensities, and numbers of transitions in the total absorption spectrum change in a very sensitive way in response to perturbations induced by the coordination environment (i.e. the ligand field) of the radionuclide ion. Thus, different species of the same metal ions possess distinctive absorption spectra. However, because the spectral transitions are parity-forbidden, the intensities are extremely low, and molar extinction coefficients (ε) below 50 M^{-1} cm^{-1} are not uncommon. This fact, coupled with the inherent low solubility of these species under solution conditions in the ground water is the cause of a formidable experimental challenge to the characterization of speciation in these actinide systems.

Photoacoustic and photothermal deflection spectroscopies and LIF have extraordinary sensitivity. For example, it has been demonstrated that LIF can detect as few as eight molecules of a substance in solution. However, most of these measurements involve probing electronic spectroscopic transitions and, as such, the spectra are notoriously difficult to relate *a priori* to specific structural features. The spectra are quite sensitive to structure, but the relationships between spectral signatures and molecular structures must generally be established empirically. It is assumed that the data obtained with this new instrumentation, showing changes in peak positions and intensities with varying conditions, will be interpretable in terms of changes in complexation of the metal center. Most recent published work in the chemistry and chemical physics literature in condensed media focuses on actinide crystalline impurity systems. These studies are of fundamental importance but limited applicability to speciation studies because only a few systems have been successfully made and characterized. The ability to fine-tune changes in structure and ligand-field strengths has not been available in any previous solid state or solution work. Accordingly, part of our task has been to establish these spectral signatures for the actinide species extant under environmentally relevant conditions.

Spectroscopic Signatures: The Model Compound Approach

In order to establish spectroscopic signatures that are applicable to interpretation of actinide solution spectra, we need the ability to fine-tune changes in structure and ligand-field strengths. The most convenient way to achieve this fine-tuning is through synthetically-tailored actinide complexes. Therefore, we have adopted a model compound approach that exploits the versatility of synthetic actinide chemistry to enable this fine-tuning of structural and electronic effects so that a clearer correlation of molecular and electronic structure can be established. Speciation information can then be extracted from subsequent spectral data (e.g., from environmental samples) with greater likelihood of success, perhaps making it possible to obtain the fundamental molecular-level characterization required to fully understand and model actinide transport and transformation processes.

Experimental activities in this model complex investigation have been proceeding along two paths. One involves the refinement of synthetic strategies and ligand sets to make available a wide range of actinide complexes with varying structural and electronic perturbations. The second is acquisition and interpretation of the electronic spectral data for these synthetically-tailored model complexes. The synthetic work has focused on alkoxide (OR^-) and alkylcarbonate (O_2COR^-) ligands. These ligands are ideal structural and electronic analogs of hydroxide (OH^-) and carbonate (O_2CO^{2-}) or bicarbonate (O_2COH^-) ligands; three ubiquitous ligands in the aqueous systems relevant to Yucca Mountain. Therefore, these synthetically-prepared complexes of the actinides should be directly related to actual environmental actinide species, both structurally and spectroscopically. The advantage afforded by the synthetic model complexes is that they provide unambiguous structures of a single species under well-controlled conditions, and can be readily characterized by a suite of spectroscopic techniques. We have utilized pulse NMR, Raman, and FTIR for the characterization of molecular speciation and structure of the complexes in solution, and single crystal X-ray diffraction for unambiguous structural characterization of solids when applicable.

The relationship between hydroxide/alkoxide and bicarbonate/alkylcarbonate ligands is illustrated qualitatively below in Figure 1. It can be seen from this figure that

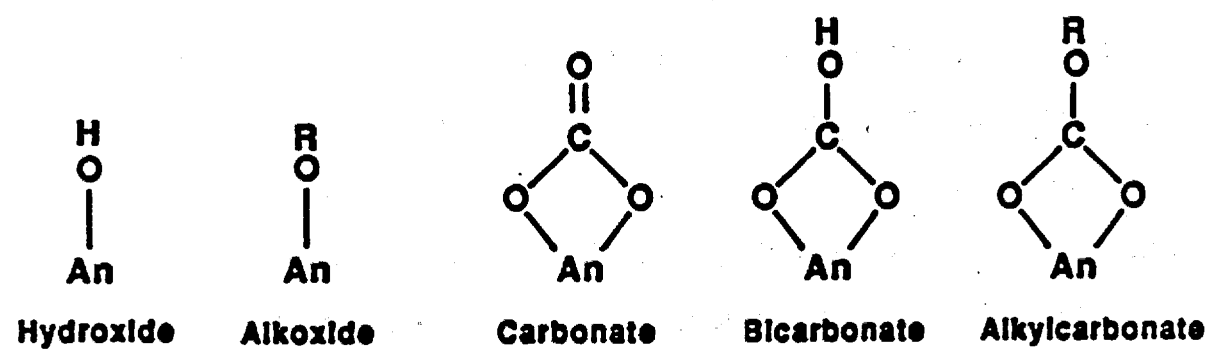


Figure 1. A comparison of actinide alkoxide and hydroxide ligands (left) and actinide carbonate, bicarbonate and alkylcarbonate ligands (right).

the hydroxide ligand is the simplest member of a large series of ligands known as alkoxides, and as such, the alkoxide ligand should serve as an ideal model for the effects of hydroxide ligation on f-element electronic structure. In a similar fashion, it can be seen from Figure 1 that the bicarbonate ligand is a simple prototype of a large series of ligands known as alkylcarbonates. Thus alkylcarbonates should serve as ideal models for the effects on carbonate/bicarbonate ligation on f-element electronic structure. A major advantage afforded by alkoxide and alkycarbonate ligands is that, by simply varying the R group, tremendous versatility is achieved in controlling the nuclearity, structure, oxidation state, and inductive electronic effects in actinide complexes. This, in turn, will have important implications in the interpretation of electronic spectroscopic data for actinide species under environmentally-relevant conditions.

The electronic structure determinations for these model compounds have been derived principally from UV-visible-near-IR electronic absorption or emission data. Attention has been devoted to understanding how the observable electronic transitions are perturbed in response to structural changes in the complexes. Additional experimental strategies will be implemented as required to clarify electronic band assignments and enhance the quality of the data. These include using low temperature glasses or doped single crystals to improve spectral resolution, and implementation of magnetic perturbations, polarization techniques, and multiphoton spectroscopies to manipulate selection rules so that detailed assignments become possible. An iterative process is evolving between spectroscopic and synthetic efforts in which new synthetic strategies will be driven by the need to tune specific spectroscopic perturbations.

It should be stressed that this model complex work is not quality effecting in any way. This work will establish the fundamental baseline spectroscopic signatures that will be used as intrepretive aids in the speciation studies of actinide ions under conditions relevant to the proposed Yucca Mountain Repository. Therefore, we have made use of known actinide alkoxide structures present in the literature, as well as new complexes developed in our laboratory. Our original experimental work has focused on thorium and uranium compounds due to the ease of handling and hence rapidity of experimental procedures. The similarity that we have observed in the chemistry of thorium and uranium is excellent evidence that our preparative strategies will work well for neptunium and plutonium complexes. Much of the spectroscopic data on uranium complexes has been collected by a collaborator, Dr. John M. Berg, a Director's Funded post doctoral fellow. Dr. Berg's collaboration in this effort has been invaluable, and his feedback on how structural perturbations affect spectroscopic band shifts has allowed us to move quickly through the pre-screening process. From these preliminary data it is clear that small structural perturbations on the synthetic compounds give rise to fairly large spectroscopic perturbations, and it appears that we are now able to identify monomeric, dimeric and trimeric uranium (IV) species in solution.

Synthesis and Characterization of Actinide Alkoxide Complexes.

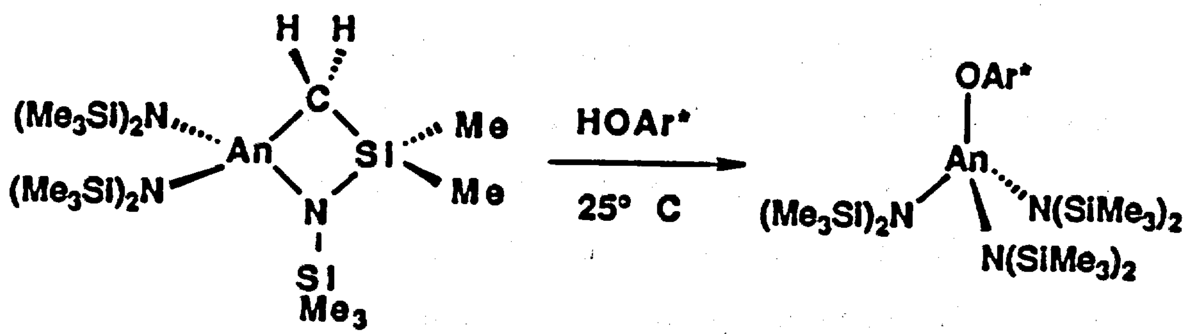
Alkoxide complexes of the actinides were first reported in the mid 1950's, during the search for volatile complexes for uranium isotope separation.[1] Much of the early work on these complexes is due to the pioneering efforts of Don Bradley whose group prepared an extensive series of tetravalent actinide alkoxides of empirical formula $An(OR)_4$ (An = Th, U).[2] Over the last decade, much new information on compounds of this type has emerged, and these new results have cleared up many earlier misinterpretations of the exact nature of these compounds in solution and in the solid state.[1c]

Our entry into compounds of this class has come about principally as a result of the discovery of large-scale synthetic routes to soluble Lewis base adducts of uranium and thorium.[3,4] We have employed these starting materials on a routine basis for the preparation of new and known tetravalent actinide alkoxide complexes.

