



**NYE COUNTY NUCLEAR WASTE
REPOSITORY PROJECT OFFICE
TECHNICAL PROCEDURE**

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COMPUTER MODELING QUALITY ASSURANCE PROCEDURE

Area 5 Radioactive Waste Management Site
Nevada Test Site
Mercury, Nevada

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1 PURPOSE¹

This Standard sets forth the requirements of the Computer Modeling Quality Assurance Procedure (CMQAP). The CMQAP shall be used by personnel responsible for simulating processes pertinent to the Area 5 Radioactive Waste Management Site (RWMS) of the Nevada Test Site (NTS) through the use of computer codes. This Standard shall be used in conjunction with Basic and Supplementary Requirements set forth in American Society of Mechanical Engineers (ASME) NQA-1-1989 edition (*ASME*, 1989a), NQA-3-1989 edition (*ASME*, 1989b), and Reynolds Electrical & Engineering Company, Inc. (REECO) Quality Assurance Program (1990) when and to the extent specified by the organization invoking this Standard.

¹Adapted from ASME NQA-1 and ASME NQA-3 (1989a and 1989b, respectively).

2 SCOPE²

The requirements set forth in this Standard apply to activities that are performed to provide the support necessary to demonstrate that a given site-specific model is valid (i.e., capable of providing meaningful site-specific Performance Assessment predictions). The requirements of this Standard are adapted in part from: 1) the Computer Program Testing Requirements promulgated by REECo (*REECo*, 1990) and the ASME (*ASME*, 1989a and 1989b). Methodologies are provided in this Standard for the following procedures:

1. Code Modification;
2. Code Compilation;
3. Code Verification;
4. Design of Site-specific Model;
5. Model Calibration;
6. Uncertainty Analysis;
7. Model Verification;
8. Predictive Simulations;
9. Sensitivity Analysis; and
10. Model Validation.

These procedures involve direct manipulation and use of computer codes designed to simulate processes pertinent to the Area 5 RWMS. Procedures for conducting the steps performed prior to manipulation and use of these codes (e.g., establishing the purpose of the modeling effort, developing the conceptual model, selecting the governing equation(s), verifying the governing equation(s), and selecting the computer code) as described in the literature (*Case and Otis*, 1988 and *Anderson and Woessner*, 1992) are not documented in this Standard.

To the extent applicable to the activities being performed, the application of this Standard, or portions thereof, and the provisions of ASME NQA-1 (*ASME*, 1989a) and ASME NQA-3 (*ASME*, 1989b) Basic and Supplementary Requirements, shall be specified in written contracts, policies, procedures, or instructions.

²Adapted from ASME NQA-1 and ASME NQA-3 (1989a and 1989b, respectively).

3 DEFINITIONS

calibration target: That region in space (one-, two-, or three-dimensional) defined by some chosen underlying statistical distribution, in which repeated measurements of a variable may approach or fall within. Simulated values must equal or approach the calibration target before calibration is deemed successful. Associated with *Model Calibration* (Section 5.5).

calibration values: Laboratory- or field-derived values of a specific parameter. Associated with *Model Calibration* (Section 5.5).

Code Compilation: The process of translating the source code (e.g., FORTRAN) into a set of machine-readable instructions.

Code Modification: The process of incorporating various changes in the code logic and/or code structure for the express purpose of improving the code (e.g., increased execution speed, inclusion of new or better physical, chemical, or biological processes).

Code Verification: Following compilation, the results obtained using the selected code for a test problem (preferably, one supplied by the author) must be compared to those obtained by the author to ensure that model predictions are not hardware- and compiler-dependent and that the code functions as advertised. A successful verification demonstrates that the code includes the documented equations and that the numerical solution algorithms are adequately accurate (*Case and Otis, 1988*).

coefficient of variation (η_x): The sample standard deviation (σ_x) divided by the sample mean (μ_x). In mathematical terms:

$$\eta_x = \frac{\sigma_x}{\mu_x} \text{ in the underlying population sense}$$

Design of Site-specific Model: The concept of building a mathematical structure which is specifically tailored to a given site (e.g., arid region concepts vs. humid region concepts).

interpolation error: The error committed in estimating "in-between" values of the value of a parameter or variable when only a set of discrete calibration values are available (e.g., linear interpolation). Associated with *Model Calibration* (Section 5.5).

