IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories WIPP Online Documents web site. A printed copy of this document may not be the version currently in effect.

NUCLEAR WASTE MANAGEMENT PROCEDURE

NP 9-1
ANALYSES
Revision 9

Effective Date: December 18, 2012

Author:	L. Eugene Safley	*Original signed by L. Eugene Safley*	*12/17/2012*
	(printed name)	(signature)	(date)

1.0 Purpose and Scope

This procedure specifies methods for controlling and documenting analyses performed by Sandia National Laboratories (SNL) for the SNL Waste Isolation Pilot Plant (WIPP) program. This procedure applies to scientific and engineering analyses (theoretical or computational). Examples of analyses covered by this procedure include:

Compliance Decision (CD) – compliance, certification, or recertification analyses whose output is relied upon to make design, analytical, operational, or compliance-based decisions with respect to the performance of the waste confinement system. These results will be used:

- in supporting an application for certification or recertification, or
- in a DOE/CBFO planned change request to activities or conditions contained in the most recent compliance determination, or
- an analysis requested by EPA (e.g., performance assessment, impact assessments, data analysis, parameter justifications).

Programmatic Decision (PD) – programmatic, scoping, or sensitivity analyses associated with programmatic decisions. These analyses may be considered as *scoping* or screening in that they apply to development, implementation, and testing of improvements to the existing methodology. Scoping calculations include evaluative efforts regarding features, events, and processes (FEPs) screening, conceptual/mechanistic model evaluation, or assessment of grid adequacy. *Sensitivity* analyses can focus on testing the impact of alternative modifications for improving capabilities for conducting performance assessments (PAs) and for communicating and explaining the results of a PA.

> Note: With written permission granted in advance by the Carlsbad Programs Group Manager relying on input from the Responsible Manager and Software Quality Assurance, some software that is required to support various analyses may need to be used prior to full qualification. Collection of quality data and subsequent analysis with software that is not fully qualified is assumed to be a risk, because completion of the required software QA documentation may require critical code modifications and may require that some programmatic decision-type calculations be redone.

Routine Calculations – simple data manipulations, detailed formulas or macros (e.g., unit conversions, interpolations, translations, rotations, or simple analytic solutions) that can be verified by hand calculations.