Tetravalent Aryloxide Complexes

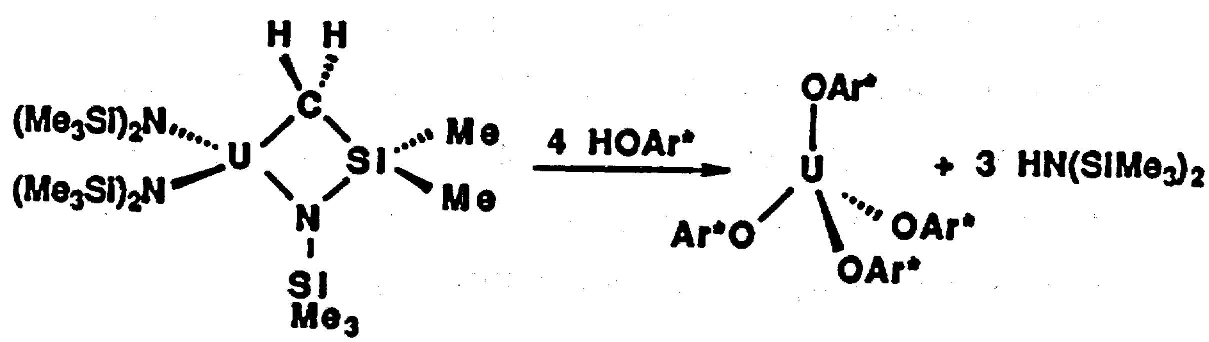
Monomeric uranium(IV) and thorium(IV) aryloxide complexes, $An(OAr)_4$, have been sought for some time. The first members of this class were prepared by Lappert and coworkers.[5] Metathesis reactions of thorium or uranium tetrachloride with lithium aryloxides gave "double alkoxide" salts, $[Li(THF)_4][An(O\text{-}2,6\text{-}i\text{-}Pr_2C_6H_3)_5]$, or incomplete metathesis products such as $AnCl(O\text{-}2,4,6\text{-}t\text{-}Bu_3C_6H_2)_3$ (An = Th, U) in good yields. In the latter case, an excess of lithium aryloxide failed to provide the homoleptic thorium complex of general formula $Th(OAr)_4$. A blue homoleptic thorium aryloxide, $Th(O\text{-}2,6\text{-}Ph_2C_6H_3)_4$, obtained from the reaction of the tetrachloride with 4 equivalents of $LiO\text{-}2,6\text{-}Ph_2C_6H_3$ in THF solution, has also been described, but no structural data was presented.

Lappert and coworkers have also examined the alcoholysis reactions of $[U(NEt_2)_4]_2$ with excess phenol. These reactions were unsuccessful vis-á-vis the preparation of $U(O\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3)_4$; only $U(NEt_2)(O\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3)_3$ could be isolated. This reaction has recently been repeated, and it was found that even in refluxing toluene, the fourth diethylamide ligand is not susceptible to alcoholysis.[6] Several years ago, Dormond *et al.*[7] described the reactions of the uranium(IV) metallacycle $[\{(Me_3Si)_2N\}_2\overline{U(CH_2SiMe_2N}SiMe_3)]$ [8] with both HO-t-Bu and HO-2,6-$Me_2C_6H_3$. They observed rapid protonation of the uranium carbon bond and isolated two complexes of general formula $U(OR)[N(SiMe_3)_2]_3$. They also noted that cleavage of uranium-nitrogen bonds occurred but was not competitive with attack on the metal-carbon bond. In agreement with Dormond *et al.*, we observed that the reaction of one equivalent of $HO\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3$ with $[\{(Me_3Si)_2N\}_2\overline{An(CH_2SiMe_2N}SiMe_3)]$ (An = Th, U) in hexane at room temperature for 1 hr. provides orange (An = U)[6] or colorless (An = Th)[9] $An(O\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3)[N(SiMe_3)_2]_3$ in essentially quantitative yield as shown in equation 1. These compounds have been characterized by elemental analyses and ^1H NMR. The room temperature ^1H NMR spectrum of the uranium complex shows non-equivalent silylamide ligands indicative of restricted rotation about the U—O and/or U—N bonds.[6] Similar behavior is not observed for the thorium complex, and may reflect the greater size of the Th(IV) center.[9]

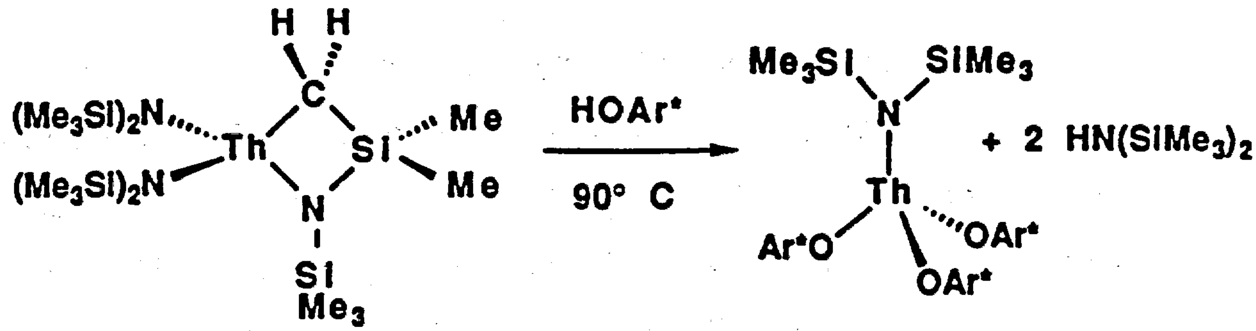
(1) 

An = Th, U; Ar* = 2,6-t-$Bu_2C_6H_3$, 2,6-$Me_2C_6H_3$

For the uranium metallacycle, reaction with slightly greater than 4 equivalents of HO-2,6-t-$Bu_2C_6H_3$ in toluene at 100°C for 6 hr provides, after solvent removal and recrystallization, orange, crystalline $U(OAr)_4$ in 80% yield according to equation 2.[6] However, the analogous reaction for thorium fails to give the homoleptic thorium aryloxide product, even after prolonged (36 hr) reflux with excess disubstituted phenol.[9] The incomplete substitution product Th[(N($SiMe_3)_2$][O-2,6-t-$Bu_2C_6H_3]_3$ can be isolated in *ca.* 80% yield as outlined in equation 3.[9]

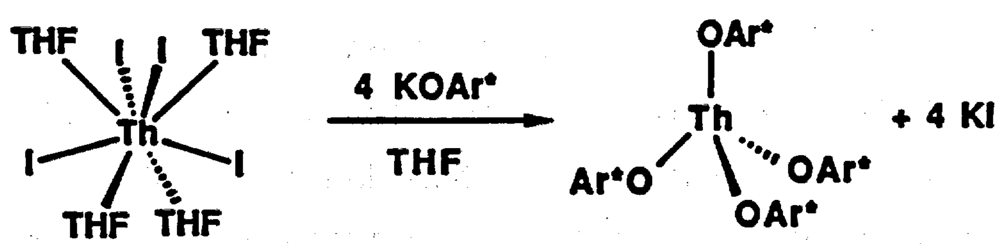
(2) 

Ar* = 2,6-t-$Bu_2C_6H_3$

(3) 

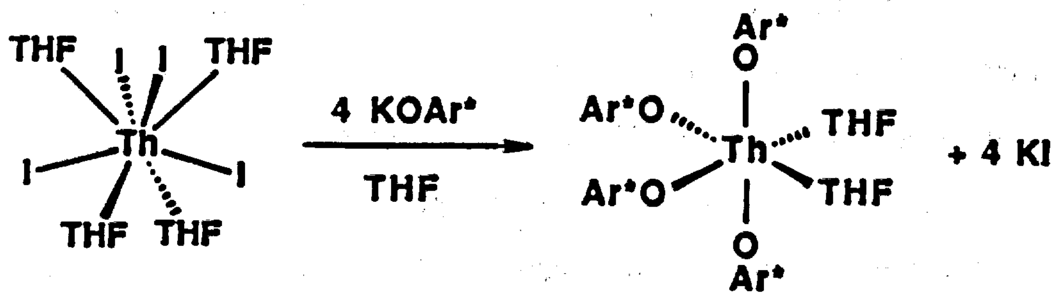
Ar* = 2,6-t-$Bu_2C_6H_3$

Upon decreasing the steric bulk of the substituted phenol HO-2,6-$R_2C_6H_3$ (R = i-Pr, Me), the alcoholysis proceeds smoothly to give the homoleptic $Th(OAr)_4$ complexes as shown (Eq. 2) for uranium. Our inability to prepare the homoleptic Th(O-2,6-t-$Bu_2C_6H_3)_4$ complex *via* this simple protonolysis reaction cannot be due to the steric requirements of the resulting $Th(OAr)_4$ compound, since the reaction of $ThI_4(THF)_4$ with four equivalents of potassium 2,6-di-*tert*-butylphenoxide in THF solution results in the formation of Th(O-2,6-t-$Bu_2C_6H_3)_4$, in *ca.* 90% isolated yield according to Equation 4.[9] In these reactions, the formation of insoluble KI may act as a driving force, and we observe complete metathesis of iodide ligands, and no formation of "ate" complexes. It is noteworthy that while this reaction is conducted in THF solution, the experimental workup procedures yield Th(O-2,6-t-$Bu_2C_6H_3)_4$ as a base-free complex, presumably due to the steric demands of the bulky 2,6-di-*tert*-butylphenoxide ligand.