Mean Error (ME): The mean of the difference between n observations of a measured variable, Q_i , and its theoretical mean. In mathematical terms:

$$ME = \frac{1}{n} \sum_{i=1}^n (Q_i - \bar{Q}), \quad \bar{Q} = \frac{1}{n} \sum_{j=1}^n Q_j$$

where:

n \equiv number of measured points
 Q_i, Q_j \equiv measured parameter value
 \bar{Q} \equiv theoretical mean of parameter value

Mean Absolute Error (MAE): The mean of the sum of the absolute deviations of n observations of a variable and its theoretical mean. In mathematical terms:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |Q_i - \bar{Q}|, \quad \bar{Q} = \frac{1}{n} \sum_{j=1}^n Q_j$$

where:

n \equiv number of measured points
 Q_i, Q_j \equiv measured parameter value
 \bar{Q} \equiv theoretical mean of parameter value

measurement error: The error in the calibration value and is associated with the accuracy of the measurement device, the personnel performing the measurement, and the location and accuracy of benchmark points. Associated with *Model Calibration* (Section 5.5).

Model Calibration: The process of adjusting model parameters so that the code output more closely matches site-specific observations.

Model Validation: The process of comparing the output of either an analytical model or a numerical model with actual field or laboratory data for the same variables.

Model Verification: The process of comparing the output from an analytical model (i.e., simple fundamental functions) with the output of a complex numerical model which has been run in the same mode as the analytical model.

Predictive Simulations: Computer runs made with prescribed input data sets purposely set outside the region of calibration with the express desire of measuring the deviation between these output values and subsequent laboratory- and/or field-derived values.

record: A hard-copy or electronic (e.g., fixed disk and floppy disk) file or document. Associated with Records Management (Section 8).

residual: The difference (or "error") between measured and simulated values.

Root Mean Square Error (RMSE): The square root of the mean of the sum of the squares of the deviations of n observations of a variable and its theoretical mean. In mathematical terms:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (Q_i - \bar{Q})^2}, \quad \bar{Q} = \frac{1}{n} \sum_{j=1}^n Q_j$$

where:

n \equiv number of measured points

\underline{Q}_j, Q_j \equiv measured parameter value

\bar{Q} \equiv theoretical mean of parameter value

scale effect error: The error in the calibration values associated with transcending scales (e.g., small to medium to large, trying to estimate effects at small scale given data at either a medium or large scale). Associated with *Model Calibration* (Section 5.5).

Sensitivity Analysis: The process of determining the relative influence of several input parameters on a specified model output. This is a useful tool for limiting the sources of uncertainty analyses and allocating resources for data collection.

transient effect error: The measurement error in a system which changes with time and may in fact, disappear with time.

Uncertainty Analysis: The process of estimating the potential variability in model output values based upon knowledge of variability of input parameters.

validation target: That region in space (one-, two-, or three-dimensional) defined by some chosen underlying statistical distribution, in which repeated measurements of a variable may approach or fall within. Simulated values must equal or approach the validation target before validation is deemed successful. Associated with *Model Validation* (Section 5.10).

verification residual: The difference between values obtained using a numerical solution and those obtained using an analytical solution.

4 RESPONSIBILITIES³

The organization invoking this Standard shall be responsible for specifying which requirements, or portions thereof, apply and appropriately relating them to specific activities. To the extent necessary, the organization invoking this Standard shall also invoke the applicable provisions of ASME NQA-1 (*ASME*, 1989a) and ASME NQA-3 (*ASME*, 1989b) Basic and Supplementary Requirements. The organization upon which this Standard, or portions thereof, is invoked shall be responsible for complying with the specified requirements.

³Adapted from ASME NQA-1 and ASME NQA-3 (1989a and 1989b, respectively).

5 PROCEDURE

The following describe the specific requirements of the CMQAP. These procedures are mandatory unless otherwise noted. All forms of documentation associated with these procedures (codes, input and output files, calculations, figures, tables, forms and checklists, batch files, maps, assumptions, and spreadsheets) shall be reviewed and signed off by responsible personnel.

