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Revision: 0



Effective Date: 1/25/2008

## Environment & Remediation Support Services Standard Operating Procedure

### for **DEVELOPMENT, REVIEW, AND DOCUMENTATION OF NUMERICAL MODELS**

#### APPROVAL SIGNATURES:

Subject Matter Expert:	Organization	Signature	Date
Ardyth Simmons	LWSP	Signature on File	
Quality Assurance Specialist:	Organization	Signature	Date
Laura Ortega	QA-IQ	Signature on File	
Responsible Line Manager:	Organization	Signature	Date
Alison M. Dorries	ERSS-DO	Signature on File	

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## 1.0 PURPOSE AND SCOPE

The purpose of this procedure is to describe the process for initiating, developing, reviewing, revising, and documenting a numerical model of groundwater or other geologic media to simulate or understand the movement and distribution of constituents in the environment with the purpose of assisting in decision-making. It ensures consistent development, use, and implementation of all modeling efforts for the Los Alamos National Laboratory (Laboratory or LANL) Water Stewardship Program (LWSP).

This procedure applies to all scales of models developed to support the understanding and prediction of movement and distribution of constituents in the environment. It includes geologic framework models, geochemical models, hydrogeologic flow and transport models, performance and risk assessment models, and visualization products of models. This procedure excludes software configuration management, verification and validation, and/or qualification. This procedure applies to all staff and contractors performing modeling work for LWSP.

## 2.0 BACKGROUND AND PRECAUTIONS

### 2.1 Background

Numerical models are a valuable component of decision support because they integrate data and physical processes on scales not accessible to direct measurement and can provide estimates of the future states of a system. Models are used to understand and predict the movement and distribution of constituents in geologic media at temporal and spatial scales that are not accessible for direct measurement in a laboratory or field study. Numerical models using site-specific data are normally used to test conceptual hypotheses or processes occurring at a site. Predictive models may be used to demonstrate the future performance of a natural or anthropogenic system. Risk assessment models may be used to evaluate the relative risks to the environment and public health posed by different anthropogenic sources or site-specific conditions.

### 2.2 Precautions

None.

## 3.0 EQUIPMENT AND TOOLS

None.

## 4.0 STEP-BY-STEP PROCESS DESCRIPTION (see flowchart in section 5 for an overview of the process)

### 4.1 Need for model development

Project Leader (PL) or other manager	1.	Notify the Conceptual Models and Data Assessment Program Manager that a modeling effort is needed or planned.
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Conceptual Models and Data Assessment Program Manager	2.	Document the decision by PLs, managers, or customers for the modeling effort, its purpose, and intended use by completing Part 1 of a Model Documentation Form (see Attachment 1).
	3.	Assign a task leader to the modeling effort and record in Part 1 of the form.
	4.	Forward the form to the assigned PL for the modeling effort.
Task Leader (TL) for Modeling Effort	5.	Meet with the Conceptual Models and Data Assessment Program Manager to select a lead modeler and record in Part 2 of the Model Documentation Form.
	6.	Meet with customers and other appropriate individuals (as determined by the scope of the modeling effort) involved in the model design, review, and use of the output to communicate the purpose and need for the model and to communicate or clarify management policies for model development, use, and implementation.
	7.	Determine and document the scope, schedule, and budget for the modeling effort (e.g., via memo, e-mail, etc.) and attach to the Model Documentation Form.
	8.	Concurrently, ensure that the scope, schedule, and budget are incorporated into the LWSP (or other programs) baseline, and, if necessary, initiate a BCP change.