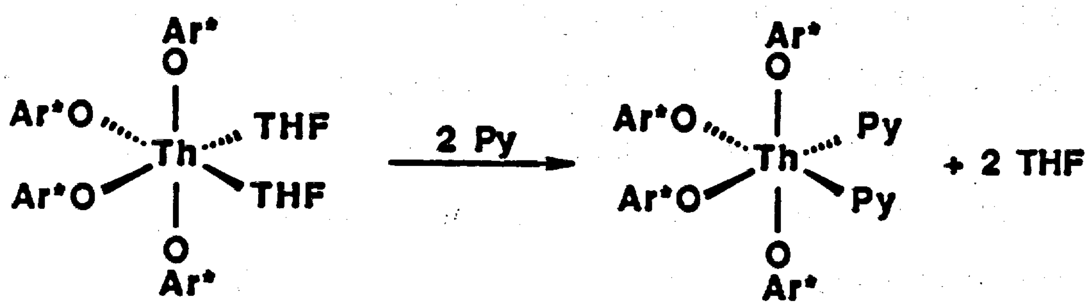
(4) 

Ar* = 2,6-t-$Bu_2C_6H_3$

For less sterically-demanding aryloxide ligands, the reaction of $ThI_4(THF)_4$ with four equivalents of KO-2,6-$R_2C_6H_3$ (R = i-Pr or Me) in THF solution results in the formation of bis-THF adducts Th(O-2,6-$R_2C_6H_3)_4(THF)_2$ in *ca.* 60 - 70% yield according to equation 5. The THF adducts readily exchange with other Lewis bases such as pyridine to give Th(O-2,6-$Me_2C_6H_3)_4(L)_2$ complexes according to equation 6. We note that Andersen has isolated and structurally characterized a related phosphine adduct of formula $Th(OPh)_4(dmpe)_2$.[10]

(5) 

OAr* = 2,6-$R_2C_6H_3$ where R = i-Pr, Me

(6) 

OAr* = 2,6-$R_2C_6H_3$ where R = i-Pr, Me

Single crystal X-ray structures have been determined for both the uranium[6] and thorium[9] An(O-2,6-t-$Bu_2C_6H_3)_4$ complexes. The compounds are isostructural and possess crystallographic $\bar{4}$ (S_4) symmetry. A view of the basic molecular structure emphasizing the S_4 symmetry is shown in Figure 2. Both sets of four An-O bond lengths are identical (2.189(6) Å, Th; and 2.135(4)Å, U), and the O-An-O angles are of two types, four of 110.46(15)° (An = Th) and two of 107.5(3)° (An = Th); the latter angles are those bisected by the C_2 (S_4) axis, and correspond to a slight flattening of the central AnO_4 core from T_d to D_{2d} symmetry. Other parameters show a strong similarity between the two structures. The structural similarity between thorium and uranium compounds leaves little doubt that we will be able to prepare the neptunium and plutonium analogues following the strategy outlined in equations 2 or 4.

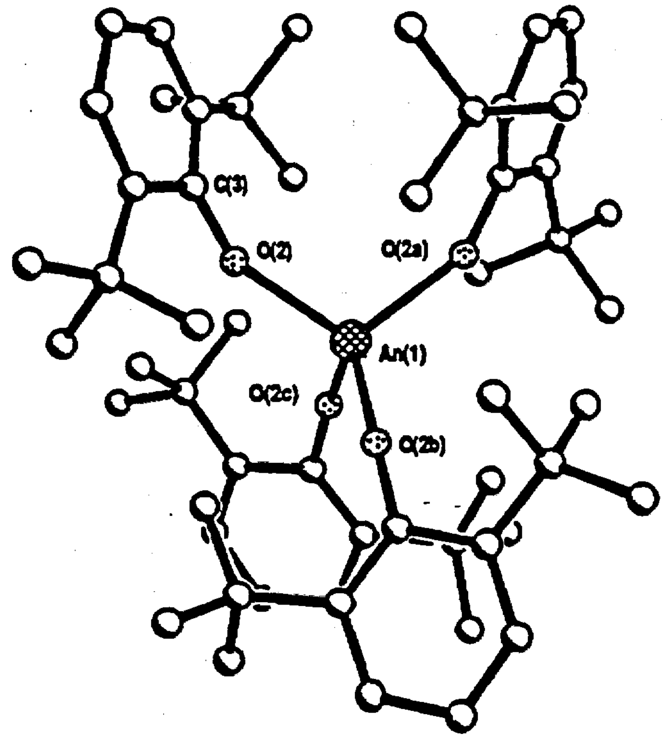


Figure 2. A drawing of the crystal structure of $An(O\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3)_4$ viewed perpendicular to the S_4 axis, emphasizing S_4 symmetry. Important bond distances [Å] and angles [°]: (An = Th) Th(1)-O(2) 2.189(6), Th(1)-O(2)-C(3) 153.5(10), O(2)-Th(1)-O(2b) 110.46(15), O(2)-Th(1)-O(2a) 107.5(3). (An = U) U(1)-O(2) 2.135(4), U(1)-O(2)-C(3) 154.0(6), O(2)-U(1)-O(2b) 110.2(1), O(2)-U(1)-O(2a) 108.0(2).

The low temperature (185K) solution ^1H NMR spectra of $An(O\text{-}2,6\text{-}t\text{-}Bu_2C_6H_3)_4$ complexes reveal chemically-inequivalent t-Bu and *meta* proton resonances, yet a single *para* proton resonance for the 2,6-di-*tert*-butylphenoxide ligand. This is indicative of S_4 symmetry in solution at low temperature in agreement with expectations based on the solid state structures. Upon raising the temperature, the *para* proton remains a sharp triplet, while the t-Bu and *meta* proton (doublet) resonances coalesce into single sharp resonances with average chemical shift values consistent with rapid rotation about An-O or O-C bonds ($\Delta G^{\ddagger} = 11.6 \pm 0.1$ kcal mol^{-1}, An = Th).[9] This variable temperature behavior is shown in Figure 3 for the t-Bu resonances of the thorium complex, and illustrates the usefulness of variable temperature NMR for determination of actinide speciation in solution. While the NMR serves as confirmation of molecular structure for these well-characterized model compounds in solution, it can serve as a structure determination tool (and hence speciation tool) for uncharacterized actinide complexes in solution.

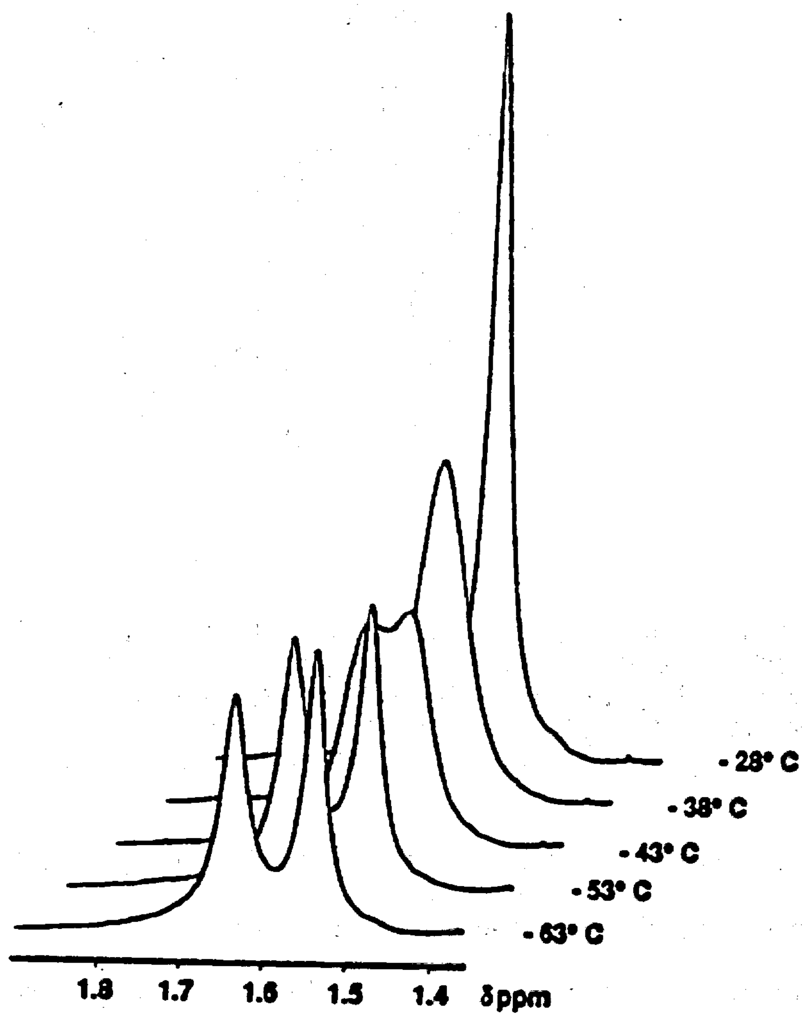


Figure 3. ^1H NMR spectra showing the variable temperature behavior of the t-Bu resonances for $Th(O\text{-}2,6\text{-}Me_2C_6H_3)_4$. The limiting spectrum obtained at -63° C is consistent with S_4 symmetry as observed in the solid state molecular structure.

A single crystal X-ray structure of the pyridine adduct $Th(O\text{-}2,6\text{-}Me_2C_6H_3)_4py_2$ displays a psuedo-octahedral geometry about the central thorium atom with the two pyridine ligands occupying *cis* positions on the octahedron (Figure 4).[9] The Th-N distances average 2.679 Å. Two different Th-O bond lengths are seen in the molecule; 2.186 Å (ave) for the aryloxide ligands *trans* to pyridine and 2.209 Å (ave) for aryloxide ligands *trans* to one another. These Th-O distances are in the same range as seen in the solid state structure of $Th(OAr)_4$ and both display relatively large Th-O-C angles. The aryloxide ligands *trans* to pyridine display the shorter Th-O distances, and exhibit the greater Th-O-C angles of 176.0° (ave), while those *trans* to one another are found to have slightly longer Th-O distances and smaller Th-O-C angles of 170.6° (ave).