5.1 Code Modification

- 5.1.1. Electronic (e.g., floppy disk) and hard copies of the unmodified and modified versions of the code shall be kept in project files.
- 5.1.2. Additional statements in the modified code and deleted statements in the original hard-copy of the code should be highlighted so as to be readily visible to reviewers and future users. Methods by which statements can be highlighted include colored (fluorescent) ink markers or readily visible or otherwise unique comment statements.
- 5.1.3. Differences between the modified and original code shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.
- 5.1.4. Initial comments in program "main" (i.e., those which provide general information regarding the code including the title, purpose(s), and original author(s)) shall be expanded to identify the author, date, and purpose(s) of the modifications. The means by which the author performing the modification may be contacted (i.e., telephone, facsimile, telex, electronic mail numbers) shall also be included in these initial comments.
- 5.1.5. All modifications shall be preceded with a comment statement noting the function, date, and author of the modification, as well as the location of files which contain supporting documentation and calculations. These comment statements shall contain a common text string (e.g., "Modification") which can be readily located by search functions.
- 5.1.6. For modifications which: a) alter the manner in which the code simulates a certain process or b) include a new process, simulations shall be performed:
 - 5.1.6.1. Before and after modification using a test problem which accesses the modified subroutine(s) to ensure that the modification produces the

desired effect. Results using the original and modified versions of the code shall be depicted graphically to clarify the effect of the modification.

- 5.1.6.2. Before and after modification using a test problem which does not access the modified subroutine(s) to ensure that the modification does not inadvertently affect the results produced by other portions of the code.
- 5.1.6.3. After modification to compare the results obtained using the modified code against those obtained using a previously verified code on a published test problem to ensure the modification(s) produce accurate results.
- 5.1.7. For modifications which: a) alter the manner in which the code reads input files and writes output files or b) increase execution speed, simulations shall be performed after modification to compare initial conditions as well as interim and final results to ensure that: a) the manner in which the input files are read and output files are written has not been corrupted and b) the manner in which the code performs calculations has not been corrupted, respectively. Initial conditions and results using the modified and original code shall be graphically depicted to ensure that the modified code performs these functions properly.
- 5.1.8. In all cases, the results of these aforementioned test simulations shall be documented as set forth in the General Requirements of this Standard and kept in the project files.

5.2 Code Compilation

- 5.2.1. Date(s), personnel, hardware, and software (including license number) associated with compilation shall be documented as well as the name of the code being compiled.
- 5.2.2. The reason(s) for using the chosen compiler as opposed to other available compilers shall be documented.
- 5.2.3. Compiler-specific commands including switches which activate certain compilation features (e.g., use of a coprocessor, optimization of loops, vectorization, etc.) shall be documented.
- 5.2.4. The compilation shall be performed in batch mode to facilitate compilation and its associated quality assurance procedures. A hard copy of the compilation batch file shall be kept in the project files.

- 5.2.5. Filenames of the compilation batch, source, object, and run-time (executable) files shall also be documented. It is recommended that a system-generated catalog listing be printed and kept in project files to facilitate this procedure.

5.3 Code Verification

- 5.5.1. A test simulation shall be performed using the compiled code to compare the results obtained by another individual (preferably the author) using different hardware and compiler software to ensure that model predictions are not hardware- and compiler-dependent and that the code functions as advertised.
- 5.3.2. It is recommended that the results obtained using the selected code for a given test case be compared to those obtained using another previously tested and confirmed code.
- 5.3.3. Test input and output files should be obtained from the other individual to facilitate this procedure.
- 5.3.4. The results of this test simulation, including notes regarding differences in the results obtained, shall be documented.

5.4 Design of Site-specific Model

5.4.1. Design of the Grid

- 5.4.1.1. The model grid shall be based on one certified hand- or computer-drawn site map supplied by a registered surveying contractor. The client and the surveying contractor shall be contacted to ensure that these individuals are aware of the version being used to develop the grid.
- 5.4.1.2. The stepwise procedure used to create the model grid shall be documented. Documentation shall include separate maps which show the rationale used in developing the grid. The first map may include grid lines drawn to define boundary conditions, the second to define wells, hydraulic structures, or other man-made boundaries, the third to define changes in conductivity, the fourth to define changes in thickness, and the fifth to define initial hydraulic conditions. Additional maps (e.g., initial concentration condition maps) shall be developed depending on the input requirements and capabilities of the model.
- 5.4.1.3. The final grid shall be developed using computer-aided-design (CAD) software to ensure accuracy. A hard-copy of the final grid shall be kept in project files.

