



*Office of Civilian Radioactive Waste Management*

QA: QA

## **PROCEDURE**

### **MODELS**

**AP-SIII.10Q**

**Revision 2 ICN 0**

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Effective Date: 09/30/2003

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9/29/03  
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## CHANGE HISTORY

<u>Revision Number</u>	<u>Interim Change No.</u>	<u>Effective Date</u>	<u>Description of Change</u>
0	0	12/21/2001	Initial issue. Models procedure prepared to separate models from scientific analyses and engineering analyses, and to address, in part, issues identified in BSC-01-C-001, LVMO-01-D-007, BSC-01-D-050, LVMO-00-D-118, BSC-01-D-078, and LVMO-00-D-119. Supersedes AP-3.10Q, <i>Analyses and Models</i> , for models. AP-3.12Q, <i>Calculations</i> , has been revised to address design/engineering calculations and analyses exclusively, and has been renamed <i>Design Calculations and Analyses</i> . AP-SIII.9Q, <i>Scientific Analyses</i> , has been prepared to address analyses and calculations subject to <i>Quality Assurance Requirements and Description</i> , DOE/RW-0333P, Supplement III.
0	1	01/25/2002	ICN to modify applicability to those documents that did not complete the requirements of Section 5.0 through Subsection 5.6 of AP-3.10Q, <i>Analyses and Models</i> , on December 21, 2001; clarify requirements of the Bechtel SAIC Company, LLC Quality Engineering Compliance check; make editorial changes; clarify role of the originator; and clarify type of validation documentation to be reviewed and initiated by the Chief Science Officer.
0	2	05/03/2002	Interim Change Notice to bring model validation requirements in line with changes to the <i>Quality Assurance Requirements and Description</i> , DOE/RW-0333P, Revision 11; require incorporation of errata per AP-15.3, <i>Control of Technical Product Errors</i> ; and renumber the outline in Attachment 2.

**CHANGE HISTORY (Continued)**

<b><u>Revision Number</u></b>	<b><u>Interim Change No.</u></b>	<b><u>Effective Date</u></b>	<b><u>Description of Change</u></b>
1	0	03/14/2003	Revision to delete references to AP-2.21Q, <i>Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities</i> ; incorporate changes to AP-SIII.2Q, <i>Use of Accepted Data and Qualification of Unqualified Data</i> ; incorporate Document Action Requests D3344, D6030, D6349, and D3424; incorporate resolution of Condition/Issue Identification and Reporting/Resolution System item 3162; and to state the requirements for incorporation of errata in accordance with AP-15.3Q <i>Control of Technical Product Errors</i> .
1	1	06/30/2003	Interim Change Notice to make explicitly clear when it is not necessary for action steps to be performed sequentially.
1	2	06/30/2003	Interim Change Notice to clarify requirements for verification data.
2	0	09/30/2003	Revision to clarify data; to change "impact reviews" to "document reviews;" to revise Attachment 2 to be consistent with input categories defined in AP-3.15Q, <i>Managing Technical Product Inputs</i> ; to clarify sequencing of action steps (Reference BSC(B)-03-D-220 and Document Action Request D10476); and to incorporate Document Action Requests D7773, D8592, D8710, D9068, D9373, D10068, D10300, D10518, D10519, and D10729.

## 1.0 PURPOSE

This procedure establishes the responsibilities and process for documenting activities that constitute scientific and performance assessment modeling that is subject to the requirements of *Quality Assurance Requirements and Description (QARD)*, DOE/RW-0333P. This procedure may also be used for models that are not subject to QARD requirements. Supplemental guidance for all scientific processes is contained in the *Scientific Processes Guidelines Manual*, MIS-WIS-MD-00001, located on the Office of Civilian Radioactive Waste Management (OCRWM) Program Documents Database under the "Manual/Handbook" icon.

## 2.0 APPLICABILITY

This procedure applies to individuals within Bechtel SAIC Company, LLC (BSC); the National Laboratories; U.S. Geological Survey; BSC subcontractors, and other contractors who perform and document modeling in support of the Office of Civilian Radioactive Waste Management Program.

Implementation of conceptual models into new mathematical models, or into mathematical models undergoing revision or change, must be documented in accordance with this procedure. Mathematical model development, validation, and initial use, as well as any related work required to accomplish these tasks, shall be documented within the model(s) document. Use AP-SIII.9Q, *Scientific Analyses*, if you are going to perform an analysis that does not require developing or revising an existing model.

Scientific analyses and calculations are documented in accordance with AP-SIII.9Q. Design analyses are documented in accordance with AP-3.12Q, *Design Calculations and Analyses*. Development, revision, configuration management, verification/validation, and/or qualification of software are documented separately in accordance with AP-SI.1Q, *Software Management*; AP-SI.2Q, *Qualification of Level A Developed or Modified Software*; and/or AP-SI.3Q, *Software Independent Verification and Validation*.

## 3.0 DEFINITIONS

- 3.1 **Abstraction**—The process of purposely simplifying a mathematical model (component, barrier, or subsystem process model) for incorporation into an overall system model of the geologic repository. The products of model abstractions may represent reduction in dimensionality, elimination of time dependence, tables obtained from more complex models, response surfaces derived from the use of more complex models, representations of a continuous process or entity with a few discrete elements, etc.
- 3.2 **Assumption**—A statement or proposition that is taken to be true or representative in the absence of direct confirming data or evidence.
- 3.3 **Checker**—A qualified individual other than the Originator, technically competent in the subject area of the document undergoing checking, responsible for confirming adequacy, accuracy, and completeness of the model documentation.