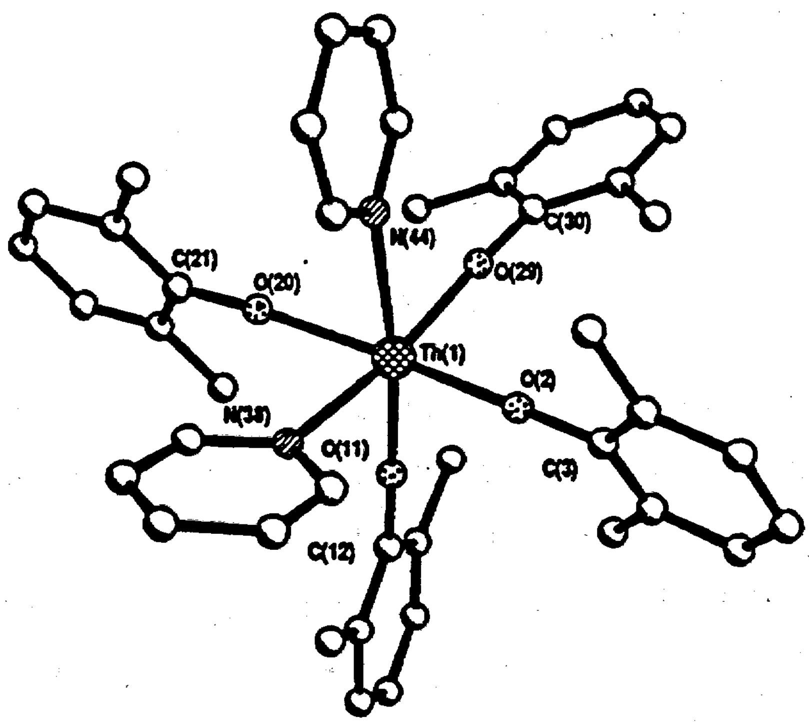
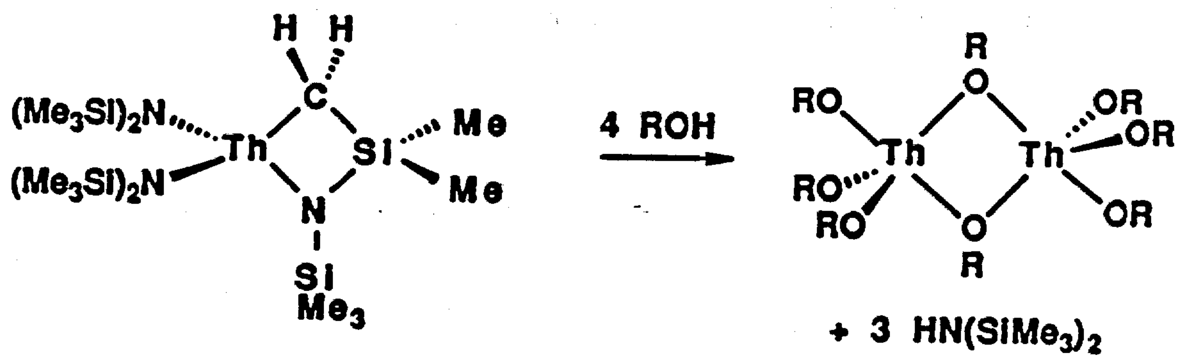


Figure 4. A drawing of the crystal structure of $Th(O\text{-}2,6\text{-}Me_2C_6H_3)_4(py)_2$ emphasizing the *cis* psuedo-octahedral symmetry. Important bond distances [Å] and angles [°]: Th(1)-O(2) 2.211(6), Th(1)-O(20) 2.206(6), Th(1)-O(11) 2.188(6), Th(1)-O(29) 2.183(6), Th(1)-N(38) 2.662(8), Th(1)-N(44) 2.696(8), Th(1)-O(2)-C(3) 169.1(7), Th(1)-O(20)-C(21) 172.0(6), Th(1)-O(11)-C(12) 175.8(6), Th(1)-O(29)-C(30) 176.2(6), N(38)-Th(1)-N(44) 78.40(24), O(2)-Th(1)-O(11) 94.37(24), O(2)-Th(1)-O(29) 93.76(23), O(11)-Th(1)-O(20) 94.99(24)

Aliphatic Alkoxide Complexes

A number of homoleptic actinide alkoxide complexes of composition $An(OR)_4$ (An = Th, U; R = Me, Et, i-Pr, n-Pr, n-Bu etc.) have been reported previously,[2] but their characterization has been limited to elemental analysis and solution molecular weight determination. We have discovered that treatment of the thorium metallacycle $[\{(Me_3Si)_2N\}_2\overline{Th(CH_2SiMe_2N}SiMe_3)]$[8] with four equivalents of either di-*iso*-propylmethanol or dimethyl-*tert*-butylsilanol in hexane at room temperature yields colorless crystals of $[Th(OR)_4]_2$ (R = $CH\text{-}i\text{-}Pr_2$, $SiMe_2\text{-}t\text{-}Bu$) in good yield according to equation 7.

(7)

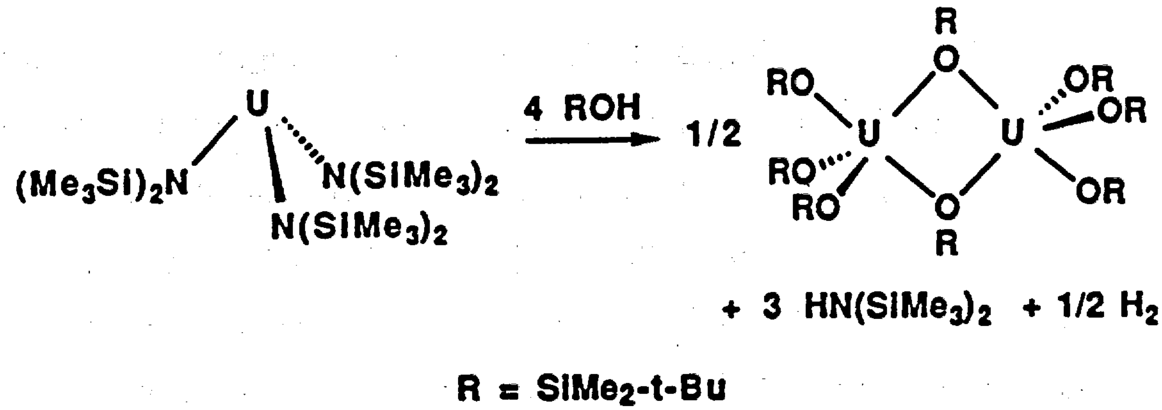


R = $CH\text{-}i\text{-}Pr_2$, $SiMe_2\text{-}t\text{-}Bu$

A similar dimeric compound has been prepared for uranium, although by a somewhat different synthetic route. Alcoholysis of $U[N(SiMe_3)_2]_3$ [11] with $HOSiMe_2\text{-}t\text{-}Bu$ leads to oxidation of the uranium(III) center and isolation of a uranium(IV) product of formula $U_2(OSiMe_2\text{-}t\text{-}Bu)_8$.[12] In order to account for oxidation of uranium(III) to uranium(IV), it is assumed that hydrogen is evolved in the reaction (Eq. 8); work is in progress to resolve this question.[12]

Single crystal X-ray structures have been determined for both $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ and $U_2(OSiMe_2\text{-}t\text{-}Bu)_8$. The structure of $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ is shown in Figure 5.[9] The compound crystallizes in the monoclinic space group $P2_1/n$ with two molecules per unit cell which reside on centers of inversion. Each thorium atom adopts a distorted

(8)



trigonal bipyramidal geometry, and the Th_2O_8 core can be viewed as two ThO_5 trigonal bipyramids joined along a common axial-equatorial edge. The three equatorial bonds are distorted from the ideal (120°) trigonal angles, the actual values

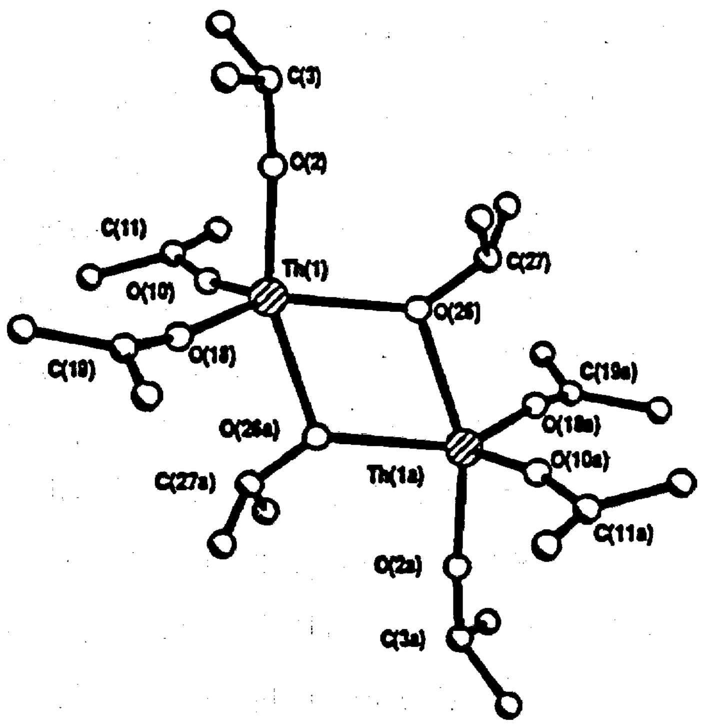


Figure 5. A view of the molecular structure of $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ emphasizing the fused trigonal bipyramidal coordination geometry. Methyl carbons of the $OCH(CHMe_2)_2$ ligands are omitted for clarity. Important bond lengths [Å] and angles [°]: Th(1)-O(2) 2.160(11), Th(1)-O(10) 2.141(11), Th(1)-O(18) 2.161(11), Th(1)-O(26) 2.408(10), Th(1)-O(26a) 2.463(11); O(2)-Th(1)-O(10) 98.2(4), O(2)-Th(1)-O(18) 94.8(5), O(2)-Th(1)-O(26) 93.9(4), O(2)-Th(1)-O(26a) 158.2(4), O(10)-Th(1)-O(18) 111.8(4), O(10)-Th(1)-O(26) 116.2(4), O(10)-Th(1)-O(26a) 98.7(4), O(18)-Th(1)-O(26) 129.2(4), O(18)-Th(1)-O(26a) 91.7(4), Th(1)-O(26)-Th(1a) 113.8(4), O(26)-Th(1)-O(26a) 66.2(4).

being 129.2(4), 111.8(4), and 116.2(4); the deviation of the trigonal ThO_3 unit from planarity is 2.8 degrees. The axial O-Th-O unit is distorted (158.2°) from the idealized 180°, and may be due to steric demands of the bridging alkoxide unit. Terminal Th-O distances are rather short at 2.154 Å (ave), and virtually identical to the Th-O distance (2.154(8) Å) observed for the 2-butene-2,3-diolate ligand in the X-ray structure of $[\{(\eta^5\text{-}C_5Me_5)_2Th(\mu\text{-}O_2C_2Me_2)\}_2]$.[13] The corresponding Th-O-C angles are large, and range from 167.4 - 171.5°.