- 5.4.1.4. The name of the computer on which the final grid resides, the software used, the directory path, and the date generated shall be contained on the hard-copy as a footnote and documented in project files.
- 5.4.1.5. Copies of the final grid shall be distributed to the client and certified surveyor for final review prior to performing site-specific simulations.
- 5.4.2. Parameters associated with Boundary Conditions, Initial Conditions, Aquifer Properties, and Stresses
- 5.4.2.1. Values for these parameters shall be based on site-specific data when available. The source(s) (i.e., names of field personnel and/or contractor) and the date(s) on which the data was obtained shall be documented. Copies of original field notes showing these data shall be kept in project files. The methods by which the data was obtained shall also be documented. Figures and tables associated with these data shall be generated and kept in project files.
- 5.4.2.2. If site-specific data regarding these parameters are not available, data supplied by local, state, and federal agencies shall be used. Supporting documentation, calculations, and assumptions associated with those parameters for which site-specific or agency-supplied values are not available (or not required for the given model application) shall be kept in project files.
- 5.4.3. Preliminary Values of Time and Convergence Parameters
- 5.4.3.1. The trial-and-error process of selecting final values for time and convergence parameters shall be documented. Final values for parameters related to initial time step size, maximum and minimum time step sizes, minimum and maximum number of iterations, and convergence criteria shall also be documented.
- 5.4.4. Modeling personnel shall maintain a logbook of all simulations related to the design of the model which shall contain the following information:
1. Complete (i.e., path included) input filename(s) and date finalized.
 2. General comments regarding the nature of the input with specific emphasis placed on alterations.
 3. Starting and ending date of simulation.
 4. Simulation run-time.
 5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
 6. General comments regarding the nature of the output and any error messages.

7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

5.4.5. The hard-copy of the final version of the input file generated as the result of the model design process shall be kept in the project files.

5.5 Model Calibration

5.5.1. Modeling personnel shall maintain a logbook of all calibration simulations which shall contain the following information:

1. Complete (i.e., path included) input filename(s) and date finalized.
2. General comments regarding the nature of the input with specific emphasis placed on alterations.
3. Starting and ending date of simulation.
4. Simulation run-time.
5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
6. General comments regarding the nature of the output and any error messages.
7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

The following procedures regarding model calibration have been adapted from *Anderson and Woessner* (1992) unless otherwise noted. The following are recommended procedures to be used in completing model calibration. Alternative procedures which accomplish the overall objective of the recommended procedures (i.e., show a logical progression of parameter adjustments leading to simulated results which show that the model can reproduce field-measured values) may be substituted at the discretion of modeling personnel.

5.5.2. The following procedures shall be performed and documented prior to conducting calibration simulations:

- 5.5.2.1. Select the parameters to be calibrated (calibration parameters).
- 5.5.2.2. Select calibration values for the calibration parameters from measured field data.

- 5.5.2.3. Estimate the errors in the calibration values based on measurement error, interpolation error, scale effect error, and errors due to transient effects.
- 5.5.2.4. Define calibration targets.
- 5.5.2.5. Estimate ranges in the values of selected parameters related to boundary conditions, aquifer properties, and stresses.
- 5.5.2.6. Divide the grid into zones and calculate the coefficient of variation (η_x) for each zone with respect to calibration parameters.
- 5.5.2.7. Prepare a map on which the locations and values of the calibration targets are overlaid on the model grid.
- 5.5.2.8. Calculate the coefficient of variation (η_x) for parameters related to boundary conditions, aquifer properties, and stresses.
- 5.5.3. The following procedures shall be performed and documented following calibration simulations:
- 5.5.3.1. Calculate the coefficient of variation (η_x) using simulated estimates of the selected parameters.
- 5.5.3.2. Calculate the mean error (ME), mean absolute error (MAE), and root mean square error (RMSE) in the selected parameters.
- 5.5.3.3. Present the spatial distribution of residuals (also referred to as "errors" or "differences") using one or more of the following:
1. Contour map showing simulated parameter values superimposed on measured parameter values.
 2. Contour map of residuals.
 3. Map showing location and values of calibration targets and simulated values.
 4. Plot of ME, MAE, and RMSE vs. calibration run number to show the approach to calibration.
- 5.5.3.4. The level of calibration shall be documented according to the following (adapted from *Woessner and Anderson*, 1990):
- | | |
|---------|--|
| Level 1 | Simulated value falls within calibration target. |
| Level 2 | Simulated value falls within two times the associated error of the calibration target. |
| Level 3 | Simulated value falls within three times the associated error of the calibration target. |

Level n Simulated value falls within n times the associated error of the calibration target.

