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Environmental Programs Directorate
Engineering Technology

Standard Operating Procedure

for DEVELOPMENT, REVIEW, AND DOCUMENTATION OF FLOW AND TRANSPORT MODELS

APPROVAL SIGNATURES:

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Quality Assurance Specialist: Paul Lowe	**Organization** QA-IQ	**Signature:**	**Date** 02/28/11
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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 simulating the flow and transport of groundwater or other subsurface fluids, contaminants, natural tracers, and geochemical constituents in the environment. The purpose of the models can be to support various characterization and environmental management activities including conceptual-model analyses, risk assessment, performance assessment, and decision making. The procedure ensures consistent development, use, implementation, and documentation of all modeling efforts for the Los Alamos National Laboratory Environmental Programs Directorate (ADEP).

This procedure applies to all scales (field and laboratory) and types of models developed to support the understanding and prediction of flow and transport of groundwater, subsurface fluids, contaminants, natural tracers, and geochemical constituents in the environment. It includes geologic framework, geochemical, parameter estimation, uncertainty quantification, risk assessment, and decision making models. This procedure applies to all staff and contractors performing modeling work for ADEP.

2.0 BACKGROUND AND PRECAUTIONS

2.1 Background

Numerical models are a valuable component of characterization and environmental management activities because they integrate data, expert knowledge, and physical processes on temporal and spatial scales potentially not accessible to direct measurement, and can provide estimates of the future states of a system. Models are used to understand and predict the flow and transport of fluids and constituents in geologic media over a wide variety of temporal and spatial scales. Models using site-specific data are often used to test conceptual hypotheses about a site. Predictive models may be used to demonstrate the future performance of natural or anthropogenically altered geologic systems. Risk and dose assessment models may be used to evaluate the relative risks to the environment and public health posed by different anthropogenic sources of contamination using realistic site-specific conditions. Decision making models may be used to guide various environmental management activities including optimal design of monitoring networks and remedy selection.

2.2 Precautions

None.

2.3 Definitions

Project Manager (PM) – The PM identifies that a flow and transport model is needed for a given project and helps define the task.

Modeling Subject Matter Expert (MSME) – The MSME is the functional lead for flow and transport modeling within the Environmental Investigations Group in ADEP, as defined on the ET-EI organization chart. The MSME must have a demonstrated background in flow and transport modeling and a sufficient background in hydrogeology. The MSME assures consistency among flow and transport modeling approaches and high quality products across the program. The MSME and the task leader (see below) may be the same person.

Task Leader (TL) – The TL supervises a given modeling project to ensure that the model meets the specified objectives and is documented appropriately. The TL must have a sufficient understanding of the modeling task to be performed. The TL and the lead modeler (see below) may be the same person.

Lead Modeler (LM) – The LM is the person that sets up and runs simulations, and analyzes and documents the model results. The LM must have a demonstrated background and experience to perform the modeling task.

Modeling Team – The modeling team assists the lead modeler with simulations, as needed, depending on the scope of the modeling task. The members of the modeling team must have a sufficient understanding of the modeling task to be performed and follow the guidance provided by the LM.

Model Reviewers –The model reviewers should have sufficient background and experience to review the modeling work. Some of the model reviewers may have expertise other than numerical modeling. For example, they may have insight into key processes, parameter distributions, or site features. The model reviewers cannot be part of the modeling team.

Modeling Report – Modeling reports provide information about the model development process and details about model execution, model input and output flies (see Attachment 2).

Model Archive File - Model Archive File provides storage of the executables, model input and output flies (see Section 4.6.3 below).

3.0 EQUIPMENT AND TOOLS

None.