The structure of $U_2(OSiMe_2\text{-t-Bu})_8$ is similar to that seen for $Th_2(OCH\text{-i-Pr}_2)_8$, and is shown in Figure 6.[12] Each uranium atom adopts a distorted trigonal bipyramidal coordination geometry, and the U_2O_8 core can be viewed as two UO_5 trigonal bipyramids joined along a common axial-equatorial edge. The molecule is distorted relative to $Th_2(OCH\text{-i-Pr}_2)_8$, with the distortion arising from a puckering in the $U_2(\mu\text{-}O)_2$ bridge, presumably due to steric interactions of the bulky $OSiMe_2$-t-Bu ligands. From Figure 6 the local trigonal bipyramidal coordination environment around each uranium atom can readily be seen. For U(1), oxygen atoms O(3) and O(43) occupy apical positions, while O(11), O(59) and O(51) lie in the equatorial plane. The three equatorial bonds are distorted from the ideal (120°) trigonal angles, the actual values being 129.4, 120.6, and 107.9; the deviation of the trigonal UO_3 unit from planarity is 2.1 degrees. The axial O(3)-U(1)-O(43) unit is distorted (162.2°) from the ideal 180°, again probably a result of steric interactions with the bridge. In a similar fashion, O(35)-U(2)-O(11) make up the principal (axial) axis, while O(27), O(19), and O(3) lie in the trigonal plane. The two trigonal bipyramids are joined through the agency of bridging alkoxide ligands with an average U-O distance of 2.401Å; the terminal U-O bonds average 2.118Å. The terminal U-O-Si angles are rather large, ranging from 156.8 - 174.3° with an average value of 165.2°.

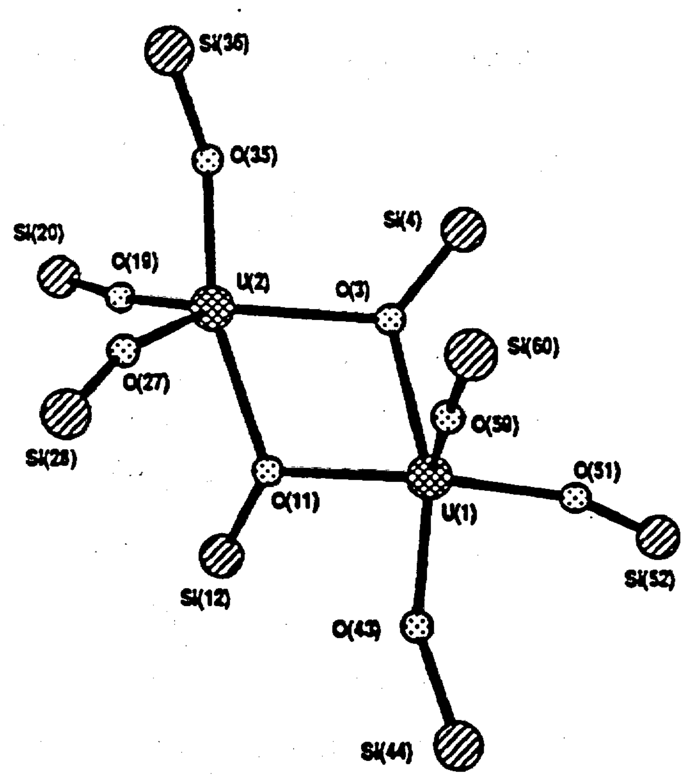
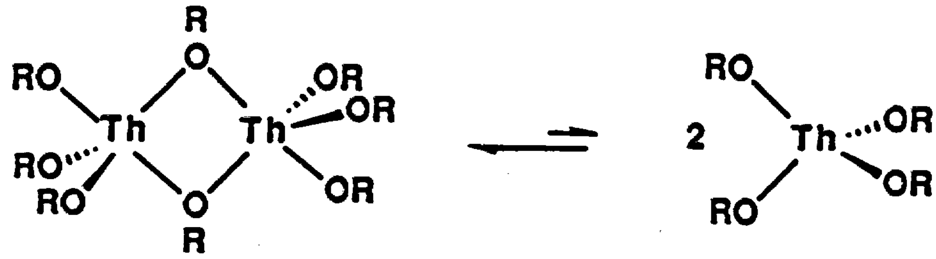


Figure 6. A view of the molecular structure of $U_2(OSiMe_2\text{-t-Bu})_8$ (from reference 12) emphasizing the fused trigonal bipyramidal coordination geometry. Carbon atoms of the $OSiMe_2$-t-Bu ligands are omitted for clarity. Important bond lengths [Å] and angles [°]: U(1) - U(2) 3.819(2), U(1)-O(3) 2.372(17), U(1)-O(11) 2.401(17), U(1)-O(43) 2.106(18), U(1)-O(51) 2.166(19), U(1)-O(59) 2.101(18), O(3)-U(1)-O(43) 162.2(6), O(3)-U(1)-O(51) 102.5(7), O(3)-U(1)-O(59) 88.7(7), . O(11)-U(1)-O(43) 95.4(6), O(11)-U(1)-O(51) 134.3(7), O(11)-U(1)-O(59) 116.6(7).

In solution, ^1H NMR spectroscopy reveals only one ligand environment for the $OSiMe_2$-t-Bu ligands in the $An_2(OSiMe_2\text{-t-Bu})_8$ compounds (An = Th, U) indicative of rapid bridge-terminal site exchange on the NMR time-scale. In contrast, room temperature ^1H NMR spectra of $Th_2(OCH\text{-i-Pr}_2)_8$ reveal resonances consistent with two species present in solution, and suggest an equilibrium between monomeric $[Th(OCH\text{-i-Pr}_2)_4]$, and its dimer $[Th(OCH\text{-i-Pr}_2)_4]_2$ as shown in equation 9.[9] The important features (of the methine regions) of the ^1H NMR spectrum are shown in Figure 7.[9] There is one set of broadened methine resonances (indicated by numeral 1

(9) 

$R = CH\text{-}i\text{-}Pr_2$

in Figure 7) consistent with only one type of alkoxide ligand, suggesting a rapid bridge-terminal exchange process for $Th_2(OCH\text{-}i\text{-}Pr_2)_8$. A smaller, sharp set of resonances, indicative of a single alkoxide environment, is also present (labeled as numeral 2 in Figure 7). Integrated intensities of *ca.* 9:1 preclude any assignment of these resonances to $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ alone. Upon heating the solution, the resonances assignable to $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ (1) diminish and those assigned to $Th(OCH\text{-}i\text{-}Pr_2)_4$ (2) increase, and at +60° C, the monomer predominates in solution (Figure 7). Upon cooling, the resonances of the dimer reappear rapidly, implying a low barrier to dimerization (Eq. 9). Low temperature ^1H NMR spectra show a further increase in the concentration of dimer (1) relative to monomer (2) as expected for an equilibrium mixture. In addition, those NMR resonances assignable to the dimer (1) broaden, and split out into two separate resonances in a 3:1 ratio consistent with maintenance of the dimeric structure in solution.

The observation of the dynamic equilibrium in solution is particularly exciting in terms of spectroscopic signatures. We are presently working on preparation of the corresponding uranium system, since it's electronic spectrum will provide a unique opportunity to measure, and deconvolute an equilibrium mixture in which we know the molecular structure of both equilibrium components.

The addition of an excess of pyridine or THF to solutions of $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ results in the formation of monomeric Lewis base adducts $Th(OCH\text{-}i\text{-}Pr_2)_4L_2$ (L = py or THF), which may be isolated as colorless crystals in good yield.[9] We assume that

Lewis bases react with monomeric $Th(OCH\text{-}i\text{-}Pr_2)_4$, shifting the equilibrium until all the dimer is consumed (Eq. 9).

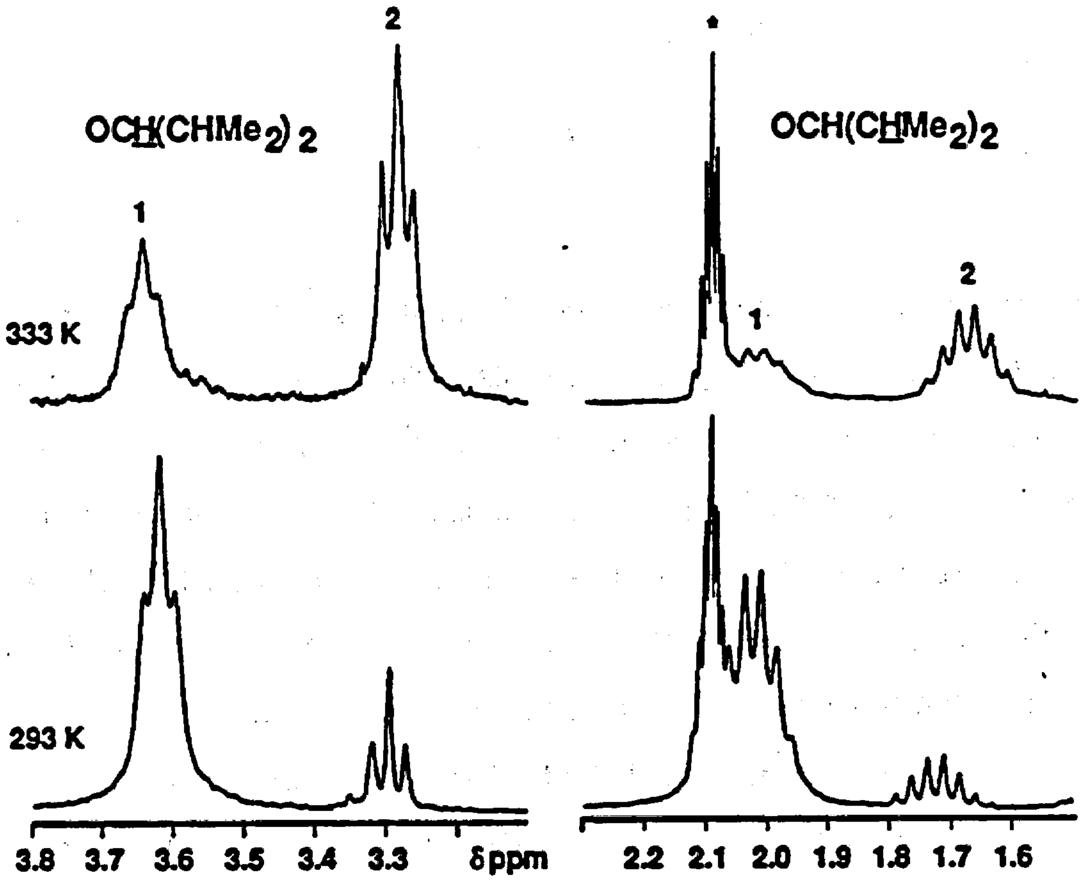
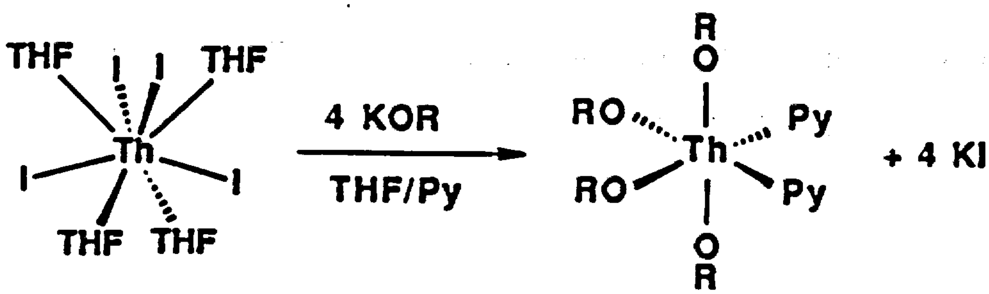