- 3.4 Editorial Correction**—Modifications made to a document such as correcting grammar, spelling, or typographical errors; renumbering sections or attachments; and updating organizational titles. Editorial corrections do not affect the chronological sequence of work or the fundamental process, or change responsibilities.
- 3.5 Interim Change Notice (ICN)**—A method for updating (e.g., updating the To Be Verified [TBV] status) or revising limited portions of approved model documentation.
- 3.6 Lead**—The individual assigned by the Responsible Manager to control a model activity and having responsibility for assignment of personnel performing activities associated with the model.
- 3.7 Model**—A representation of a system, process, or phenomenon, along with any hypotheses required to describe the process or system or explain the phenomenon, often mathematically (QARD). Model development typically progresses from conceptual to mathematical models. Mathematical model development typically progresses from process, to abstraction, and to system models.
- 3.8 Model, Abstraction**—A product of the abstraction process that meets the definition of a mathematical model (QARD).
- 3.9 Model, Conceptual**—A set of hypotheses consisting of assumptions, simplifications, and idealizations that describes the essential aspects of a system, process, or phenomenon (QARD). Such a model may consist of concepts related to geometrical elements of the object (size or shape); dimensionality (one-, two-, or three-dimensional); time dependence (steady-state or transient); applicable conservation principles (mass, momentum, energy); applicable constitutive relations, significant processes, natural laws, and boundary conditions; and initial conditions. Conceptual models may be implemented into mathematical models.
- 3.10 Model, Mathematical**—A mathematical representation of a conceptual model (system, process, or phenomenon) that is based on established scientific and engineering principles and from which the approximate behavior of a system, process, or phenomenon can be calculated within determinable limits of uncertainty (QARD).
- 3.11 Model, Process**—A mathematical model that represents an event, phenomenon, process, component, etc., or series of events, phenomena, processes, or components, etc. A process model may undergo an abstraction for incorporation into a system model (QARD).
- 3.12 Model, System**—A collection of interrelated mathematical models that represent the overall geologic repository or overall component subsystem of the geologic repository (QARD).
- 3.13 Model Validation**—A process used to establish confidence that a mathematical model and its underlying conceptual model adequately represents with sufficient accuracy the phenomenon, process, or system in question (QARD).
- 3.14 Originator**—A technically competent individual designated to perform a model activity and to prepare the model documentation and assigned the responsibility for ensuring the

adequacy, accuracy, and completeness of the model documentation. For the purpose of this procedure, an all-inclusive term for a preparer, modeler, or investigator.

- 3.15 *Responsible Manager***—The individual having management responsibility for a model activity, for assigning a Lead to the model activity, and for approving the model documentation.
- 3.16 *Scientific Analysis***—A documented study that 1) defines, calculates, or investigates scientific phenomena or parameters; 2) evaluates performance of components or aspects of the overall geologic repository; or 3) solves a mathematical problem by formula, algorithm or other numerical method. A scientific analysis may involve numerical manipulations that are not part of a previously developed and validated mathematical model (per AP-SIII.10Q) if the choice of method is evident from standard scientific practice, approach, or method. A scientific analysis may also use a previously developed and validated mathematical model (per AP-SIII.10Q), within the mathematical model's intended use and stated limitations, but may not revise the mathematical model in order to complete the scientific analysis. An analysis can be performed as part of a model developed in accordance with this procedure (AP-SIII.10Q) or using AP-SIII.9Q.
- 3.17 *Sensitivity***—The degree to which the model results are affected by changes in a selected model input.
- 3.18 *Software***—Computer programs, procedures, rules, and associated documentation pertaining to the operation of a computer system (QARD).
- 3.19 *To Be Verified (TBV)***—The Identification of information that is preliminary, needs to be re-evaluated, and/or needs confirmation.
- 3.20 *Traceability***—The ability to trace the history, application, or location of an item, data, or sample using recorded documentation (QARD).
- 3.21 *Transparency***—The attribute of producing documents that are sufficiently detailed as to purpose, method, assumptions, inputs, conclusions, references, and units, such that a person technically qualified in the subject can understand the documents and ensure their adequacy without recourse to the originator.

#### **4.0 RESPONSIBILITIES**

- 4.1** The Chief Science Officer (CSO) is responsible for the preparation, change, and approval of this procedure.
- 4.2** The following organizations or positions are responsible for activities identified in Section 5.0 of this procedure:
- a) Responsible Manager
  - b) Lead
  - c) Originator
  - d) CSO

- e) Checker
- f) Quality Engineering Representative (QER)
- g) Reviewing Organization

## 5.0 PROCESS

Modeling, by its nature, is an iterative process. This procedure establishes in the specific subsections those action steps that must be completed sequentially but does not require all action steps to be completed in sequential order. Specific action steps that must be completed before other action steps may begin are identified. Acronyms and abbreviations used in this procedure are defined in Attachment 1, Acronyms and Abbreviations.