## 4.2 Conceptual Model Development

TL for Modeling Effort	1.	Arrange one or more meetings, as necessary, to define the conceptual model(s) to be used and its development and review; include customers, modelers, other project and program personnel, regulators, and other stakeholders, as determined by the Conceptual Models and Data Assessment Program Manager, based on the scope of the modeling effort.
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TL for Modeling Effort (Continued)

3. Document (e.g., via memo, e-mail, or other formal document) the following information about the conceptual model and attach to the Model Documentation Form:
  - types of media being modeled and relationships between media;
  - justification of assumptions;
  - level of realism (preferred) vs. conservatism (define and consider);
  - existing data to be used as input;
  - uncertainties and pedigree of existing data;
  - existing models that may be used or modified;
  - alternative conceptual models, if any;
  - desired or intended accuracy and uncertainty of results;
  - other information as appropriate for the complexity, importance, or customer needs of the model; and
  - resources needed.

[NOTE: This phase of model development should be repeated if major changes are needed at later phases. Agreement on the conceptual model and approach by all customers is critical to acceptance of the model results. Stakeholder agreement is highly desirable.]

4. Select appropriate reviewers to technically and administratively review the model at each stage of development and approval; choose the number of reviewers, type of reviewers, and individual reviewers by considering the complexity, type, and importance of the modeling effort (graded approach).
5. Record the names of the reviewers in Part 2 of the Model Documentation Form and inform them of their selection as reviewers.

Lead Modeler

6. Meet with the programmer or other modeling team members to discuss the computer resources needed, data needs, personnel assignments, and other logistics.
7. Communicate any needed changes to the PL for modeling effort.
8. Obtain review and concurrence on the approach or results via email, paper copy, or memo from the reviewers listed on the Model Documentation Form, and attach to the Model Documentation Form.

### 4.3 Formulation of Model Into Numerical Algorithms

Modeler

1. If not already defined, test and screen potential codes, choose the software to be used, decide on code modifications needed, and/or decide if new code is needed.
2. Consult data subject matter experts (e.g., those who collected or use the data) to understand sources and uncertainties of the data and its limitations to define data needs for the input, calibration, and validation phases.
3. Obtain spatial data only from a controlled and validated GIS data system, as available (e.g., the ADEP GIS data system).

4. Construct or modify existing algorithms.
5. Document (e.g., in memos, papers, e-mails) all work performed in sufficient detail to allow another similarly qualified individual to understand the work and reasons for any decisions.
6. Obtain review and concurrence on the approach or results from the reviewers listed on the Model Documentation Form.
7. Attach appropriate documentation (e.g., memos, papers, e-mails) of the reviewers' concurrence.

#### 4.4 Coding of Model

- |            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Programmer | <ol style="list-style-type: none"> <li>1. Follow all applicable LANL software quality policies and best practices for writing, testing, and documenting all modified or new software code (see <a href="http://erinternal.lanl.gov/ADEP-SQM/">http://erinternal.lanl.gov/ADEP-SQM/</a>).</li> <li>2. If test files were used, confirm that the test files correctly implement the data sets that define the numerical model set up.</li> <li>3. During development, clearly identify on all output from the model each version or revision of the model using a suitable method (e.g., version numbers, dates, or other method) and document all changes in a version or revision history table.</li> <li>5. If code changes are required, prepare a new or revise an existing user manual for the software code.</li> </ol> |
|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

#### 4.5 Calibration of Model

- |         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Modeler | <ol style="list-style-type: none"> <li>1. If appropriate for the type, purpose, and context of the model being used, calibrate the model code using agreed upon calibration data (from Section 4.3 Step 8).<br/><br/>[NOTE: Calibration involves the identification of parameters that need adjustment to achieve the desired accuracy and uncertainty, as defined in Section 4.2.]</li> <li>2. Document the source and pedigree of all data used.</li> <li>3. Describe any modifications to the model based on the calibration data.</li> <li>4. Make a copy (if directed by the modeling PL or review team) of the calibration data set on suitable storage media (e.g., DVD).</li> <li>5. If major changes to the code, conceptual model, or algorithms are deemed necessary, contact the modeling PL and revise the conceptual model according to Section 4.2 above.</li> </ol> |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

6. Obtain review and concurrence on the results via email, paper copy, or memo from the reviewers listed on the Model Documentation Form, and attach to the Model Documentation Form.