4.0 STEP-BY-STEP PROCESS DESCRIPTION

4.1 Definition of Modeling Objectives

Modeling Subject Matter Expert (MSME)	4.1.1	The MSME and the TL (see below) define the model intent and objectives, The model intent needs to be short and concise with follow up descriptions of the model objectives; for example, “Test Conceptual Hypotheses”, “Predict Future Performance”, “Risk Assessment”, “Scoping Analysis”, etc. If needed, the PM and MSME will also define how the modeling work will be presented in a deliverable document (a standalone regulatory document or an appendix in a project report; this document can be in addition to the Modeling Report as defined in Section 4.6.2 below). The TL and the MSME may be the same person; in this case, the MSME will not be part of the team of model reviewers.
Task Leader (TL)	4.1.2	Works with the MSME to document the objectives of the modeling effort on a Model Documentation Form (see Attachment 1).
	4.1.3	Meet with the MSME to select a Lead Modeler (LM), if different from the MSME, and Model Reviewers. The TL and the LM may be the same person. Record the selection on the Model Documentation Form. The reviewers should be familiar with the type of modeling to be performed, as they will ultimately be peer reviewers for the Modeling Report or overall document containing the description of the modeling effort (see SOP-4005, *Peer Review Process*).
	4.1.4	Together with the MSME, meet with appropriate individuals (as determined by the objectives and scope of the modeling effort, including geologists, hydrologists, and geochemists) involved in the model setup, development, review, and use of the output to communicate the objectives and need for the model. The TL should communicate management policies for model setup, development, review, use, and implementation.

4.2 Conceptual Model Development

TL

4.2.1 In agreement with the PM and MSME, arrange one or more meetings, as necessary, to define the conceptual model(s) to be used in the modeling effort based on the modeling objectives and the available site data; include customers, modelers, project and program personnel, regulators, and stakeholders based on the scope of the modeling effort.

4.2.2 A model-description document shall be prepared, taking into account model intent and objectives. The model description document should include, as applicable, the following information:

- types of media being modeled and their relationships;
- conceptualizations of various model elements, including alternatives (if any) and uncertainties; the considered conceptual model elements should include dimensionality, governing process, phases, model domain, initial/boundary conditions, heterogeneity of the subsurface flow and transport medium, medium properties, etc.
- justifications of assumptions related to various conceptual model elements;
- desired level of realism vs. conservatism to be applied in the modeling effort depending on the modeling objectives;
- preferences regarding formulation of the numerical model (e.g. numerical vs. analytical techniques) and applied computational codes;
- desired properties and resolution of the computational grid(s) and spatial/temporal discretization of the simulated process;
- desired representation of geological framework model (GFM), and heterogeneity associated with the subsurface flow and transport media in the model;
- existing data to be used as model inputs, calibration and validation data;
- calibration approach;
- uncertainties and pedigree of existing data, including prior probability distributions;
- existing models and/or codes that may be used or modified;
- development of new codes and scripts;
- desired accuracy and uncertainty in the modeling results;
- approaches for analyses of the modeling results including residual analysis, quantification of uncertainty in model predictions, model-parameter sensitivity, posterior uncertainty in model parameters (posterior probability distributions), information content in existing data, etc.
- resources needed; and
- work scope.

The model-description document should be updated if major changes are needed during the later stages of model development.

4.2.3 Obtain review and concurrence on the prepared model-description document (Section 4.2.2) from the MSME and reviewers listed on the Model Documentation Form. If proposed by the PM and MSME, obtain review and concurrence on the prepared model-description document by responsible managers, customers, and stakeholders.

TL (cont.)	4.2.4	Meet with the LM and any other members of the modeling team to discuss the computer resources needed, personnel assignments, and other logistics. 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. Communicate any proposed changes in the work scope to the PM and MSME.
4.3 Formulate Model		
LM/Modeling Team	4.3.1	Document the source and pedigree of all the data applied in the modeling process. Obtain data from a controlled data source, if possible. Define uncertainties and limitations associated with the data applied in the design, calibration, and validation phases of the modeling effort. If needed, consult subject-matter experts (e.g., those who collected or use the data) to understand sources and uncertainties of the data that will be applied in the model development.
	4.3.2	Taking into account modeling objectives and existing data, formulate the numerical model based on existing, modified or newly developed codes and algorithms.
	4.3.3	Obtain review and concurrence on the approach for development of the numerical model and the expected modeling results from the MSME, TL, and reviewers listed on the Model Documentation Form.
4.4 Implement Model		
LM/Modeling Team	4.4.1	Keep a log of the model outputs from each version or revision of the model that provided important information in the process of model development using a suitable method (e.g., version numbers, dates, or other method) and document all changes in a version or revision history table to be included in the Modeling Report. Document pertinent intermediate results, if applicable, at a level of detail sufficient to allow an independent, appropriately-trained expert to reproduce the modeling work. Use visualization techniques to represent the model structure and important modeling results.
	4.4.2	Follow all applicable LANL software quality policies and best practices for writing, testing, and documenting all modified or newly developed codes.
	4.4.3	If appropriate for the type, objectives, and context of the model, calibrate the model using agreed upon calibration approach and data. **NOTE**: Calibration involves the identification and adjustment of parameters to achieve the desired modeling accuracy, as defined in Section 4.2.2
	4.4.4	Verify that the model implementation is consistent with the objectives and scope of the modeling work, and follows the model-description document (Section 4.2.2). If there are deviations, contact the MSME and the TL, and propose revisions of the model-description document (Section 4.2.2).
	4.4.5	If the process of model implementation suggests major changes to the conceptual model, computational code, or algorithms, contact the MSME and the TL, and propose revisions to the conceptual model or numerical solution according to Section 4.2.1.