### PROCESS OUTLINE

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## 5.1 PLANNING

The Technical Work Plan (TWP) must be completed before beginning action steps in Paragraph 5.1.1.

### 5.1.1 Responsible Manager:

- a) Control the development, validation, checking, documentation, revision, change, and key technical activities of the model activity in accordance with the requirements of this procedure. A Lead may be assigned to control these functions.
- b) If a Lead has been assigned, provide the Lead with the applicable TWP prepared in accordance with AP-2.27Q, *Planning for Science Activities*.

### **5.1.2 Responsible Manager or Lead:**

- a) Review the TWP for the Work Package associated with the model to be developed. If the TWP requires revision, ensure that it is completed in accordance with AP-2.27Q.
  - 1) Ensure the applicable TWP includes adequate planning for model validation, including the identification of the intended purpose of the model, the needed level of confidence for the model, the criteria to be used to determine that the appropriate level of confidence has been met, the plans for independent technical review per Subsection 5.4 (if any), and the plans for post-development model validation activities. Supplemental guidance is contained in the *Scientific Processes Guidelines Manual* located on the OCRWM Program Documents Database under the "Manual/Handbook" icon.
  - 2) If a previously developed model is to be used outside of its intended use, limitation, or range of validity, justification and plans for validation shall be provided in the applicable TWP.
  - 3) Ensure that the applicable TWP includes adequate planning (per AP-SIII.2Q, *Qualification of Unqualified Data*) for any required data qualification activities.
- b) Assign an Originator to perform the modeling activity (the Lead may assume the Originator's responsibilities; however, the Lead may not assume the Checker's or Reviewer's responsibilities when acting as the Originator) and provide the originator the applicable TWP.

## **5.2 DOCUMENTATION**

It is not necessary for the action steps to be performed sequentially.

### **5.2.1 Originator:**

- a) The modeling activity and associated tasks shall be performed in accordance with the applicable TWP and all applicable procedures. Scientific notebooks may be used in the modeling activity in accordance with AP-SIII.1Q, *Scientific Notebooks*.
- b) Obtain a document identifier (DI) for the model documentation from Document Control in accordance with AP-6.1Q, *Document Control*.
- c) Record the DI and revision/change number on each page of the model documentation unless the conditions for attachments, as specified in Attachment 2, Model Documentation Outline, apply.



- d) Document the model using the annotated outline in the Model Documentation Outline. If a section in the annotated outline is not applicable, indicate that it is not applicable after the title and provide a rationale for non-applicability.
- e) If any information with regard to Naval fuel is included in the model document, have the Resident Manager for the Naval Nuclear Propulsion Program review the model to ensure no unauthorized Naval Reactors information is included in the model document.
- f) Document product input in accordance with AP-3.15Q, *Managing Technical Product Inputs*, using the Document Input Reference System (DIRS).
- g) Use alphanumeric revision designators (e.g., Rev. 00a, Rev. 00b) to denote different drafts or versions in the development of the model documentation prior to the version submitted for final approval.
- h) Complete the appropriate sections of Attachment 3, Model Cover Sheet, and Attachment 4, Model Revision Record, in accordance with the instructions for each attachment.
- i) Ensure documentation is legible and in a form suitable for reproduction, filing, and retrieval.
- j) Ensure each page is sequentially numbered, beginning with the cover page as page 1 and the revision page as page 2.
- k) Ensure attachments to documentation developed using the annotated outline in the Model Documentation Outline are identified by Roman numerals (e.g., Pages I-1 through I-7), except as noted in the instructions for Block 6 of the Model Cover Sheet.
- l) Software used to develop and perform the model must be controlled and documented in accordance with AP-SI.1Q, AP-SI.2Q, and/or AP-SI.3Q.
- m) Commercial software used during model validation shall be controlled and tracked in accordance with AP-3.15Q and AP-SV.1Q, *Control of the Electronic Management of Information*, but may not need to be qualified.
- n) Document software used in the model as described in Section 3 of the Model Documentation Outline.
- o) Document the qualification of unqualified data, developed in accordance with AP-SIII.2Q, as described in Section 6 of the Model Documentation Outline.

**5.2.2 Responsible Manager or Lead:**

If the modeling activity produces preliminary output, submit in accordance with AP-SIII.3Q, *Submittal and Incorporation of Data/Technical Information to the Technical Data Management System*.

**5.3 MODEL VALIDATION**

It is not necessary for the action steps to be performed sequentially.

**5.3.1 Originator:**

- a) Identify and document the intended purpose, and any limitations for the model as described in Section 1 of the Model Documentation Outline.
- b) Document the criteria used to determine that the needed level of confidence for the model has been met as described in Section 7 of the Model Documentation Outline.
  - 1) The criteria used to establish the adequacy of the scientific basis for the model must be consistent with the intended use of the model and must be justified in the documentation.
  - 2) The criteria used to demonstrate that the model is sufficiently accurate for its intended use must be consistent with parameter uncertainties and must be justified in the documentation.
- c) If validation activities are to extend beyond the documented completion of the current model, include a description of future activities that are to be completed and a justification for extending model validation in accordance with Section 7 of the Model Documentation Outline.
- d) Validate the model to the level of confidence required in accordance with the TWP and Paragraph 5.3.3c) of this procedure.
- e) Document model validation as described in Section 7 of the Model Documentation Outline.
- f) Submit draft documentation of the results of the validation activities to the CSO for review.