- 5.5.4. Differences between the input files used to conduct calibration simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.

5.6 Uncertainty Analysis

- 5.6.1. Modeling personnel shall maintain a logbook of all uncertainty analysis simulations which shall contain the following information:

1. Complete (i.e., path included) input filename(s) and date finalized.
2. General comments regarding the nature of the input with specific emphasis placed on alterations.
3. Starting and ending date of simulation.
4. Simulation run-time.
5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
6. General comments regarding the nature of the output and any error messages.
7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

The following procedures regarding uncertainty analysis have been adapted from *Anderson and Woessner* (1992) unless otherwise noted. The following are recommended procedures to be used in completing the uncertainty analysis. Alternative procedures which accomplish the overall objective of the recommended procedures (i.e., show the effect which the statistical variability associated with the values of selected parameters has on model predictions) may be substituted at the discretion of modeling personnel.

- 5.6.2. The following procedures shall be performed and documented for uncertain parameters:

- 5.6.2.1. Select the parameters to be evaluated (uncertain parameters) and the dependent variable(s) (e.g., hydraulic head, travel-time, point-of-compliance concentration).
- 5.6.2.2. Systematically change one parameter at a time within the previously established range to determine its effect on predicted values of the dependent variable.

- 5.6.2.3. Systematically change a combination of parameters to generate the broadest range of predictions (e.g., minimum travel-times may be generated by using the largest values of hydraulic conductivity combined with the largest values of hydraulic gradient and *vice versa*).
- 5.6.2.4. Present the results of these uncertainty analyses using one or more of the following:
1. Contour map of residuals of the dependent variable for each value of the uncertain parameter.
 2. Plot of ME, MAE, and RMSE of dependent variable vs. percent change in the uncertain parameter.
- 5.6.3. Differences between the input files used to conduct uncertainty analyses simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.

5.7 Model Verification

- 5.7.1. Modeling personnel shall maintain a logbook of all verification simulations which shall contain the following information:
1. The name and source of the analytical model used to perform the verification.
 2. The published derivation of the analytical solution used to perform the verification, if available.
 3. Complete (i.e., path included) input filename(s) and date finalized.
 4. General comments regarding the nature of the input with specific emphasis placed on alterations.
 5. Starting and ending date of analytical and numerical simulations.
 6. Analytical and numerical simulation run-times.
 7. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
 8. General comments regarding the nature of the output and any error messages.
 9. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
 10. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

The following are recommended procedures to be used in completing model verification. Alternative procedures which accomplish the overall objective of the recommended

procedures (i.e., show that the model can reproduce results obtained using simple fundamental functions when run in the same mode as the analytical model) may be substituted at the discretion of modeling personnel.

5.7.2. The following procedures shall be performed and documented prior to conducting model verification simulations:

5.7.2.1. Select the parameters to be verified (verification parameters).

5.7.2.2. Select the input parameters to be varied to determine their influence on the verification parameters.

5.7.3. The following procedures shall be performed and documented following model verification simulations:

5.7.3.3. Present the difference between the numerical and analytical results using one or more of the following:

1. Contour maps or x-y plots showing numerically-simulated parameter values superimposed on analytically-simulated parameter values.
2. Contour map of verification residuals.

5.7.3.4. The level of verification shall be documented according to the following (patterned after *Woessner and Anderson, 1990*):

- Level A Numerically-simulated value falls within 5 % of the analytically-simulated value.
- Level B Numerically-simulated value falls within 10 % of the analytically-simulated value.
- Level C Numerically-simulated value falls within 20 % of the analytically-simulated value.
- Level D Numerically-simulated value falls within 50 % of the analytically-simulated value.

5.7.4. Differences between the input files used to conduct verification simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.