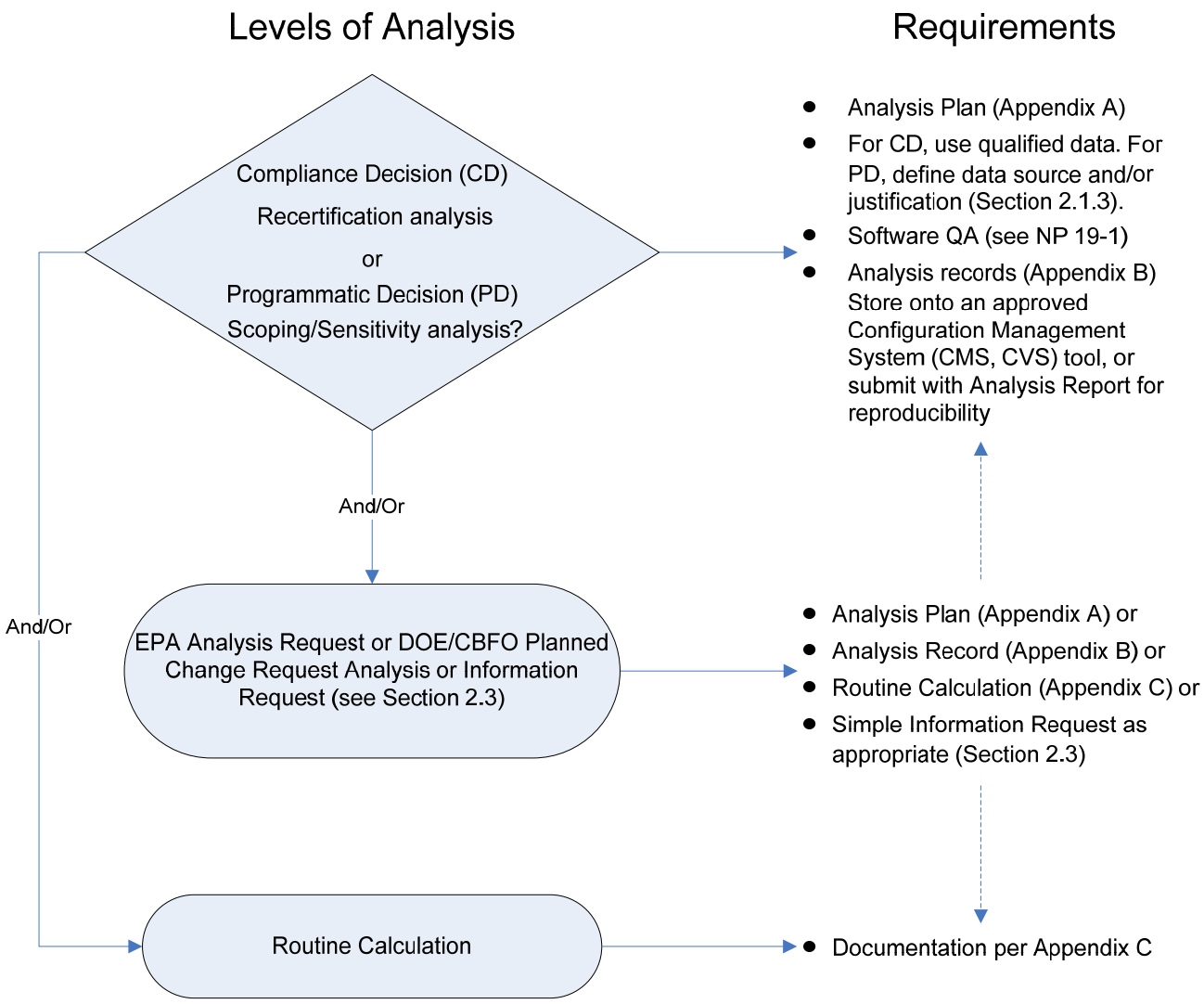
This procedure governs only the conduct of the analysis, not the process for qualifying software used in an analysis (see NP 19-1).

Acronyms and definitions for terms used in this procedure may be found in the Glossary located at the Sandia National Laboratories (SNL) WIPP Online Documents web site.

2.0 Implementation Actions

2.1 General

Below is an overview of the requirements for conducting the various levels of analysis:



2.1.1 Analysis Plan Preparation and Approval

The author (e.g., Principal Investigator, analyst, designee) prepares an Analysis Plan (AP) consistent with requirements found in Appendix A. The author then submits the plan for technical, QA, and management review and approval, following the flow chart in Appendix D (Analysis Plan/Revision Review and Approval). The author shall submit the AP for issuance as a controlled document in accordance with NP 6-2.

2.1.2 Analysis Plan Changes/Revisions

Documentation shall be provided for deviations from the original AP. Deviations include the performance of activities not described in the plan as well as activities defined in the plan that were not performed. Deviations can be documented as part of the final analysis records (Appendix B) or by revising the plan (Appendix D). When revising the AP, the author shall ensure that changes to the AP are clearly indicated with vertical change bars in the margin of the revised plan (Note: change bars will indicate changes for the current revision only). Changes to an AP shall receive technical, QA, and management review in accordance with NP 6-1 and shall be issued as a controlled document in accordance with NP 6-2.

2.1.3 Analysis Plan Implementation

The author shall:

- Oversee implementation of the AP.
- For software that was executed on an approved CMS, the software configuration management system (SCMS) Librarian or software configuration management for Unix (SCMU) Run Master will ensure that the source code, input and output files, scripts and any other information needed to re-run the calculation are stored onto the centralized storage system (e.g., COMPAQ/DEC CMS or Linux/CVS). The SCMS Librarian or SCMU Run Master is responsible for performing compliance runs and checking in the results. The specific responsibilities of the SCMS Librarian or SCMU Run Master are contained in Long, 2003 and Kirchner, 2012.
- For software that is not executed on an approved CMS, the author ensures that all files necessary to re-run the calculation are submitted with the Analysis Report.
- Justify the use of all data and inputs. Assure that assumptions are stated clearly and lead logically to the conclusions presented in the work product.
- For a CD Performance Assessment calculation, all data and derived parameters must be justified by an Analysis Plan, Report, or Routine calculation. The new parameter information is to be provided (in a table if appropriate) with the following attributes for entry into the PA Parameter Database (See NP 9-2 Parameters), as appropriate:
  - Material (add description or long name as appropriate with an abbreviation)
  - Property (add description or long name as appropriate with an abbreviation)
  - Constant Value (if known)
  - Units
  - Distribution [if not a constant, calculated per (Tierney, 1990)]
    i. Data values and probability supporting the distribution (as applicable)
    ii. Mean
    iii. Mode (triangular distribution only)
    iv. Standard Deviation
    v. Minimum
    vi. Maximum
- Programmatic decision calculations do not require qualified data, but the source and or derivation of the data and or parameter should be provided in the Analysis report.
- Oversee preparation of the analysis records as described in Appendix B.

- Ensure proper review of the analysis records (see Appendix E Flow Chart) and submittal to the SNL WIPP Records Center. **Note:** For compliance decision analyses, only qualified software, data, and inputs shall be used.

2.2 Routine Calculations

Routine calculations are meant to cover straightforward calculations or decisions like reasoned arguments involving no calculations. This type of analysis can include memos documenting decisions or simple calculations and can use tools like Microsoft Excel, Access, Mathematica, MATLAB, and simple code/utility implementations.

Routine calculations are also used to verify software that is exempt from the QAPD requirements for software development. In these cases as outlined in Appendix C, the input and output files, platform information, and code listing, are captured along with an illustration of how to get the correct results for the specified range of input (e.g., a verification problem and/or a clear description of the steps used).

2.2.1 Documentation of Routine Calculations

Documentation for routine calculations shall follow the criteria in Appendix C.

2.2.2 Review of Routine Calculations

Routine calculations shall receive both technical and QA review and approval.
The technical review may be accomplished using one of the following methods as appropriate:

- Separate independent calculations of the original work.
- A check of the steps in the original calculations.
- A spot or random check of the original calculations.

Both the Technical and QA review shall be conducted per NP 6-1.

Note: Routine calculations normally stand alone; however, several routine calculations may be conducted under an AP. In the latter case, the routine calculations can be reviewed as part of the analysis records and do not require a separate review as described above.

2.3 Other Analysis or Information Requests

Compliance Decision Analysis may be initiated by SNL Management to address DOE/CBFO planned-change requests and for analyses to address requests for information from the WIPP EPA Regulators.

For most planned change requests or EPA analysis requests, the analysis may be conducted without the development of an AP provided the Analysis Report follows Appendix B and/or Appendix C criteria as appropriate. If in-depth analyses are needed to address these requests, an AP should be developed per Section 2.1.1. If a Routine calculation can address the request, the calculation or decision can be performed per the criteria of Appendix C and documented in a memo format. In these cases, the AP, Analysis Report, or Routine calculation memo must reference the SNL Management Request, or the DOE/CBFO directive (milestone number, letter, e-mail, etc.), or the EPA request (letter, meeting notes, phone conversation, e-mail request, etc.) for additional analyses. These references must be submitted as records per NP 17-1 prior to being referenced in the AP, Analysis Report, and/or Routine calculation memo.

To obtain concurrence with the methodology and/or approach, our DOE/CBFO customer may request an informal EPA Regulator review prior to our completion of the plan or report. In those cases, the DOE/CBFO request is to be submitted to Records.

At times, different WIPP stakeholders [EPA, DOE/CBFO, project participants (e.g., WTS, LANL, etc.) and academia] may request information on already-completed analyses. In these cases, the request shall be reported to SNL Management for approval. If they approve (verbal), the information requested is to be appropriately copied by the SNL WIPP Records Center and delivered to the requesting party.