**5.3.2 CSO:**

- a) Review draft documentation of the validation activities to determine if the appropriate level of confidence, as identified in the applicable TWP, has been obtained.

- b) If the appropriate level of confidence has been obtained, initial or sign and date on the first page of the draft model validation documentation or indicate acceptance by electronic mail.
- c) Return the documentation, with any recommendations, to the Originator.

**5.3.3 Responsible Manager or Lead:**

- a) Ensure mathematical models are validated for their intended purpose and stated limitations, and to the level of confidence required by the model's relative importance to the potential performance of the repository system. Validation is required for all mathematical models and their underlying conceptual models (validation is not required for conceptual models not implemented in mathematical models).
- b) Ensure that validation of the mathematical model and its underlying conceptual model includes documentation of decisions or activities that are implemented to generate confidence in the model during model development, including the following:
  - 1) Selection of input parameters and/or input data, and a discussion of how the selection process builds confidence in the model.
  - 2) Description of calibration activities, and/or initial boundary condition runs, and/or run convergences, and a discussion of how the activity or activities build confidence in the model. Include a discussion of impacts of any run non-convergences.
  - 3) Discussion of the impacts of uncertainties to model results.
- c) Ensure that mathematical models undergo model validation activities after the model has been developed. The model validation activity/activities completed after the model has been developed shall be dependent upon and consistent with the model's intended use and required level of confidence and shall include one or more of the following:
  - 1) Corroboration of model results with data acquired from the laboratory, field experiments, analog studies, or other relevant observations, not previously used to develop or calibrate the model
  - 2) Corroboration of results with alternative mathematical models
  - 3) Corroboration with information published in refereed journals or literature
  - 4) Peer Review per AP-2.12Q, *Peer Review*

- 5) Technical review, planned in the applicable TWP, by reviewers independent of the development, checking, and interdisciplinary review of the model documentation (the Originator, Responsible Manager/Lead, Checker, QER, and interdisciplinary reviewers assigned to the model document/activity may not serve as an independent post-development model validation technical reviewer)
  - 6) Corroboration of abstraction or system model results to the results of the validated mathematical model(s) from which the abstraction or system model was derived, including corroboration with results of auxiliary analyses used to provide additional confidence in system model results
  - 7) Corroboration of pre-test model predictions to data collected during subsequent, associated testing.
- d) Technical review through publication in a refereed professional journal or review by an external agency, documented by the external agency, may be used to demonstrate additional confidence in the model, if publication or review is used in conjunction with one or more of the model validation activities described in Step 5.3.3c).

#### **5.4 CHECK AND REVIEW**

It is not necessary for the action steps to be performed sequentially. However, all action steps through Paragraph 5.4.6 must be completed before beginning action steps in Paragraphs 5.4.7 through 5.4.12.

##### **5.4.1 Responsible Manager or Lead:**

Assign a Checker to check the model documentation.

- 1) The Originator may not perform the checking function.
- 2) If no other technically competent individual is available, the Lead may perform checking.

##### **5.4.2 Originator:**

Provide to the Checker and QER (an optional Models Checklist, Form 1098 on the BSC Intranet Automated Form System, may be completed by the Originator):

- 1) Check copies of the model documentation. Clearly indicate on the Model Cover Sheet one copy as the "Checker check copy" and one copy as the "QER check copy," initial, and date.
- 2) The DIRS report.

- 3) Other supporting information and documentation that may be requested by the Checker or QER. (Lengthy or large supporting documentation or files may be provided to the checker or QER in advance of the check package submittal.)
- 4) The draft model validation documentation initialed or signed by the CSO during the validation documentation review or copy of electronic mail indicating CSO acceptance (Paragraph 5.3.2).

**5.4.3 Checker:**

- a) Check the model documentation ensuring that (an optional Models Checklist, Form 1098 on the BSC Intranet Automated Form System, may be completed by the Checker):
  - 1) The content and output of the model are technically adequate, complete, and correct.
  - 2) Software, if used, is adequate for its intended use; is identified by the software tracking number, title, and revision/version number; and has been controlled and documented in accordance with AP-SI.1Q, AP-SI.2Q, and/or AP-SI.3Q.
  - 3) Appropriate technical product inputs were selected, correctly identified in the model documentation and on the DIRS report, cited, and incorporated in the modeling activity in accordance with AP-3.15Q.
  - 4) Corroborating data, models, or information is clearly identified and is documented in accordance with AP-3.15Q.
  - 5) Any assumption, data undergoing qualification per AP-SIII.2Q, or other input values are clearly identified and justified.
  - 6) TBV tracking numbers and Unresolved Reference Number tracking numbers, if required, are included in DIRS in accordance with AP-3.15Q.
  - 7) The implications of uncertainties and restrictions are discussed and are evaluated within the model documentation.
  - 8) The assumptions, constraints, bounds, or limits on the inputs are identified in the model documentation, and their impact on the results are described and assessed in the documentation.
  - 9) The discussion of scientific approach and/or technical methods is documented.
  - 10) The referencing is thorough, accurate, and complete, including appropriate project tracking numbers (e.g., records accession numbers

and/or Data Tracking Numbers [DTNs]) and is consistent with the DIRS report.