#### 4.6 Running the Model

- |         |                                                                                                                                                                                                                |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Modeler | 1. Produce the final model(s) output using agreed-upon input data (from Section 4.3 Step 2).                                                                                                                   |
|         | 2. Save intermediate results at a level of detail sufficient to allow another similarly qualified individual to resume or repeat the work without recourse to the individual who initially performed the work. |
|         | 3. Document the source and pedigree of all input data used for running the model.                                                                                                                              |
|         | 4. Describe any modifications to the input data.                                                                                                                                                               |
|         | 5. If directed by the Task Leader, make a copy of or otherwise store the data set on suitable storage media (e.g., DVD).                                                                                       |

#### 4.7 Validation of the Model (optional)

- |              |                                                                                                                                                                                                                                                                                                                                                                 |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Lead Modeler | 1. If appropriate for the type, purpose, and context of the model being used (as determined during the conceptual model development phase), perform validation runs of the model to validate the final output.<br><br>[NOTE: Validation involves running the model to determine if the results match other known results or expected accuracy and uncertainty.] |
|              | 2. If major changes to the code, conceptual model or algorithms are deemed necessary, contact the assigned PL for the modeling and revise the conceptual model according to Section 4.2 above.                                                                                                                                                                  |
|              | 3. Document the source and pedigree of all input data used during model validation.                                                                                                                                                                                                                                                                             |
|              | 4. Describe any modifications to the validation data.                                                                                                                                                                                                                                                                                                           |
|              | 5. Confirm that input files correctly implement the data sets that define the numerical model set up.                                                                                                                                                                                                                                                           |
|              | 6. Make a copy of or otherwise store (if directed) the computer input files on suitable storage media (e.g., DVD).                                                                                                                                                                                                                                              |
|              | 7. Obtain review and concurrence on the approach or results via email, paper copy, or memo from the reviewers listed on the Model Documentation Form, and attach to the Model Documentation Form.                                                                                                                                                               |

#### 4.8 Reporting on Results and Interpretation

Lead Modeler

1. Using input and contributions from other modeling participants as needed and documentation from earlier phases, document the model results and interpretation in a final report for the PL with the content given in the Content of Model Documentation Final Report (see Attachment 3). An alternate format may be specified by the PL.

[NOTE: Some elements of the attachment are not required for reports that will be included in another document (e.g., a submittal to the NMED).]

2. If the report is subject to the scope of EP-ERSS-SOP-4002, *Document Development*, follow this procedure for preparation of the report.

3. Present the results using visualization tools suitable for displaying the scale and dimensionality of the model.

[NOTE: The visualization and accompanying text explanation must reflect the level of uncertainty of the model analysis.]

4. Document the capability of the visualization tools used, assumptions made, and manipulations performed on the data for the visualization.

5. If the report is a stand-alone document, add to the checklist (Attachment 2) any additional review criteria for the reviewers in the spaces provided. Include as reviewers all involved managers, the requesting PL or the Conceptual Models and Data Assessment Program Manager, and any additional reviewers listed on the Model Development Form.

6. Send the report with included visualization output and Attachment 2 for peer review pursuant to EP-ERSS-SOP-4005, *Peer Review Process*.

7. If the report will be part of another document and the PL determines that it will be reviewed as part of a peer review of that document, forward the report to the PL with recommendations on additional review criteria and suggested reviewers.

8. Follow the peer review process to resolve comments and edits and forward the final report to the Task Leader for the modeling effort.