Draft or incomplete work information requests (analysis plans, reports, calculations, presentations, etc.) that is requested by DOE/CBFO and needed by the Regulator or for a qualification activity (e.g., peer review) that is to be delivered outside of the SNL WIPP team shall be appropriately annotated stating that the work is preliminary or draft and is not to be cited. SNL WIPP Management and QA concurrence (verbal) shall be obtained prior to delivery of draft or incomplete work.

2.4 References

Kirchner, T., (2012) WIPP Performance Assessment Software Configuration Management Under UNIX (SCMU) Plan, Version 1.1. Sandia National Laboratory-Carlsbad. November 12, 2012. ERMS 558444

Long, J., (2003) WIPP Performance Assessment (PA) Software Configuration Management System (SCMS) Plan, Revision 2.0. Sandia National Laboratory-Carlsbad. September 15, 2003. ERMS 524707

Tierney, M.S., “Constructing probability distributions of uncertain variables in models of the Performance of the Waste Isolation Pilot Plant: the 1990 performance simulations.” SAND 90-2510

3.0 Records

The following QA records, generated through implementation of this procedure, shall be prepared and submitted to the SNL WIPP Records Center in accordance with NP 17-1 (Records).

QA Record

- The final, approved new/revised Analysis Plan (per Appendix A)
- Analysis Records (per Appendix B)
- Analysis Records DRC forms (NP 6-1-1)
- Routine Calculation documentation (per Appendix C)
- Data reports from other WIPP project participants (per Appendix B, Item 5, bullet 3)
- Analysis/Information Request (per Section 2.3)

4.0 Appendices

Appendix A: Analysis Plan Content and Format
Appendix B: Analysis Records
Appendix C: Routine Calculation Requirements
Appendix D: Analysis Plan/Revision Review and Approval Flow Chart
Appendix E: Analysis Records Flow Chart

Appendix A
Analysis Plan Content and Format

Analysis Plans are to include the following as appropriate:

- **Cover page**
  - Title of Analysis
  - Effective date (assigned by Document Control)
  - Author (name, signature, date)
  - Technical, QA and Management Reviewers (name, signature, date)

- **Document Control Header** – To be included on the upper right-hand side of each page.
  - Analysis plan number (obtained from Document Control)
  - Revision Number
  - Page (number) of (total number)

- **Content Requirements** – The following shall be included, unless the nature of the work does not involve the item/concept.

  1. **Introduction and Objectives.** A description of the scope of the analysis, the objectives to be achieved or hypotheses to be tested, and the initial assumptions:
     - discussion of the conditions, scenarios and general purpose of the analysis
     - description of assumptions relating to the implementation of any conceptual models
     - identification of potential sources of error and uncertainty and how they will be controlled
     - type of analysis to be performed (i.e., compliance decision or programmatic decision)

  2. **Approach.** A description of the analytical approach, including a discussion of the computer codes and parameter input or justifications to be used in the analyses.

  3. **Software List.** List software expected to be used.

  4. **Tasks.** A listing of the primary tasks and how they will be documented, the identity of the individuals who will perform the tasks, task deliverables and expected completion date.

  5. **Special Considerations.** The identification of prerequisites, special controls, processes, skills and certification requirements.

  6. **Applicable Procedures.** The identification of any applicable controlling documents, such as program procedures (e.g., NPs) or project procedures (e.g., SPs).

Appendix B
Analysis Records

Analysis records shall provide sufficient documentation so that a qualified technical person could reconstruct the work and reproduce the results. The following information shall be included by the author (e.g., Principal Investigator, analyst, SCM librarian or run master, designee) in the analysis records, unless the nature of the work does not involve the item/concept:

1. Provide reference to the analysis plan and any revisions.

2. Provide detailed explanation of the scientific approach or technical method used to perform the analysis.
   - A discussion and sketch of the grid for any scientific codes.
   - Boundary conditions and initial conditions.
   - Time period of analysis.
   - Any other aspects of the approach necessary to provide traceability and reproducibility.
   - Assumptions for all decisions need to be clearly explained as to why the assumption is needed and how the assumption is or may be conservatively bounding or representative of the data being analyzed.