- 11) Justification and model validation documentation are provided for using a previously developed model outside of its intended purpose, limitations, or range of validity.
  - 12) Data used as direct input are verified to be the same as those in the Technical Data Management System (TDMS).
  - 13) Validation has been completed in accordance with the applicable TWP and the requirements of this procedure.
  - 14) All errata, initiated in accordance with AP-16.1Q, *Condition Reporting and Resolution*, and documented against previous model document revisions/changes, if any, are incorporated in the model documentation.
- b) Clearly and legibly write, or mark electronically, all comments on the Checker check copy or indicate that there are no comments (comments may be documented separately if keyed to the check copy and if comment documentation is signed, dated, and attached to the check copy).
  - c) Initial and date the Checker check copy of the Model Cover Sheet and return the documentation to the Originator.

**5.4.4 QER:**

- a) For models subject to the QARD, perform a quality assurance (QA) check to ensure compliance with this procedure and the applicable TWP.
- b) Clearly and legibly write, or mark electronically, all comments on the QER check copy or indicate that there are no comments (comments may be documented separately if keyed to the check copy and if comment documentation is signed, dated, and attached to the check copy).
- c) Initial and date the check copy of the Model Cover Sheet and return the documentation to the Originator.

**5.4.5 Originator:**

- a) Resolve all comments with the Checker and QER and document the resolution by mark up of the applicable check copy, including the rationale for comments not incorporated or only partially incorporated. Use insert pages as necessary. (Resolution may be documented separately if keyed to the applicable check copy.)
- b) Elevate unresolved comments to the next levels of management of the Originator and Checker/QER until resolution is achieved and document the

resolution. (Resolution may be documented separately if keyed to the applicable check copy.)

- c) Modify the original model documentation, as required, to incorporate comment resolution.
- d) Denote the modified model documentation by revising the alphanumeric revision number.
- e) Provide the modified copy, DIRS report, and applicable check copy to the Checker and QER.

**5.4.6 Checker and QER:**

- a) Check the modified model documentation by comparing it to the applicable check copy.
- b) Indicate acceptance of the resolution of any comment that was not incorporated or was only partially incorporated by accepting the Originator's rationale or by providing separate justification. Initial and date the response, and sign and date the applicable check copy.
- c) Return the documentation to the Originator.

**5.4.7 Originator:**

Prepare a review copy of the model documentation and forward it to the Responsible Manager.

**5.4.8 Responsible Manager:**

- a) Initiate a review in accordance with AP-2.14Q, *Document Review*. Reviews of ICNs are limited to the changes and the portions of the documentation affected by the changes.
- b) Include the CSO, organizations/disciplines providing input to the model documentation, customer organizations/disciplines for the model documentation, and organizations/disciplines affected by the model documentation as mandatory reviewers on AP-2.14Q reviews of the model documentation.

**5.4.9 Reviewing Organization:**

- a) Complete a review of the model documentation in accordance with AP-2.14Q.
- b) If the model does not affect the reviewing organization, indicate "not applicable" and return the review documentation.

**5.4.10 Originator:**

- a) Resolve all comments with the reviewers in accordance with AP-2.14Q. Elevate unresolved comments to the next levels of management of the Originator and reviewers until resolution is achieved and document the resolution.
- b) Develop a concurrence draft by modifying the AP-2.14Q review copy of the model documentation, as required, to incorporate changes resulting from the comment resolution.
- c) After the AP-2.14Q comments have been closed, provide the final concurrence copy of the model documentation to the Lead, CSO, Checker, and QER.

**5.4.11 Lead, CSO, Checker, and QER:**

- a) Ensure that the AP-2.14Q review comments, as resolved, have not adversely affected the model documentation.
- b) Resolve any adverse impacts with the Originator and the Reviewing Organization.
- c) Indicate acceptance by signing and dating the documentation. Return the documentation to the Originator.

**5.4.12 Originator:**

Request lock-out of changes to links in DIRS in accordance with AP-3.15Q.

**5.5 PRODUCT OUTPUT**

**Originator:**

- a) Submit the following to the TDMS in accordance with AP-SIII.3Q:
  - 1) Product output that replaces or supersedes product output currently in the TDMS.
  - 2) Data that have undergone a status change as a result of a qualification within the model documentation.
  - 3) Other output may be submitted, as directed by the Responsible Manager.
- b) Finalize or supersede preliminary product output, if any, in accordance with AP-SIII.3Q.



## **5.6 CONCURRENCE AND APPROVAL**

### **5.6.1 Originator:**

- a) Prepare the model documentation by changing the alphanumeric designator to a numeric designator (i.e., the initial model documentation designator is "00," and subsequent revisions are "01," etc.) and updating the revision history, as necessary.
- b) Complete the Model Cover Sheet in accordance with the instructions in Attachment 3.
- c) Submit model documentation records to the Records Processing Center in accordance with Section 6.0.

### **5.6.2 Responsible Manager:**

- a) If modifications are required as a result of the U.S. Department of Energy's review (AP-7.5Q, *Submittal, Review and Acceptance of Deliverables*), including increasing the revision/change level indicator, ensure the development and change process defined by this procedure is followed.
- b) If the model documentation resolves TBVs/Unresolved Reference Numbers, process them in accordance with AP-3.15Q.