Figure 7. [1]H NMR spectra of the methine region of a mixture of $Th_2(OCH\text{-}i\text{-}Pr_2)_8$ (1) and $Th(OCH\text{-}i\text{-}Pr_2)_4$ (2) at 293K (bottom) and 333K (top). Left and right spectra not to scale. The resonance marked with an asterisk denotes the [1]H impurity in toluene-d_8. Methine resonances assigned to 1 and 2 are labeled.

Lewis base adducts of general formula $Th(OR)_4py_2$ may also be prepared directly by the addition of four equivalents of potassium alkoxide to $ThX_4(THF)_4$ (X = Br, I)[4] in THF or THF/pyridine, followed by crystallization as indicated in equation 10.[9]

For example, reaction of the tetrahydrofuran adduct of thorium tetraiodide with four equivalents of potassium *tert*-butoxide in the presence of pyridine leads to the isolation of $Th(O\text{-}t\text{-}Bu)_4(py)_2$. A single crystal X-ray diffraction study on $Th(O\text{-}t\text{-}Bu)_4(py)_2$ revealed a psuedo-octahedral geometry about the central thorium atom with

(10) 

R = t-Bu, CH-i-Pr$_2$

the two pyridine ligands occupying *cis* positions. The molecular structure of Th(O-t-Bu)$_4$(py)$_2$ is shown in Figure 8. Like its aryloxide analogue, two significantly different Th - O bond lengths are seen in the molecule; 2.16 Å for the *tert*-butoxide ligands *trans* to pyridine, and 2.20 Å for the *tert*-butoxide ligands *trans* to one another. The two pyridine ligands exhibit a thorium - nitrogen distance of 2.76 Å. The relatively large Th - O - C angles are indicative of a significant degree of π-donation from oxygen lone pairs to the thorium metal center, and are dependent on the *trans* influence and π-donor properties of the *trans* ligand. Thus the *tert*-butoxide ligands *trans* to pyridine (which has a relatively weak *trans* influence) exhibit Th - O - C angles of 172° while those *trans* to one another are found to have smaller Th - O - C angles of 163°.

Room-temperature ^{1}H NMR spectra reveal only one type of alkoxide ligand for Th(OR)$_4$py$_2$, presumably due to a dynamic exchange process in solution. The dynamic exchange is so facile that low temperature NMR spectroscopy is unable to freeze out a limiting structure, even at -185 K. We note the isolation, by Bradley *et al.*, of the complex Th(OCMe$_2$CCl$_3$)$_4$py$_2$,[2e] although no mention was made of the stereochemistry of the molecule, and the preparation by Andersen and co-workers of the related uranium species U{OCH(CF$_3$)$_2$}$_4$(THF)$_2$,[17] U{OC(CF$_3$)$_3$}$_4$(THF)$_2$[17] and U(OCH -t-Bu$_2$)$_4$.[18]

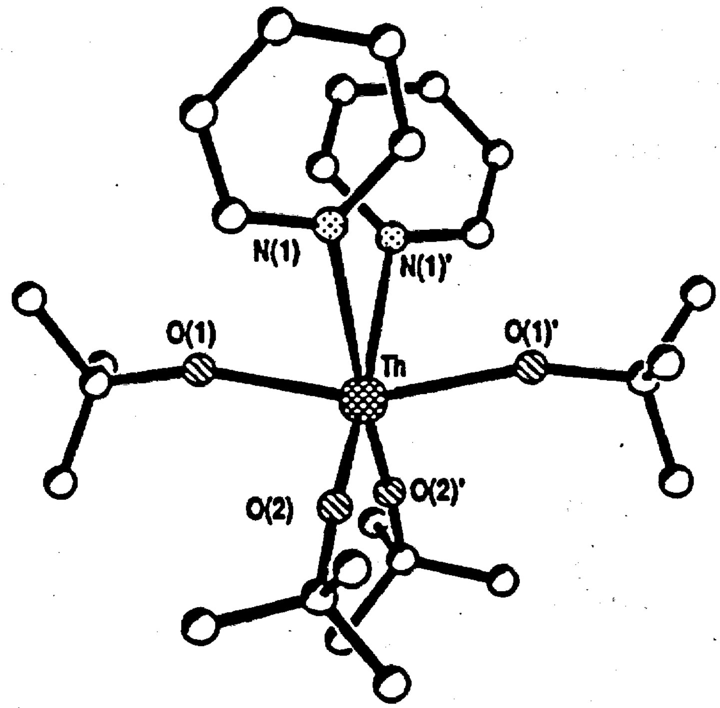
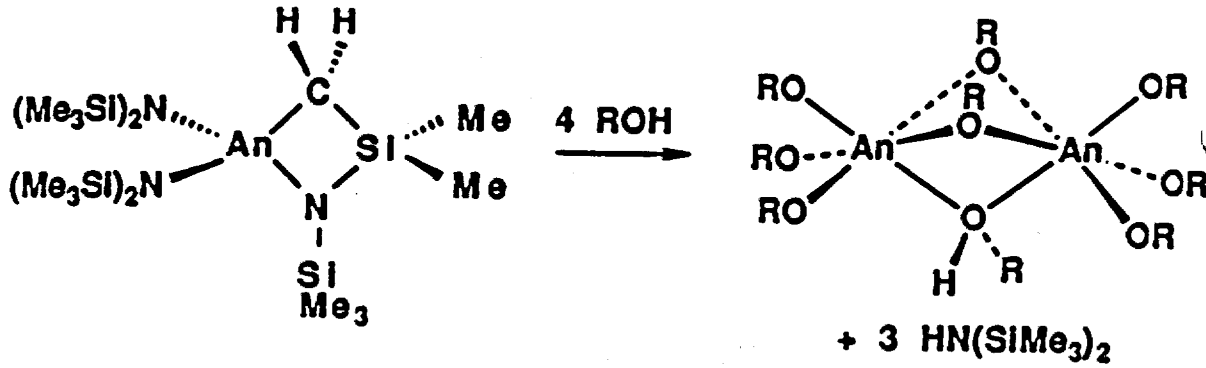
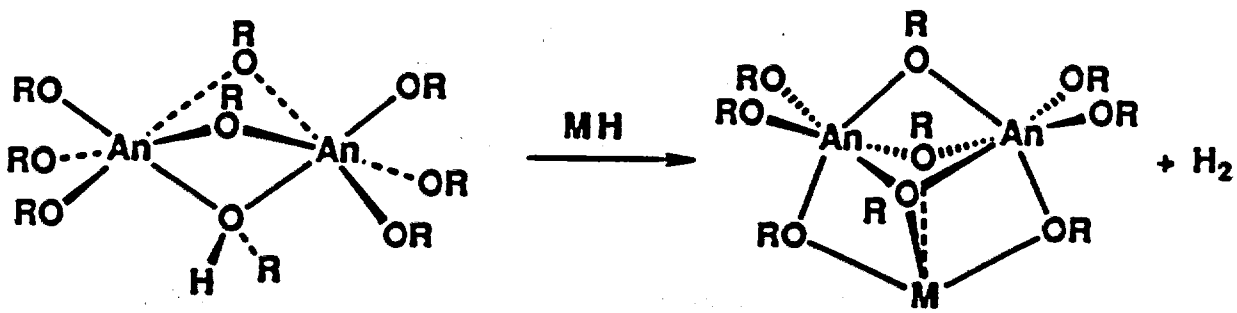


Figure 8. A drawing of the molecular structure of $Th(O\text{-}t\text{-}Bu)_4(py)_2$ emphasizing the cis pseudo-octahedral symmetry about the central thorium atom. Important bond distances [Å] and angles [°]: Th(1)-O(1) 2.194(6), Th(1)-O(2) 2.157(6), Th(1)-N(1) 2.753(8), Th(1)-O(1)-C(1) 163,0(7), Th(1)-O(2)-C(5) 172.1(6)

Treatment of the metallacyclic species $[\{(Me_3Si)_2N\}_2\overline{An(CH_2SiMe_2N}SiMe_3)]$ with four equivalents of *tert*-butanol in toluene at room temperature produces the dimeric alcoholate formulated as $An_2(O\text{-}t\text{-}Bu)_8(HO\text{-}t\text{-}Bu)$ for both An = Th[9] and U.[12] as outlined in equation 11. The compound is formulated as $An_2(O\text{-}t\text{-}Bu)_8(HO\text{-}t\text{-}Bu)$ based on elemental analyses, solution NMR, IR, and UV-visible-NIR spesctroscopy. The combined data are all consistent with a fused confacial bioctahedral coordination geometry as illustrated in equation 11. Deprotonation of the alcoholate complex with alkali metal hydride or alkoxide generates the corresponding alkali metal salt $M'An_2(O\text{-}t\text{-}Bu)_9$ where An = Th and M' = Na,[9] or An = U, and M' = K[14] as shown in equation 12.