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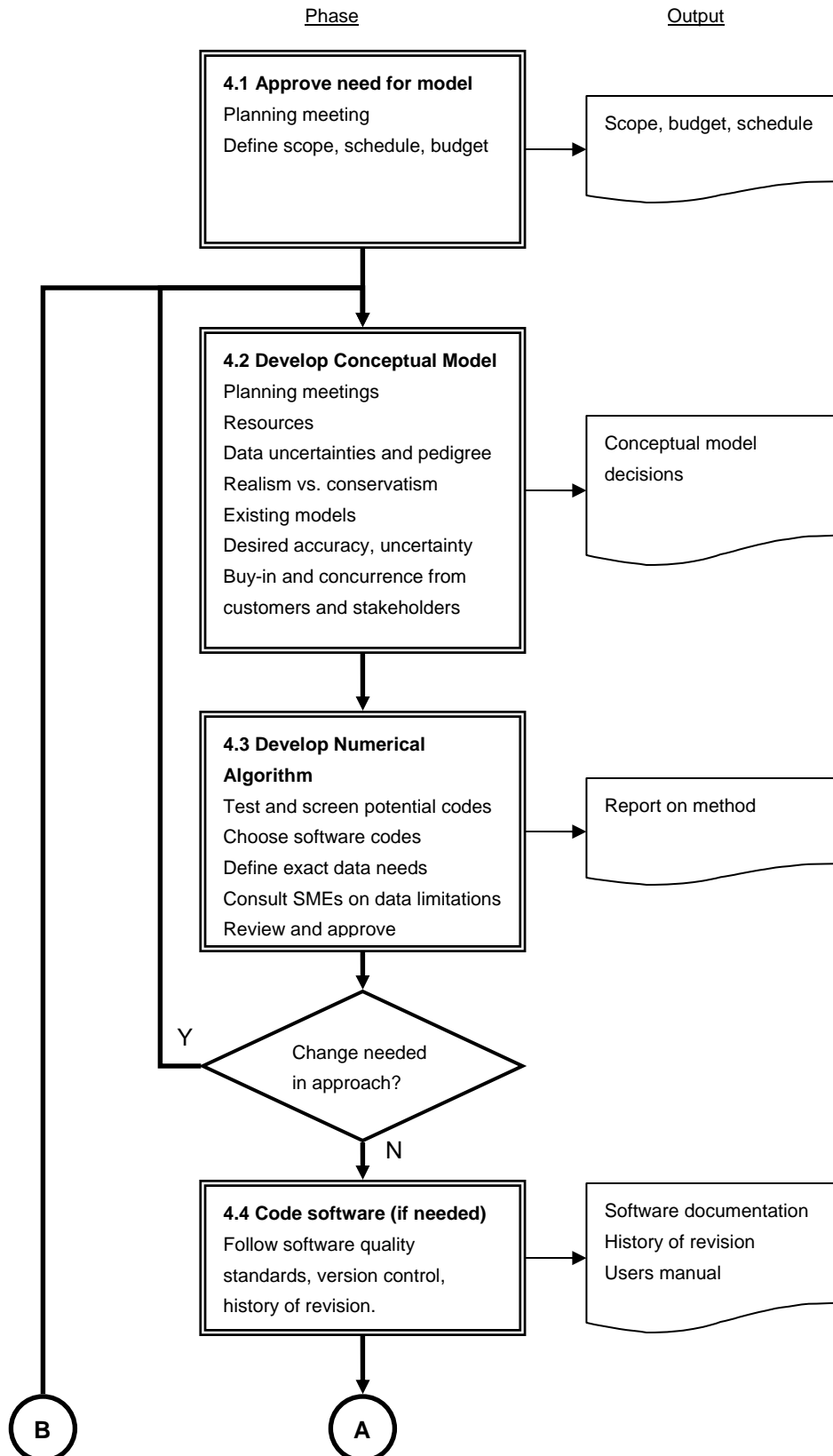
- 
9. Forward the following records generated from this procedure to the PL for modeling effort:
- Numerical algorithm formulation (see Section 4.3);
  - Software code with included documentation and history of revision (if developed or modified) (see Section 4.4);
  - User manual (see Section 4.4);
  - Description of source and pedigree of calibration (see Section 4.5 – optional), input (see Section 4.6), and validation data (optional) (see Section 4.7 – optional);
  - Final model output and pertinent intermediate results and output that might be useful for future modelers, as appropriate (see Section 4.6);
  - Final report (see Section 4.8);
  - Visualization output and documentation of visualization tools used, assumptions made, and manipulations performed on the data (see Section 4.8); and
  - Other documentation, as appropriate, for the type and purpose of the model that would allow an independent person to understand the work done.
- 