## **5.7 EDITORIAL CORRECTIONS**

### **Originator:**

- a) If the model documentation requires editorial corrections after approval but before distribution by Document Control, change the in-process master as follows:
  - 1) Mark the change(s) by drawing a single line through the change(s) (i.e., pen/ink or electronic changes) and/or inserting the new or correct information.
  - 2) Initial and date the change(s).
  - 3) Note the change(s) in the Remarks section (Block 13) of the Model Cover Sheet.
- b) Obtain the Responsible Manager's/Lead's approval of the change(s) adjacent to the notation on the Model Cover Sheet.

## **5.8 REVISIONS OR CHANGES**

### **Responsible Manager:**

- a) Determine whether the model documentation will be modified as a revision or as an ICN. Reviews of ICNs are limited to the changes and the portions of the documentation affected by the changes.

- b) When initiating a revision or change to an existing document, notify Document Control of the impending action to ensure version control.
- c) Issue no more than five ICNs against a documentation revision.
- d) Process a revision or change in accordance with requirements of Section 5.0 and indicate revisions or interim changes in the model documentation using one of the following:
  - 1) A black vertical line in the margin of the page and notes on the Model Revision Record, clearly indicating which individual sections or subsections were revised, as applicable, and a brief description of the revision or change on the Model Revision Record
  - 2) A note on the Model Revision Record indicating the entire model documentation was revised because the changes were too extensive to use Step 5.8d)1).
- e) Address any applicable errata, documented in accordance with AP-16.1Q in the appropriate section of the model document. List any errata addressed in the Remarks section of the Model Cover Sheet.
- f) Cancel models that are no longer relevant to the project in accordance with AP-6.1Q.

## **6.0 RECORDS**

The records listed in Subsections 6.1 and 6.2 shall be collected and submitted to the Records Processing Center in accordance with AP-17.1Q, *Records Management*, as individual records or included in a records package, as specified. The records listed in Subsection 6.3 shall be dispositioned by the Records Coordinator in accordance with AP-17.1Q.

### **6.1 QA RECORDS**

Records Package for Models Subject to the QARD:

Draft model validation documentation or electronic record of acceptance initialed or signed and dated by the CSO

Checker and QER check copies of the model documentation

Comments or comment sheets; review copy signed and dated by Responsible Manager/Lead, CSO, Checker, and QER; and all documents generated by the AP-2.14Q reviews

Final copy of the DIRS report

Approved Model Report

## 6.2 NON-QA LONG-TERM RECORDS

Records Package for Models Not Subject to the QARD:

Draft model validation documentation or electronic record of acceptance initialed or signed and dated by the CSO

Checker check copy of the model documentation

Comments or comment sheets; review copy signed and dated by Responsible Manager/Lead, CSO, Checker, and QER; and all documents generated by the AP-2.14Q reviews

Final copy of the DIRS report

Approved Model Report

## 6.3 NON-QA SHORT-TERM RECORDS (THREE YEARS OR LESS RETENTION)

Models Checklist(s), if completed by the Originator, Checker, and/or QER

## 7.0 REFERENCES

- a) *Quality Assurance Requirements and Description, DOE/RW-0333P*
- b) *AP-2.12Q, Peer Review*
- c) *AP-2.14Q, Document Review*
- d) *AP-2.22Q, Classification Analyses and Maintenance of the Q-List*
- e) *AP-2.27Q, Planning for Science Activities*
- f) *AP-3.12Q, Design Calculations and Analyses*
- g) *AP-3.15Q, Managing Technical Product Inputs*
- h) *AP-6.1Q, Document Control*
- i) *AP-7.5Q, Submittal, Review and Acceptance of Deliverables*
- j) *AP-16.1Q, Condition Reporting and Resolution*
- k) *AP-17.1Q, Records Management*
- l) *AP-SI.1Q, Software Management*
- m) *AP-SI.2Q, Qualification of Level A Software*
- n) *AP-SI.3Q, Software Independent Verification and Validation*

- o) AP-SIII.1Q, *Scientific Notebooks*
- p) AP-SIII.2Q, *Qualification of Unqualified Data*
- q) AP-SIII.3Q, *Submittal and Incorporation of Data/Technical Information to the Technical Data Management System*
- r) AP-SIII.4Q, *Development, Review, Online Placement, and Maintenance of Individual Reference Information Base Data Items*
- s) AP-SIII.9Q, *Scientific Analyses*
- t) AP-SV.1Q, *Control of the Electronic Management of Information*
- u) *Scientific Process Guidelines Manual*, MIS-WIS-MD-000001

## **8.0 ATTACHMENTS**

Forms and templates attached to this procedure are controlled and distributed as full-size pages separate from this procedure and may be copied for use when implementing this procedure.

Attachment 1 - Acronyms and Abbreviations

Attachment 2 - Model Documentation Outline

Attachment 3 - Model Cover Sheet

Attachment 4 - Model Revision Record (Form ASIII10-2)

BSC	Bechtel SAIC Company, LLC
CSO	Chief Science Officer
DI	Document Identifier
DIRS	Document Input Reference System
DTN	Data Tracking Number
ICN	Interim Change Notice
OCRWM	Office of Civilian Radioactive Waste Management
QA	quality assurance
QARD	Quality Assurance Requirements and Description
QER	Quality Engineering Representative
TBV	To Be Verified
TDMS	Technical Data Management System
TWP	Technical Work Plan

## MODEL DOCUMENTATION OUTLINE

If any of the following sections are not applicable to a particular model, a brief statement of non-applicability is required for documentation purposes under each heading. The document may include additional sections (e.g., an Executive Summary) to assist “users” of the model. Information presented in the model documentation shall be transparent and traceable. Document any deviation from the TWP in the appropriate section and provide justification for the deviation.