5.8 Predictive Simulations

5.8.1. Modeling personnel shall maintain a logbook of all predictive simulations which shall contain the following information:

1. Complete (i.e., path included) input filename(s) and date finalized.

2. General comments regarding the nature of the input with specific emphasis placed on alterations.
 3. Starting and ending date of simulation.
 4. Simulation run-time.
 5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
 6. General comments regarding the nature of the output and any error messages.
 7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
 8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.
- 5.8.2. Differences between the input files used to conduct predictive simulations and those used to calibrate the model shall be documented in the logbook described in Section 5.8.1. Since the purpose of the predictive simulations is to measure the deviation between output values obtained using input data sets purposely set outside the region of calibration and subsequent laboratory- and field-measured values, it is recommended that a separate section in the logbook be devoted to these differences to facilitate validating the model (Section 5.10).
- 5.8.3. Differences between the input files used to conduct predictive simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.
- 5.8.4. It is recommended that simulations be accomplished via batch processing to facilitate: 1) the process of performing multiple simulations and 2) tracking of input and output files (in addition to notes kept in the modeling logbook described in Section 5.8.1.). Batch files used shall be reviewed and initialed by responsible personnel.
- 5.8.5. It is recommended that screen dumps be redirected to internal or external disk drives in order to decrease the simulation run-time and facilitate analysis of model output.
- 5.8.6. All files associated with the predictive simulations shall remain on the active system (i.e., "on-line") until the project is completed (i.e., client and/or agency-approved). If necessary, the files may be compressed ("zipped") to save space. The names and the contents of compressed files must be recorded in the modeling logbook described in Section 5.8.1.
- 5.8.7. Following completion of predictive simulations (or once per week, whichever is more frequent), all of the associated input and output files shall be stored on a backup system or other internal or external storage device.

5.9 Sensitivity Analysis

5.9.1. Modeling personnel shall maintain a logbook of all sensitivity analysis simulations which shall contain the following information:

1. Complete (i.e., path included) input filename(s) and date finalized.
2. General comments regarding the nature of the input with specific emphasis placed on alterations.
3. Starting and ending date of simulation.
4. Simulation run-time.
5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
6. General comments regarding the nature of the output and any error messages.
7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

The following procedures regarding sensitivity analysis have been adapted from *Anderson and Woessner (1992)* unless otherwise noted. The following are recommended procedures to be used in completing the sensitivity analysis. Alternative procedures which accomplish the overall objective of the recommended procedures (i.e., show the effect which varying selected uncertain parameter values and stresses have on results of the predictive simulations) may be substituted at the discretion of modeling personnel.

5.9.2. The following procedures shall be performed and documented:

5.9.2.1. Select the parameters to be evaluated (uncertain parameters) and the dependent variable(s) (e.g., hydraulic head, travel-time, point-of-compliance concentration).

5.9.2.2. Systematically change one parameter at a time within the previously established range (see Section 5.5) to determine its effect on predicted values of the dependent variable.

5.9.2.3. Systematically change a combination of parameters to generate the broadest range of predictions (e.g., minimum travel-times may be generated by using the largest values of hydraulic conductivity combined with the largest values of hydraulic gradient and *vice versa*).

5.9.2.4. Present the results of these analyses using one or more of the following:

1. Contour map of residuals of the dependent variable for each value of the varied parameter.

2. Map showing location and values of calibration targets and simulated values of the dependent variable for each value of the varied parameter.
3. Plot of ME, MAE, and RMSE of dependent variable vs. percent change in the varied parameter.

5.9.3. Differences between the input files used to conduct sensitivity analyses simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.

5.10 Model Validation

5.10.1. Modeling personnel shall maintain a logbook of all validation simulations which shall contain the following information:

1. Complete (i.e., path included) input filename(s) and date finalized.
2. General comments regarding the nature of the input with specific emphasis placed on alterations.
3. Starting and ending date of simulation.
4. Simulation run-time.
5. Complete (i.e., path included) output filename(s) (including screen dumps) and date finalized.
6. General comments regarding the nature of the output and any error messages.
7. General comments (including dates and locations) describing discussions with other modeling personnel, clients, and regulatory personnel regarding model results.
8. Complete (i.e., path included) compressed filename(s), date of compression, and contents.

The following procedures regarding model validation have been patterned after the model calibration procedure adapted from *Anderson and Woessner* (1992) outlined in Section 5.5. The following are recommended procedures to be used in completing model validation. Alternative procedures which accomplish the overall objective of the recommended procedures (i.e., show that the results obtained from the predictive simulations were correct) may be substituted at the discretion of modeling personnel.