LM/Modeling Team (cont.)	4.4.6	Communicate the modeling progress to the TL and MSME.
4.5 Evaluate Model Performance		
LM	4.5.1	If appropriate for the intent, objectives, and context of the modeling effort, compare field or reference data to modeling results to analyze their uncertainties and limitations.
	4.5.2	If the comparison of the modeling results against the existing data suggests major changes to the conceptual model, input parameters, computational code or algorithms, contact the MSME and the TL and propose revisions to the conceptual model, parameters, or numerical methods according to Section 4.2.
	4.5.3	Communicate the modeling results and conclusions to the TL and MSME.
4.6 Model Documentation, Reporting and Reviewing		
LM	4.6.1	Communicate modeling results to the TL and MSME. If requested by the PM and MSME, communicate the modeling results and conclusions to project and program managers, regulators, and stakeholders.
	4.6.2.	Write a Modeling Report or applicable section of a document that presents the results of the modeling work. The sections and level of documentation in the report will be defined by the TL and MSME based on the modeling objectives and nature of the report. The modeling can be reported as a standalone document or electronic interactive document. The content should include descriptions of: • modeling objectives and scope of work; • conceptual model elements and their uncertainty; • assumptions related to development of conceptual and numerical models; • source, pedigree and uncertainty of the model inputs, calibration and validation data (if used); • process of model development; • appropriate visualization of the model structure and important modeling results; • input and output files; • codes, scripts, and algorithms used for simulation, preprocessing, postprocessing, and data analysis; if the applied codes and scripts are not documented elsewhere provide execution instructions and/or manuals, revision history, verification and validation runs; software codes such as Mercurial (http://mercurial.selenic.com) and Doxygen (http://www.doxygen.org) are recommended for tracking the version history and developing the modeling and software documentation; and • summary and conclusions. The information provided in the report should be sufficient to allow an independent, appropriately-trained expert to understand and replicate the modeling effort. Additional information about the content of the report is provided in Attachment 2 below (Suggested Outline for Model Reporting). In addition, the modeling work may be summarized in a separate deliverable document (standalone regulatory deliverable document or an appendix in a project report; see Section 4.1.1)

LM (cont.)	4.6.3.	Prepare a single compressed Model Archive File. This should combine various types of information about the modeling effort including relevant input and output files in electronic form. The Model Archive File should include: • the Modeling Report (standalone or embedded as an appendix in a project report or regulatory deliverable document as described in Section 4.6.2); • complete set of input files required to execute versions of the model discussed in the Modeling Report; • final and pertinent intermediate modeling results discussed in the Modeling Report in the form of output files; if the sizes of some of the input/output files are such that they prevent their inclusion in the Model Archive File (e.g., on the order of GB's), abstracted information should be provided that is sufficient for comparisons of independent model executions; if the input/output files are stored in proprietary binary format, a plain-text (ASCII) version of the input/output files should be provided as well; and • source and executable files of the applied software codes and scripts (if not documented and stored elsewhere with appropriate version control).
	4.6.4.	Submit the completed Model Documentation Form and Model Archive File to the ADEP Records Processing Facility (RPF). If the work is performed within the Earth and Environmental Sciences (EES) Division, the Model Archive File may also be stored in the EES Model Repository.
TL, MSME and Reviewers	4.6.5.	Ensure that the Model Archive File contains the items required (see Section 4.6.3), and that the level of documentation is sufficient to allow the work to be replicated by an independent appropriately trained expert.
Documents Team	4.6.6.	Ensure that the Model Documentation Form is complete and correct.
	4.6.7.	Following existing procedures to submit the Model Archive File to ADEP Records Processing Facility.
	4.6.8.	Add the reviewers listed on the Model Documentation Form to the list of experts that will provide Peer Review of the document containing the modeling results, the Modeling Report, and the Model Archive File.
Reviewers	4.6.9	The reviewers in their review should address the following questions: 1. Are the conceptual model, assumptions, model setup, results and conclusions consistent with the model intent and objectives? 2. Are the model assumptions and choices clearly stated and well justified? 3. Are calculations correct and described in sufficient detail to permit their reproduction by an independent, appropriately-trained expert? 4. Are the utilized data, model input and output clearly labeled and traceable? 5. Is the description of work performed complete and accurate? 6. Is the description of obtained results complete and accurate? 7. Does the Model Archive File provide a complete and accurate representation of the model files? 8. Are the caveats, restrictions and limitations associated with the modeling work well identified?