Task Leader  
for Modeling  
Effort

11. Assemble a records package of all records with the Model Development Form as the cover for the records package.
- 
12. Submit the records package, including the following records, to the Records Processing Facility:
- Model Development Form;
  - Documentation of conceptual model development and concurrence; and
  - All records produced by the lead modeler.
-



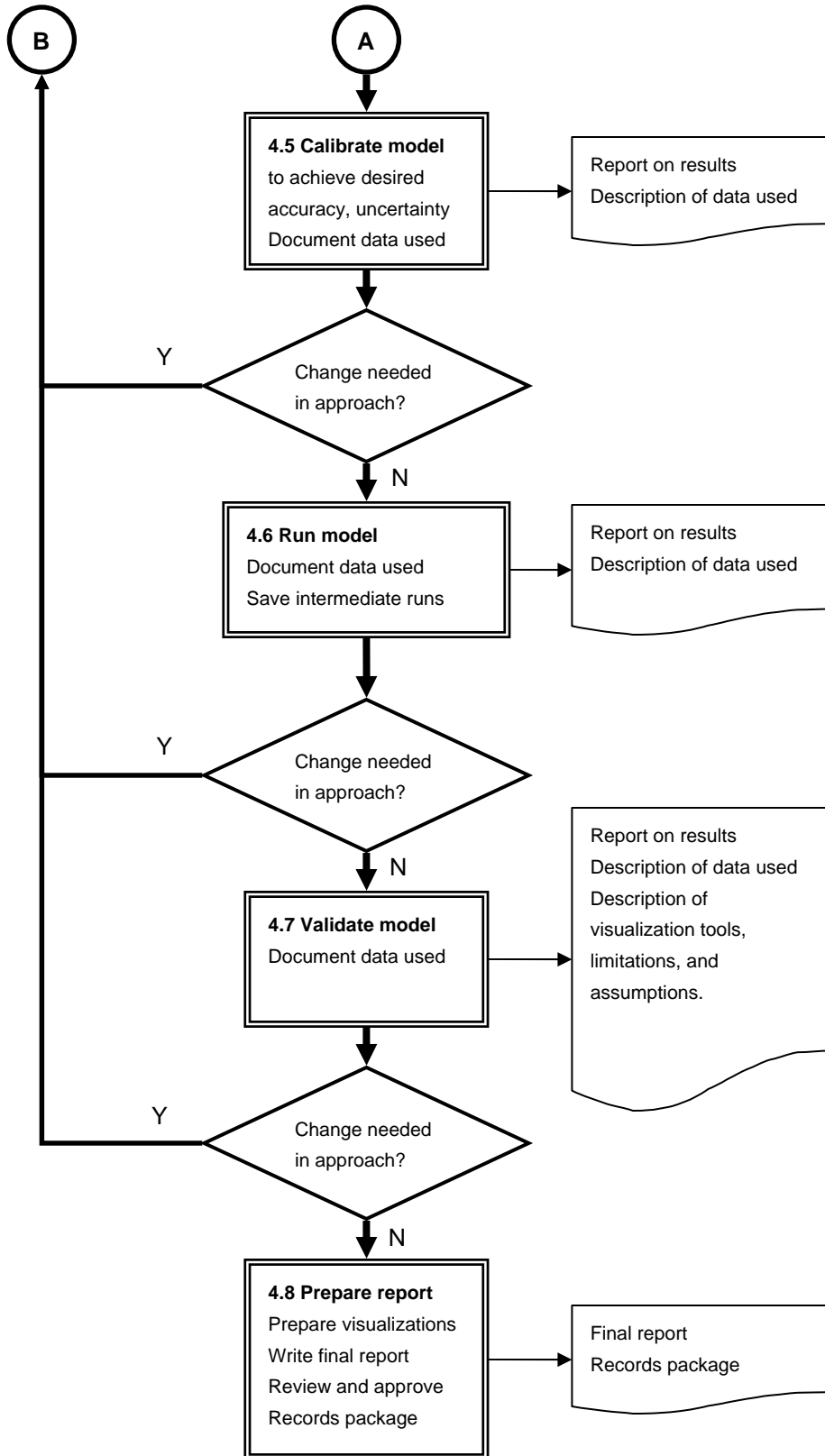
**5.0 PROCESS FLOW CHART**



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6.0



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## ATTACHMENTS

- Attachment 1 5128-1 Model Documentation Form (1 page)
- Attachment 2 5128-2 Checklist for Model Reviewers (1 page)
- Attachment 3 5128-3 Content of Model Documentation Final Report (3 pages)

## 7.0 REVISION HISTORY

Author: Ardyth Simmons

Revision No. <i>[Enter current revision number, beginning with Rev.0]</i>	Effective Date <i>[DCC inserts effective date for revision]</i>	Description of Changes <i>[List specific changes made since the previous revision]</i>	Type of Change <i>[Technical (T) or Editorial (E)]</i>
0.0		New Document	T

[Using a CRYPTOCard, click here to record "self-study" training to this procedure.](#)

If you do not possess a CRYPTOCard or encounter problems, contact the ERSS training specialist.

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**5128 - ATTACHMENT 1: MODEL DOCUMENTATION FORM**

**This form is used to document model development and may be used as the cover for the record series for the model documentation.**

**Part 1** (completed by Conceptual Models and Data Assessment Program Manager):

Assigned Project Leader:

Purpose and need for model:

**Part 2** (completed by assigned Project Leader):

Assigned Modeler:

Reviewer(s) for Conceptual Design:

Reviewer(s) for Calibration Methods:

Reviewer(s) for Numerical Design:

Reviewer(s) Visualization Tools:

Reviewer(s) for Final Report:

PL Signature:

PL Printed Name:

Date:

**Part 3** (completed by assigned modeler):

Phase	Started	Reviewed	Finished	Revised? (Date)	List Documentation Attached
Conceptual Design					
Numerical Design					
Calibration					
Visualization Tools					
Final Report					

List Attached Pages:

Modeler Signature:

Modeler Printed Name:

Date:

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**5128 - ATTACHMENT 2: CHECKLIST FOR MODEL REVIEWERS**

**Peer Review Criteria for Model Output**

Is the document technically adequate, correct, complete, accurate, applicable, and implementable?	Y / N
Is the conceptual model appropriate for the problem to be solved?	Y / N
Is the visualization method clear and appropriate for presenting the results?	Y / N / NA
Is the uncertainty of the model results appropriately addressed?	Y / N
Does the visualization reflect the appropriate level of uncertainty of the model results?	Y / N / NA
Are calculations or methodology correct and described in sufficient detail to permit reproduction without recourse to the originator?	Y / N
Is the level of documentation sufficient to allow similarly-qualified individuals to understand and repeat the work?	Y / N
Are software codes adequately identified to permit reproduction without recourse to the originator?	Y / N / NA
Are table headings correct and figures and tables numbered and referenced correctly in the text?	Y / N
Is the document consistent with applicable regulatory requirements?	Y / N / NA
Have all impacts on other program elements been communicated and addressed?	Y / N

**Other Review Criteria Supplied by Lead Modeler or Project Leader for the Modeling Effort**

	Y / N
	Y / N
	Y / N
	Y / N
	Y / N
	Y / N
	Y / N
	Y / N
	Y / N
	Y / N

Reviewer: All my comments have been addressed or resolved to my satisfaction.