1. **Purpose**—This section shall provide the intended use of the model, the model limitations (e.g., data available for model development, valid ranges of model application, spatial and temporal scaling), and scope of the model documentation. It shall also refer to the TWP for the activity.
2. **Quality Assurance**—This section shall include the applicability of the QA program, including evaluation of associated activities in accordance with appropriate implementing procedures. If the modeling activity or tasks included in the modeling activity have been determined not to be subject to the QARD, provide justification. This section shall include the safety category of items and natural barriers if classified in accordance with applicable implementing procedures (e.g., AP-2.22Q, *Classification Analyses and Maintenance of the Q-List*). Reference the TWP for the determination of accountability of the QARD. If the modeling activity investigates an item or barrier on the Q-List, identify the item or barrier and its safety category (Category 1, Category 2, Beyond Category 2, or Non-Safety Category). This section shall identify the method(s) used to control the electronic management of data in accordance with the controls specified in the TWP and will describe any variance from the planned method(s).
3. **Use of Software**—This section shall include a list of all controlled and baselined software used in model development, performance, and validation as described in AP-SI.1Q, AP-SI.2Q, or AP-SI.3Q. Software shall be identified in the scientific analysis/model documentation by software title, software tracking number, and version number.

If the solution to the calculation or analysis package used to support this technical product is obtained using the standard functions of a commercial off-the-shelf software program (e.g., EXCEL, MATHCAD, EARTHVISION, etc.) and the results are not dependent on the software program used, this software does not need to follow AP-SI.1Q. If the results are not dependent on the software program, the actions performed (as indicated below) shall be documented in sufficient detail in this technical product to allow an independent reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the Originator:

- The formula or algorithm used
- A listing of the inputs to the formula or algorithm
- A listing of the outputs from the formula or algorithm

- Other information (e.g., operating environment information) that would be required in order any independent person to reproduce the work.
- 4. Inputs**–Project data shall be referenced by the DTN. Technical product inputs shall be correctly selected, identified in the model documentation, correctly cited and incorporated. This section may contain applicable inputs as described in the following subsections.
- 4.1 Direct Input**–The appropriateness of technical product inputs (data, models, or technical product output) directly used to develop the model shall be documented and substantiated in this section.
- Provide lists or tables of technical product inputs that were used directly in the development of the model.
  - If the present study uses, revises, or changes a previously developed and validated model to complete the present study, list associated DTNs, accession numbers, documentation titles, and document identifying numbers, if applicable.
- 4.2 Criteria**–List criteria identified in Section 3 of the TWP, including requirements contained in applicable Requirement Documents (such as design interface documents) and any relevant acceptance or completion criteria. (Model Validation criteria should be documented in Section 7 of the model document.)
- 4.3 Codes and Standards**–Provide a list of the applicable codes (only if the model directly addresses federal or other code requirements) and standards (e.g., American Society for Testing and Materials or Occupational Safety and Health Administration standards) used in the model by name, number, and date, including applicable revision status, using date or revision designator.
- 5. Assumptions**–This section shall provide a list of the assumptions used to perform the model activity. Discuss assumptions in immediately preceding upstream documentation or input documentation that may significantly impact the results of the present model. Document the assumptions made to develop the model and the rationale for the assumptions. State whether the assumption requires confirmation. If an assumption is determined not to require further confirmation, provide justification. Identify the subsections where assumptions are used. For frequently used assumptions, the comment “used throughout” may be substituted instead of individual references. Assumptions that require confirmation by testing, analysis, or design must also be designated in accordance with AP-3.15Q.
- 6. Model Discussion**–Include a description of the system, process, or phenomenon conceptual model and the scientific, engineering, and mathematical concepts/principles on which the mathematical model is based. Establish the appropriateness of the model for the purposes and within the limitations stated in Section 1 of this attachment.

The use of a scientific notebook(s) in accordance with AP-SIII.1Q, as applicable, is allowed for documenting the model activities, but final model documentation shall be completed to the requirements of this procedure. The documentation can refer to the scientific notebook(s) by title, number, organization, records accession number, or similar information.

Provide lists or tables of corroborating/supporting data, models, or product output used to develop the model. Identify the sources of the corroborating/supporting information. Include additional discussions to substantiate input used in this section if not included in Section 4. Address any differences in direct input values between values brought forward in Section 4 and values used in this section.

The following topics shall be included in this section, as applicable, when documenting a model:

- A detailed description of the conceptual model and the conceptual model implementation (mathematical model)
- Results of literature searches or other background information
- A discussion of uncertainties, sources of uncertainties, and impacts of uncertainties on model output
- Alternate models that were not used and the rationale for not selecting them
- Units of measurement
- Description of the input data used to generate input files for each model simulation
- A discussion of initial and/or boundary conditions
- A discussion of mathematical formulations, equations, algorithms, and numerical methods used
- A discussion of the results of model testing, sensitivities, and calibration activities
- Intended use of the model output
- Other software/computational methods considered and the rationale for not selecting them.