3. List name, version and platform of any computer software used in performing the analysis and indicate if calculation was or was not executed on the CMS/CVS.
   - Provide all files, including the location of these files on the CMS/CVS, necessary to reproduce the calculations (e.g., source code, macros, inputs, outputs, executables) with the Analysis Report, and
   - Provide an explanation of how control of use was accomplished, and a description of the execution environment, including:
     - Execution flow (e.g., hardware, operating system version)
     - Code flow
     - Run control

4. Identify inputs and input sources (i.e., variables that affect interrelated scientific investigations) to assure comparability among the related variables, and documentation of the appropriate control of these variables. Provide:
   - For Performance Assessment calculations, all parameters must be justified per NP 9-2 Parameters and the new parameter information should be provided in a table as specified in Section 2.1.3 (bullet 5).
   - Each parameter (with brief description) by computer code.
   - Map of each model parameter to the grid for each computer code. The mapping between computational grid and material regions may be used along with a listing of the model parameters required for each material region.
   - Identification and discussion of the choices of numerical control variables and other values that are input to the codes via input files.
   - Identification of the values of variables that are hard-wired into computer codes and are significant to the results.
   - Discussion of the use of input variables which result from other codes; reference the analysis plan or other documents describing the analysis that produced the results used as input to this analysis.

5. Provide qualification/justification for data/input:
   - For **programmatic decision** analysis, identify source of data or justification of values used if no data exists.
   - For **compliance decision** analysis, identify qualification and basis for input used.
   - For data reports that come from other project participants (LANL, WTS, etc.) who have DOE/CBFO-approved QA programs a copy of the completed work product (memo, e-mail, report, etc.) is to be submitted to the SNL WIPP Record Center and cited in the report.

6. Describe the work performed and the results obtained, including:
   - Tables, plots and discussion of results. Provide sufficient detail to demonstrate to an equally qualified technical person that the results of the analyses adequately meet the purpose of the analysis. Conclusions and assumptions need to be supported in specific detail. All logic and analyses needs to be clearly presented.
   - Discussion of any other items necessary for traceability, transparency, and reproducibility.

7. Provide documentation of any changes from the analysis plan that occurred during the performance of the analysis, including the reason for the changes (note: not necessary if the plan was revised and re-issued).

8. Provide Document Review and Comment forms (DRCs) used to document the review of the work.

Appendix C
Routine Calculation Requirements

Documentation of routine calculations is intended to provide sufficient detail to allow reproducibility of the calculation, spreadsheet, auxiliary/utility code or decision (e.g., reasoned argument) by an independent technical person. Documentation of routine calculations can be in any format (e.g., memo, scientific notebook, Appendix in an Analysis report, etc.). The author (e.g., Principal Investigator, analyst, designee) shall ensure the following information is included as appropriate:

1. Title of calculation.

2. Associated planning document identifier (e.g., analysis plan, test plan, EPA letter, planned change request title, milestone number, etc.), as applicable.

3. A clear description of each step or clear definition of each algorithm used in the calculation, spreadsheet, or auxiliary/utility code. Assumptions are to be clearly stated and lead logically to the conclusions presented.