(11) 

An = U, Th; R = t-Bu

(12) 

An = U, M' = K; An = Th, M' = Na; R = t-Bu

Solution ^{1}H NMR data displayed four types of alkoxide ligands in a 4:2:2:1 ratio consistent with a static confacial bioctahedral $Th_2(O\text{-}t\text{-}Bu)_9^-$ anion bridged by a sodium cation as illustrated in equation 12. This structural hypothesis was confirmed by a single-crystal X-ray structure determination on $NaTh_2(O\text{-}t\text{-}Bu)_9$, and a view of the solid state structure is shown in Figure 9. Thorium - oxygen bond lengths are found to be 2.15 and 2.23 Å for the terminal *tert*-butoxide ligands, and 2.48 Å (average) for the bridging alkoxide ligands. The sodium ion is coordinated to four oxygen atoms of the *tert*-butoxide ligands, two of these occupying bridging positions and two being terminal ligands, with sodium - oxygen distances of 2.42 and 2.61 Å, respectively. The isostructural uranium analogue of formula $KU_2(O\text{-}t\text{-}Bu)_9$ has been reported by Cotton and co-workers.[15] The uranium analogue can also be prepared in good yield directly from uranium tetrachloride and 4.5 equivalents of potassium tertbutoxide.

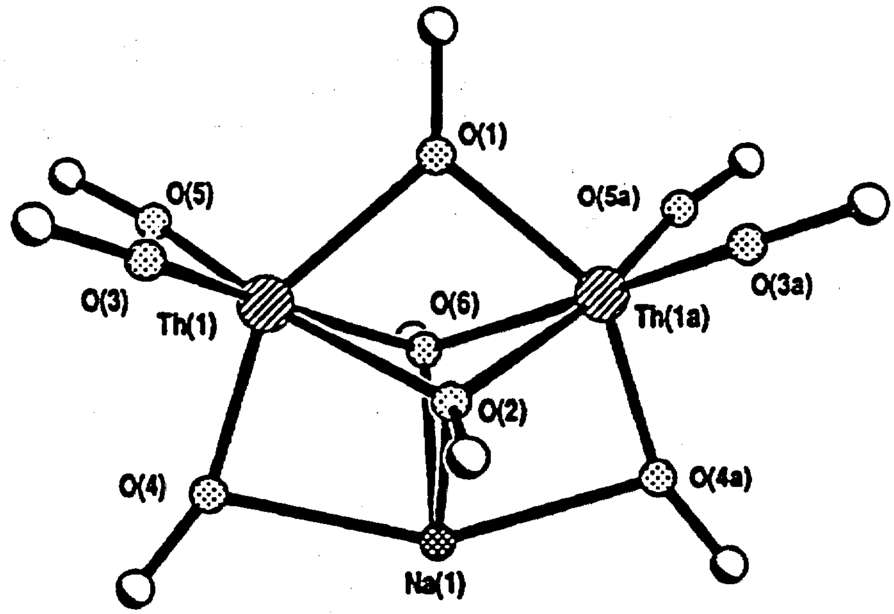
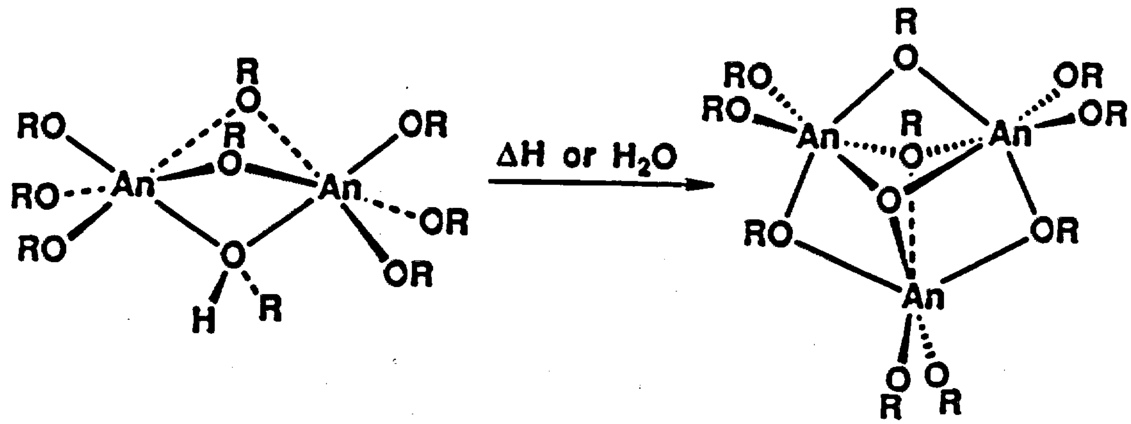


Figure 9. A drawing of the molecular structure of $NaTh_2(O\text{-}t\text{-}Bu)_9$ emphasizing the confacial bioctahedral dimeric structure, with the sodium ion cradled by two bridging and two terminal oxygen atoms. Important bond distances [Å] and angles [°]: Th(1)-O(1) 2.448(8), Th(1)-O(2) 2.498(8), Th(1)-O(6) 2.477(8), Th(1)-O(3) 2.146(9), Th(1)-O(4) 2.266(12), Th(1)-O(5) 2.164(9), Na(1)-O(4) 2.61 Na(1)-O(2) 2.42.

If the actinide metallacycle $[\{(Me_3Si)_2N\}_2\overline{An(CH_2SiMe_2N}SiMe_3)]$ is treated with an excess of *tert*-butanol (6 equivalents) in refluxing toluene, the trimeric complex $An_3O(O\text{-}t\text{-}Bu)_{10}$ may be obtained according to equation 13. For the uranium analogue it has been shown that hydrolysis via one equivalent of H_2O will also generate the trimer shown in equation 13. ^1H NMR spectroscopy reveals a characteristic 3:3:3:1 pattern of *tert*-butoxide resonances indicative of an M_3X_{11} structure as indicated in equation 13. An X-ray structure determination has been reported for the uranium analogue by Cotton and co-workers.[16] A drawing of the molecular structure of $U_3O(O\text{-}t\text{-}Bu)_9$ is shown in Figure 10.

(13) 

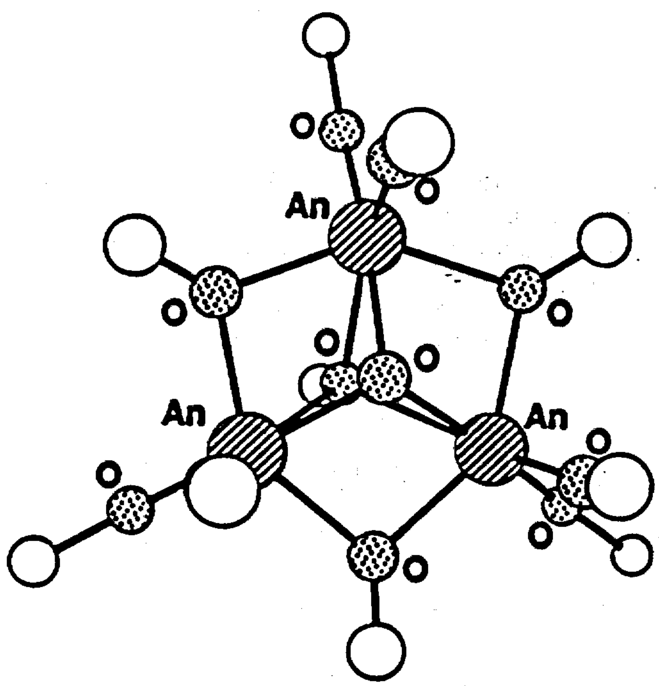


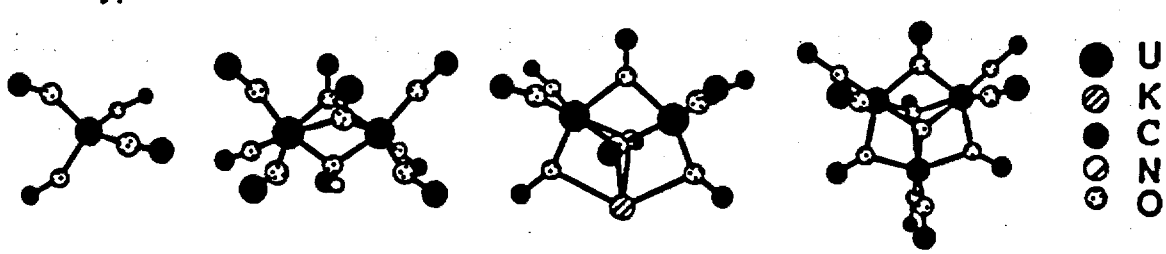
Figure 10. A drawing of the molecular structure of $An_3O(O\text{-}t\text{-}Bu)_9$ emphasizing the octahedral coordination environment around each actinide atom. The structure reveals six terminal alkoxide oxygens, three doubly bridging oxygens, one triply bridging alkoxide oxygen, and one triply bridging oxo ligand on the front of the molecule as shown here.

Summary of Model Compound Synthesis

In environmental groundwaters, the slow polymerization of actinide ions may be attributed to the kinetically slow polymerization of metal-oxygen bonds in direct analogy to the slow polymerization observed in many metal alkoxide complexes. We have shown, that in general, a decrease in the steric bulk about the actinide metal center will promote oligomerization of metal-oxygen bonds. Thus by careful control of steric bulk on the supporting alkyl group in the actinide alkoxide, one can control oligomerization in the model complexes as exemplified by the X-ray structures of $An(OAr)_4$, $An_2(OR)_8$ and $An_3O(OR)_{10}$. Many of the same structural types have been prepared and characterized for both Th(IV) and U(IV), indicating a high liklihood for success in preparation of analogous Np(IV) and Pu(IV) complexes for spectroscopic study.

Spectroscopic Study of Actinide Electronic Structure

The synthetic studies have established that we can indeed control the local coordination geometry about the central actinide ion, and we have built a fairly extensive database of X-ray structural data. Solution NMR studies have demonstrated that these structural types are maintained in solution, and thus electronic absorption spectra obtained on pure compounds will be indicative of each structural type in solution. For the discussion of optical spectroscopic data, we have chosen representative examples from the variety of structures discussed in the earlier section. The structural types chosen for a discussion of spectroscopic signatures include four-coordinate monomers of structural type **1**, six-coordinate dimeric species of structural types **2** and **3**, and the six-coordinate trimer of structural type **4**. These important structural types are indicated for reference below.