**7. Validation**—The model validation documentation shall include:

- Lists or tables of corroborating/supporting data, models, or information used to complete model validation activities. Identify the sources of the corroborating/supporting information.



- Documentation and discussion of activities performed in Subsection 5.3 of this procedure
- Results of the validation activities
- Model validation criteria for ensuring the appropriate level of confidence has been obtained, consistent with Subsection 5.3 and the applicable TWP
- Rationale for determining that the validation criteria have been met
- Any future activities that need to be accomplished for model validation and a justification for extending model validation beyond the documented completion of the current model.

Because model validation may consist of a sequence of separate activities, each model validation activity should be documented in accordance with the requirements of this procedure upon its completion.

8. **Conclusions**—This section shall provide a summary of the modeling activity. The conclusions, including the DTNs and/or tables or lists of product output as well as any decisions or recommendations based on the modeling activity, shall be presented in this section. Conclusions shall include any uncertainties and restrictions for subsequent use.
9. **Inputs and References**—Sources of inputs, software, DTNs, and cited references (including references used to justify assumptions) shall be listed in this section. Inputs and references include materials that support the conclusions of the model. These may include published reports, technical papers, scientific notebooks, literature searches, or other background information. The online Style Manual may be used as guidance on formatting reference lists and citations.

**Attachments**—Supporting documentation, such as computer output, that are lengthy or cannot be conveniently included within the main text of the documentation may be included as attachments. Computer output may be attached as hardcopy, read-only disk, or compact disk (read only memory), but must meet the requirements of AP-17.1Q. Computer output files included as attachments are exempt from page numbering, DI, and revision number requirements provided the total number of pages in each attachment (for hardcopy) or complete file information, including all file names, file dates and times, and file sizes, are documented on the attachment. In case of printed attachments, the total page count for each attachment shall be documented on the Model Cover Sheet. Where the attachment is on computer media, the quantity and type of media shall be clearly identified on the Model Cover Sheet.

<b>OCRWM</b>	<b>MODEL COVER SHEET</b>	1. QA: Page      of	
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2. Type of Mathematical Model

☐ Process Model
 ☐ Abstraction Model
 ☐ System Model

Describe Intended Use of Model

EXAMPLE

  

3. Title			
4. DI (including Rev. No. and Change No., if applicable):			
5. Total Attachments		6. Attachment Numbers - No. of Pages in Each	
	Printed Name	Signature	Date
7. Originator			
8. CSO			
9. Checker			
10. QER			
11. Responsible Manager/Lead			
12. Responsible Manager			
13. Remarks			

**INSTRUCTIONS FOR MODEL COVER SHEET**

***Originator***

1. Enter QA designator and total number of pages.
2. Check the model type and describe the intended use of the model.
3. Enter the title of the model.
4. Enter the DI, including revision number (alphanumeric before approval, e.g., Rev. 00a, 01a) and change number, if applicable.
5. Indicate the total number of attachments.
6. Indicate the number of pages in each attachment (e.g., I-11, II-5, and III-20). Computer output may be included as hardcopy or as electronic data files contained on appropriate media. In the case of printed attachments, document the total page count for each attachment. If the attachment is on computer media, identify the quantity and type of media attached. If necessary, this information may be placed in Block 13, Remarks, with a reference to Block 6.

Steps 7 through 13 occur after checking is completed and the revision/change designator is changed to a numeric designator. Names may be preprinted.

7. Print or type name; sign and date.

***CSO***

8. Print or type name; sign and date, indicating acceptance of the model documentation.

***Checker***

9. Print or type name; sign and date when all comments have been resolved and changes have been incorporated into the model documentation.

***QER***

10. Print or type name; sign and date when all comments have been resolved and changes have been incorporated into the model documentation.

***Responsible Manager/Lead***

11. Print or type name; sign and date when all reviews have been completed and all issues have been resolved. (If a Lead was not assigned, the Responsible Manager should complete this box.)

***Responsible Manager***

12. Print or type name; sign and date to signify approval.

***Originator, Checker, Lead, Responsible Manager, QER***

13. Include remarks or supplemental information on attachments from Block 6, if required. Indicate any other limitations on the use of the model. The Remarks section of the review copy may also be used to document those draft documents that are in concurrent review and that were used as input (TBV).

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT MODEL REVISION RECORD	
1. Page:      of:	
2. Model Title:	
3. DI (including Rev. No. and Change No., if applicable):	
4. Revision/Change No.	5. Description of Revision/Change
<div style="font-size: 100px; opacity: 0.5;">EXAMPLE</div>	

**INSTRUCTIONS FOR MODEL REVISION RECORD**

***Originator***

1. Enter the page number and total number of pages.
2. Enter the title of the model.
3. Enter the DI.
4. Enter the revision number(s) and change number, if applicable (date is optional).
5. Identify any revisions or changes to this model documentation, in order, starting with Rev 00 and continuing through to the latest revision or change. Indicate the difference from the previous numeric revision by writing a brief description, including the reason for the change (e.g., "This revision incorporates changes to the model based on verification of the assumptions"), and include a brief description of the changes (e.g., "added Attachments I and II").