4. Identification/listing of input, input sources, parameter justifications, and output.

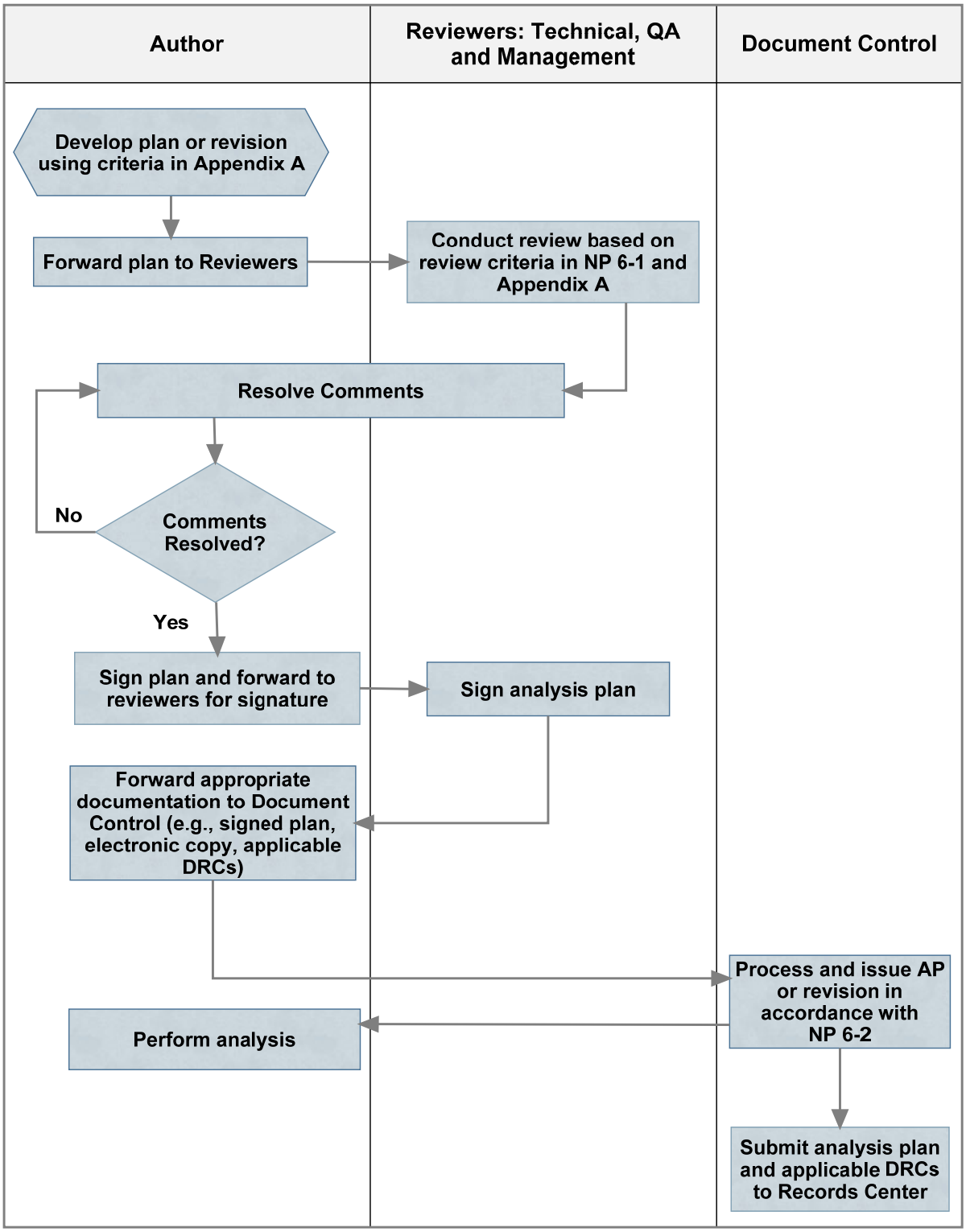
5. Data qualification or justification:
   - For **programmatic decision** analysis, identify source of data or justification of values used if no data exists.
   - For **compliance decision** analysis, identify qualification and basis for input used.
   - For data reports that come from other project participants (LANL, WTS, etc.) who have DOE/CBFO-approved QA programs, a copy of the completed work product (memo, e-mail, report, etc.) is to be submitted to the SNL WIPP Records Center and cited in the report.

6. If software was used to do the calculation (e.g., a spreadsheet, database, or graphing program), identify the name and version of the software, the platform on which it was run, and illustrate how the specific application provides the correct results for the specified range of input parameters.

   Note: The software used for routine calculations should be submitted as part of the documentation, if needed for reproducibility.

7. Dates and results of reviews, along with the names and signatures of the analyst and reviewers (technical and QA).

Appendix D
Analysis Plan/Revision Review and Approval Flow Chart



Appendix E
Analysis Records Flow Chart