1 **2** **3** **4** **Key**

For the electronic spectra of the actinide model compounds, the narrow absorption peaks observed in visible and near-infrared spectra are due to transitions between states which are predominantly metal $5f^n$ in origin. A large number of states originate from this manifold even for cases such as U(IV) which has only two f electrons. Figures 11 and 12 show representative spectra that we have obtained for six synthetically-tailored U(IV) model complexes of the four structural types listed above. Since one must consider ligand field effects in addition to the strong interactions within the $5f^n$ manifold in interpreting spectra, the problem of understanding the electronic structure of all but the most simple actinide complexes begins to appear forbiddingly difficult.

Fortunately, the energies of the states within the $5f^n$ configuration are determined principally by electron-electron repulsion and spin-orbit interactions, which are heavily dependent on the metal ion and its oxidation state. This leads to a qualitative similarity of spectra of actinide complexes in the same oxidation state and makes low level assignments of the gross peak structure possible. Indeed the spectra shown in Figure 11 share many common characteristics with each other and with U(IV) in crystalline impurity systems and in aqueous solution. Ligand-field effects, which are weaker than in transition metal complexes, can be approached initially as perturbations on this dominant structure. The synthetic control discussed above allows us to manipulate these perturbations with a subtlety not approached by other classes of complexes, such as crystalline halide salts. Thus we have a unique opportunity to provide one key to an integrated understanding of overall electronic structure.

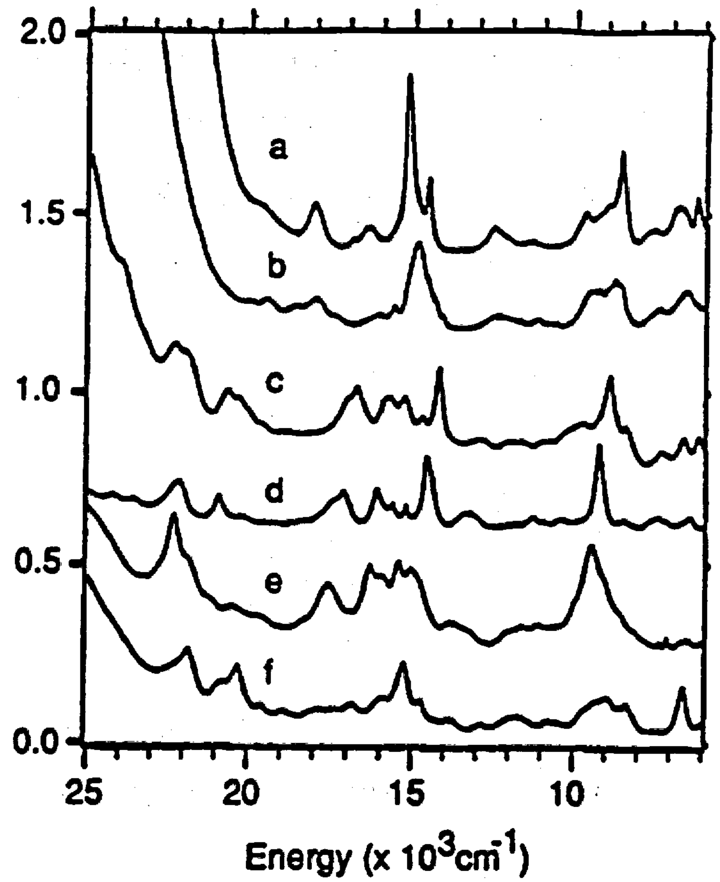


Figure 11. Room temperature UV-VIS-NIR spectra for six uranium (IV) model complexes obtained at 293 K. Compounds are as follows: a = $U(OAr^*)_4$, b = $U[N(SiMe_3)_2](OAr^*)_3$, c = $U_2(O\text{-}t\text{-}Bu)_8(HO\text{-}t\text{-}Bu)$, d = $KU_2(O\text{-}t\text{-}Bu)_9$, e = $(NBu_4)U_2(O\text{-}t\text{-}Bu)_9$, f = $U_3O(O\text{-}t\text{-}Bu)_{10}$.

The differences between the spectra shown in Figures 11 and 12 already illustrate interesting aspects of the influence of the ligand field on the structure of the $5f^n$ configuration. The top two spectra (**a** and **b**) in Figure 11 are of monomeric complexes with approximately tetrahedral symmetry about the U(IV) center (structure type 1). The third, fourth, and fifth spectra (**c**, **d**, and **e**) are of dimeric complexes with 6-coordinate U(IV) centers and approximately octahedral symmetry (structure types 2 and 3). The last spectrum (**f**) is of the trimer with 6-coordinate U(IV) centers which are slightly distorted from octahedral symmetry (structure type 4). We submit that the spectra in Figure 11 naturally fall into groupings by coordination number and symmetry, with **a** and **b** having similar appearances which are distinct from **c**-**e**, and with the trimer **f** showing qualitative differences from all the others. The low temperature spectra in Figure 12 accentuate these differences. Within these groupings by symmetry, changes due to different ligand identities are evident. For instance, the shift to higher energies of the major peaks in spectra c-e correlates with decreasing ligand polarizability.

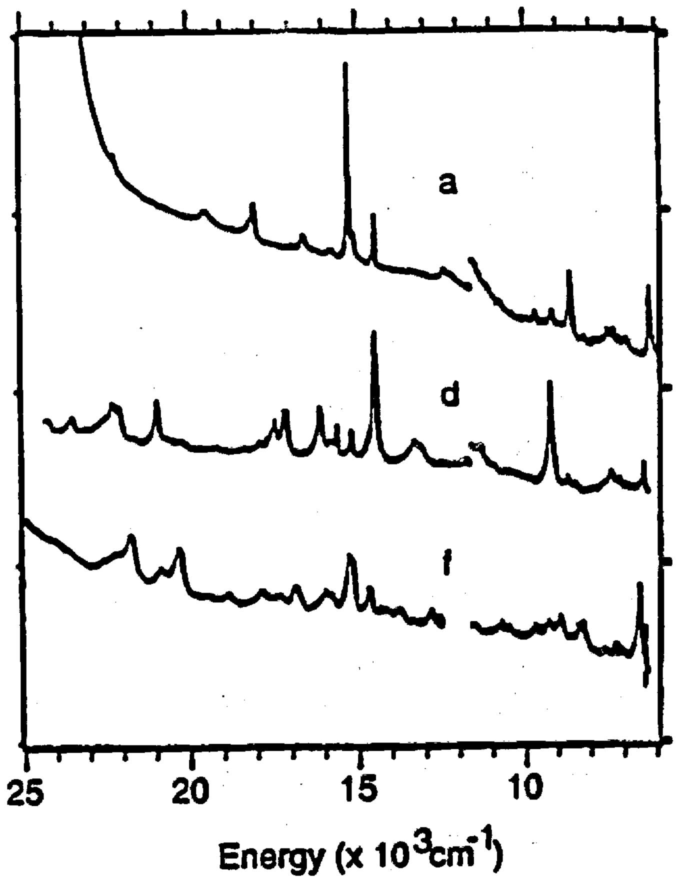


Figure 12. Low temperature UV-VIS-NIR spectra for six uranium (IV) model complexes obtained at 77 K. Compounds are as follows: a = $U(OAr^*)_4$, d = $KU_2(O\text{-}t\text{-}Bu)_9$, f = $U_3O(O\text{-}t\text{-}Bu)_{10}$.

Further design and synthesis of similar complexes with controlled variation in the factors which influence the absorption spectra will enable us to strengthen and fine-tune correlations between spectra and ligation to the point where absorption-based techniques become more useful molecular structure tools. The degree of control within our existing synthetic capabilities gives this work unique promise to provide a level of understanding of actinide electronic structure which will compliment and in many ways exceed that which has been achieved through the studies of crystalline impurity systems.

Concluding Remarks

A great deal of effort has been devoted to the development of sensitive spectroscopic techniques for the study of actinide speciation based on the sensitivity of f-f electronic absorption bands to oxidation state and ligation of the actinide ions. These efforts assume that data obtained in such studies will be interpretable in terms of changes in complexation of the metal center. However, our current understanding of 5f electronic structure is based on data from solid state doped single crystals. In these studies the local coordination geometry about the central actinide ion is maintained in an almost perfect high-symmetry environment, and will have little relevance for species in solution where deviations from perfect high symmetry tend to be the rule rather than the exception. Accordingly, part of our task has been to establish these spectral signatures for the actinide species extant under environmentally relevant conditions.

In order to establish spectroscopic signatures that are applicable to interpretation of actinide solution spectra, we need the ability to fine-tune changes in structure and ligand-field strengths. The most convenient way to achieve this fine-tuning is through synthetically-tailored actinide complexes. Therefore, we have adopted a model compound approach that exploits the versatility of synthetic actinide chemistry to enable this fine-tuning of structural and electronic effects so that a clearer correlation of molecular and electronic structure can be established. Speciation information can then be extracted from subsequent spectral data (e.g., from environmental samples) with greater likelihood of success, perhaps making it possible to obtain the fundamental molecular-level characterization required to fully understand and model actinide transport and transformation processes.

Experimental activities in this model complex investigation have involved both the refinement of synthetic strategies to make available a wide range of actinide complexes with varying structural and electronic perturbations, and acquisition and interpretation of the electronic spectral data for these synthetically-tailored model complexes. We have synthesized and characterized well over 40 new actinide alkoxide complexes, and are confident that our methodology will be applicable to the preparation of the analogous neptunium and plutonium complexes. The neptunium and plutonium chemistry is expected to be underway this summer with completion of a new hotlab chemistry facility.

These model complexes have been used to determine how observable electronic transitions are perturbed in response to structural changes in the complex in solution. From the spectra obtained for these model complexes, we have found that the f-f transitions naturally fall into obvious groupings by coordination number and symmetry by which we can now differentiate between monomeric, dimeric, and trimerc actinide species in solution. It is noteworthy that the f-f transitions in the homoleptic alkoxide complexes differ from those observed in a mixed oxo-alkoxide complex of the same coordination number and local site symmetry.

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