5.10.2. The following procedures shall be performed and documented prior to conducting model validation simulations:

5.10.2.1. Select the parameters to be validated (validation parameters).

5.10.2.2. Select values for the validation parameters from measured field data.

- 5.10.2.3. Estimate the errors in the values based on measurement error, interpolation error, scale effect error, and errors due to transient effects.
 - 5.10.2.4. Define validation targets.
 - 5.10.2.5. Estimate ranges in the values of selected parameters related to boundary conditions, aquifer properties, and stresses.
 - 5.10.2.6. Divide the grid into zones and calculate the coefficient of variation (η) for each zone with respect to these selected parameters.
 - 5.10.2.7. Prepare a map on which the locations and values of the validation targets are overlaid on the model grid.
 - 5.10.2.8. Calculate the coefficient of variation (η) for parameters related to boundary conditions, aquifer properties, and stresses.
- 5.10.3. The following procedures shall be performed and documented following model validation simulations:
- 5.10.3.1. Calculate the coefficient of variation (η) using simulated estimates of the selected parameters.
 - 5.10.3.2. Calculate the mean error (ME), mean absolute error (MAE), and root mean square error (RMSE) in the selected parameters.
 - 5.10.3.3. Present the spatial distribution of residuals using one or more of the following:
 - 1. Contour map showing simulated parameter values superimposed on measured parameter values.
 - 2. Contour map of residuals.
 - 3. Map showing location and values of validation targets and simulated values.
 - 5.10.3.4. The level of validation shall be documented according to the following (patterned after *Woessner and Anderson, 1990*):
 - Level 1 Simulated value falls within validation target.
 - Level 2 Simulated value falls within two times the associated error of the validation target.
 - Level 3 Simulated value falls within three times the associated error of the validation target.
 - Level n Simulated value falls within n times the associated error of the validation target.

- 5.10.4. Differences between the input files used to conduct validation simulations shall be electronically checked using a user-generated program or appropriate operating system commands (e.g., the "diff" command for UNIX-based systems). Output produced by such programs or commands shall be kept in project files.
- 5.10.5. The following procedures shall be performed if calibrated parameter values are changed during model validation:
- 5.10.5.1. The calibration simulation shall be performed again to ensure that the new parameter values can successfully reproduce the calibration targets.
 - 5.10.5.2. If the calibration targets cannot be reproduced using parameter values that were changed during model validation, the validation process must be repeated until a set of parameter values is found which can successfully reproduce calibration and validation targets.

6 REFERENCES

American Society of Mechanical Engineers (ASME) (1989a): *Quality Assurance Program Requirements for Nuclear Facilities - ASME NQA-1-1989 Edition*; An American National Standard; The American Society of Mechanical Engineers, New York, New York; 69 pp.

American Society of Mechanical Engineers (ASME) (1989b): *Quality Assurance Program Requirements for Nuclear Facilities - ASME NQA-3-1989 Edition*; An American National Standard; The American Society of Mechanical Engineers, New York, New York; 19 pp.

Anderson, M.P. and W.W. Woessner (1992): *Applied Groundwater Modeling - Simulation of Flow and Advective Transport*; Academic Press, Inc., San Diego, California; 381 pp.

Case, M.J. and M.D. Otis (1988): *Guidelines for Radiological Performance Assessment of DOE Low-Level Radioactive Waste Disposal Sites*; National Low-Level Radioactive Waste Program, Idaho Falls, Idaho; Prepared for the U.S. Department of Energy, Idaho Operations Office under DOE Contract No. DE-AC07-76ID01570; July.

National Research Council (1990): *Ground Water Models - Scientific and Regulatory Applications*; National Academy Press, Washington, D.C.; 303 pp.

Perry, W.E. (1991): *Quality Assurance for Information Systems - Methods, Tools, and Techniques*; QED Technical Publishing Group, Wellesley, Massachusetts; 814 pp.

Reynolds Electrical & Engineering Company, Inc. (REECo) (1990): *Quality Assurance Program*; Chapter I; Nevada Operations; 568-DOC-122 - Revision D; reviewed and approved August 1, 1990 - effective date November 1, 1990.