Signature:	Printed Name:	Date:
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**5128 – ATTACHMENT 3: CONTENT OF MODEL DOCUMENTATION FINAL REPORT**

**CONTENT OF MODEL DOCUMENTATION FINAL REPORT**

**Sections to be included in the final report documentation of a model.**

Executive Summary	Brief 1-page summary of report contents, including significant results and conclusions.
Introduction and Purpose	Describe the objectives of the modeling activity. 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.
Codes, Standards, and Regulations	Identify all the applicable codes (only if the model directly addresses federal or other code requirements), standards (e.g., American Society for Testing and Materials or Occupational Safety and Health Administration standards), and regulations used in the model by name, number, and date, including applicable revision status, using date or revision designator.
Assumptions*	Describe the assumptions used, in the absence of direct confirming data or evidence, to perform the model activity.
Discussion*	<p>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 the Introduction and Purpose section. Identify all the corroborating/supporting data, models, or product output used to develop the model. Identify the sources of the corroborating/supporting information.</p> <p>Where appropriate, include the following topics in this section when documenting a model:</p> <ul style="list-style-type: none"> <li>• A detailed description of the conceptual model, including features, events, and processes simulated by the model. The description should include model domain, dimensionality, initial conditions, and boundary conditions, as appropriate;</li> <li>• Description of the mathematical model generally expressed in the form of relevant governing equations;</li> <li>• Description of the numerical model, including analytical or numerical methods, solution technique, and numerical grid, as appropriate;</li> <li>• If a previously developed model was used outside of its intended use, limitation, or range of validity, provide justification for the new/revised intended use;</li> <li>• Results of literature searches or other background information; and</li> <li>• Discuss constraints or limits on inputs and any impacts on model outputs.</li> <li>• Describe uncertainties, sources of uncertainties, and impacts of uncertainties on modeling results.</li> <li>• Verify that all input ranges are within the range of validity of the model or provide appropriate justification.</li> <li>• Alternate models that were not used and the rationale for not selecting them.</li> <li>• Identification of any conservatisms used, and demonstration that other approaches were not</li> </ul>

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	<p>feasible.</p> <ul style="list-style-type: none"> <li>• Description of the input data used to generate input files for each model simulation.</li> <li>• A discussion of initial and/or boundary conditions and an assessment of impacts of boundary conditions on model output.</li> <li>• A discussion of model assumptions and the impact of key assumptions on model output.</li> <li>• A description and source for mathematical formulations, equations, algorithms, and numerical methods used in model development.</li> <li>• 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.</li> <li>• A discussion of the results of model testing, sensitivities, and calibration activities, as applicable. Sensitivity of model results to the numerical methods, including grid resolution and time-step size should be discussed, as appropriate.</li> <li>• Intended use of the model output, including any uncertainties and restrictions for subsequent use.</li> <li>• Comparison between the preliminary and final outputs, as applicable.</li> <li>• Other software/computational methods considered and the rationale for not selecting them, as applicable.</li> <li>• The use of any expert judgments, regardless of whether the judgments were obtained using formal or informal elicitation methods and the reasoning used to arrive at and support the judgments.</li> </ul>
<p>Validation (if done)*</p>	<p>The model validation documentation will include:</p> <ul style="list-style-type: none"> <li>○ Identification of corroborating/supporting data, models, or information used to complete model validation activities. Identify the sources of the corroborating/supporting information</li> <li>○ Level of model importance and required level of confidence</li> <li>○ Discussion of model validation activities performed and results</li> <li>○ Model validation criteria explicitly specified for ensuring the appropriate level of confidence has been obtained. These criteria must address adequacy of the scientific basis and accuracy of the model consistent with intended use.</li> <li>○ Text demonstrating that validation criteria are met consistent with the stated level of confidence required for the model.</li> </ul>
<p>Conclusions*</p>	<p>Provide a summary of the modeling activity. Present the conclusions, including the product output and any decisions or recommendations based on the modeling activity. Include any restrictions for subsequent use. The conclusion section should contain no new information, but only provide a summary of information already presented in previous sections of the document.</p>
<p>Appendices (optional)</p>	<p>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 appendices. Computer input or output may be attached as hardcopy, read-only disk, or compact disk (read only memory). Where the appendix is on computer media, clearly identify</p>

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	the quantity and type of media.
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\* Indicates elements required for a modeling report that is to be included in another document; all elements are required for a stand-alone modeling report.