5.0 ATTACHMENTS

Attachment 1 EP-DIV-SOP-10011-1 - Model Documentation Form (1 page)

Attachment 2 EP-DIV-SOP-10011-2 - Suggested Outline for Modeling Report (1 page)

6.0 REVISION HISTORY

Revision No. *[Enter current revision number, beginning with Rev.0]*	Effective Date *[DCC inserts effective date for revision]*	Description of Changes *[List specific changes made since the previous revision]*	Type of Change *[Technical (T) or Editorial (E)]*
0	3/8/11	New document number assigned; Supersedes EP-ERSS-SOP-5128, R0	T/E

Using a CRYPTO Card, click here for "Required Read" credit.

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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 the **Task Leader** (**TL**) assigned to manage modeling effort by **MSME**)

Task Leader (**TL**) :

Objectives and requirements for modeling effort:

Lead Modeler (LM):

Modeling Subject Matter Expert (to be included in any later Peer Review):

Model Reviewers (to be included in any later Peer Review):

Name of final report or other final document containing the modeling results and analyses:

Part 2 (completed by **Lead Modeler (LM)** based on input from **MSME** and **TL**)

Specify the level of documentation in the Modeling Report, and how the modeling work will be documented and presented in a deliverable document (a standalone regulatory deliverable document or an appendix in a project report):

Program Manager (PM) Signature:	Printed Name:	Date:
Modeling Subject Matter Expert (MSME) Signature:	Printed Name:	Date:
Task Leader (TL) Signature:	Printed Name:	Date:
Lead Modeler (LM) Signature:	Printed Name:	Date:

ATTACHMENT 2: SUGGESTED OUTLINE FOR MODELING REPORT	
Executive Summary	Briefly summarize the report contents, including results and conclusions.
Intent and Objectives	Describe the model intent and objectives.
Introduction	Describe the scope of the modeling work.
Standards and Regulations (if applicable)	If the model directly addresses federal, state, or other requirements, standards, and regulations, list the applicable information (e.g., document name, number, date, revision, version number, etc.).
Model Conceptualization and Assumptions	Describe the model conceptualization and assumptions; provide justifications for assumptions related to various conceptual model elements. Discuss level of realism vs. conservatism applied in the modeling effort depending on the modeling objectives. Describe alternate conceptual models that were not used and the rationale for not using them. Identify all the corroborating data, models, documents/publications or expert knowledge used to justify the selected conceptual model(s).
Methodology	Describe the modeling approach including references to relevant documents and publications. As appropriate, describe the numerical model, including computational domain, initial/boundary conditions, computational grid, computational methods, solution technique, etc. If needed, identify corroborating data, models, documents/publications or expert knowledge used to justify the approach for model development.
Model Verification and Validation (if applicable)	If the applied codes and scripts are not already verified and validated, provide verification and validation runs that demonstrate their applicability for the modeling effort.
Model Inputs	Present and describe model inputs. Describe pedigree and uncertainties associated with all the model inputs. Verify that all the model inputs are within the range of validity of the applied model or provide appropriate justification.
Modeling Results	Present and describe modeling results. If appropriate, compare the results to previous or other relevant modeling analyses (published in the literature or documented elsewhere). Describe accuracy and uncertainties associated with modeling results. Verify that all the model outputs are within the range of validity of the applied model or provide appropriate justification. If appropriate, compare obtained modeling results against existing data. Discuss the obtained residuals.
Conclusions and Caveats	Summarize decisions or recommendations based on the modeling effort. Present limitations and caveats associated with modeling effort (e.g., data availability, valid ranges of model simulation and predictions, spatial and temporal scaling). Discuss any restrictions for subsequent use of the modeling results.
Appendices	Source files of applied code and scripts (if not documented and stored elsewhere with appropriate version control); execution instructions and documentation of applied code and scripts (if not documented and stored elsewhere with appropriate version control); input and output files; modeling workflow.