Woessner, W.W. and M.P. Anderson (1990): "Setting calibration targets and assessing model calibration - Room for improvement: An example from North America"; In *Calibration and Reliability in Groundwater Modeling* (K. Kovar, ed.), IAHS Pub. 195, pp. 279-290.

7 FORMS

This section contains the forms which shall be completed upon performing the required procedures specified in this document. These forms, in addition to notes, logbook(s), and calculation sheets maintained by modeling personnel, provide the documentation necessary to comply with the requirements set forth in this Standard and to ensure timely completion of computer modeling projects. The format of these forms may be changed to facilitate conversion for use with other word processing software packages; however, the general content of the forms should not be changed.

CMQAP FORM 1

CODE MODIFICATION (Section 5.1)

PROJECT FILE REQUIREMENTS

- | Yes | No | |
|--------------------------|--------------------------|--|
| <input type="checkbox"/> | <input type="checkbox"/> | Electronic copy of original ("unmodified") code in project file |
| <input type="checkbox"/> | <input type="checkbox"/> | Electronic copy of modified code in project file |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of original ("unmodified") code in project file |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of modified code in project file |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of modified code properly highlighted |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of output produced by user-generated program or system command program designed to find differences in codes in project file |

CODE-SPECIFIC REQUIREMENTS

- | Yes | No | |
|--------------------------|--------------------------|---|
| <input type="checkbox"/> | <input type="checkbox"/> | Initial comments in program "main" expanded to include information pertinent to the modification(s) |
| <input type="checkbox"/> | <input type="checkbox"/> | Comment statements preceding all modified statements |

CODE TESTING REQUIREMENTS

For modifications which alter the manner in which the code simulates a certain process or include a new process...

- | Yes | No | |
|--------------------------|--------------------------|--|
| <input type="checkbox"/> | <input type="checkbox"/> | Simulations to clarify the effect of the modification performed using original and modified versions of the code |
| <input type="checkbox"/> | <input type="checkbox"/> | Simulations to ensure that the modifications do not affect other portions of the code |
| <input type="checkbox"/> | <input type="checkbox"/> | Compare results obtained with modified code to those obtained with previously verified code |
| <input type="checkbox"/> | <input type="checkbox"/> | Results of test simulations documented and graphically depicted |

For modifications which alter the manner in which the code reads input files and writes output files...

- | Yes | No | |
|--------------------------|--------------------------|---|
| <input type="checkbox"/> | <input type="checkbox"/> | Graphical comparison of initial conditions using original and modified code |
| <input type="checkbox"/> | <input type="checkbox"/> | Graphical comparison of final conditions using original and modified code |
| <input type="checkbox"/> | <input type="checkbox"/> | Results of test simulations documented |

Signatures (Dated)

QA Manager _____
 Project Manager _____

CMQAP FORM 2
CODE COMPILATION (Section 5.2)

Date _____
Personnel _____

Hardware _____

Software _____

Reason(s) for using the above software _____

Compiler-specific commands/switches and their function(s) _____

Yes No
 Hard-copy of compilation batch file in project file

Name of compilation batch file _____

Name of source file _____

Name of object file _____

Name of run-time (executable) file _____

Signatures (Dated)

Project Manager _____

QA Manager _____

CMQAP FORM 3
CODE VERIFICATION (Section 5.3)

Date _____

Personnel and Employer(s) _____

In-house hardware _____

Verification hardware _____

Name of source file _____

Name of run-time (executable) file _____

Name of verification input file(s) _____

Name of verification output file(s) _____

General comments regarding code verification _____

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 4

DESIGN OF SITE-SPECIFIC MODEL (Section 5.4)

DESIGN OF THE GRID

Yes No
 Grid based on certified site map

Surveying contractor name _____

Surveying contractor address _____

Surveying contractor phone number _____

Yes No
 Hard-copy of certified site map in project files
 Electronic copy of certified site map in project files
 Client notified as to which version of the site map is being used to generate model grid
 Surveying contractor notified as to which version of the site map is being used to generate model grid

Yes No NA
 Boundary conditions used to develop grid documented in project files
 Hydraulic structures used to develop grid documented in project files
 Hydraulic conductivity values used to develop grid documented in project files
 Heat conductivity values used to develop grid documented in project files
 Transmissivity values used to develop grid documented in project files
 Media thicknesses used to develop grid documented in project files
 Initial hydraulic conditions used to develop grid documented in project files
 Initial concentration conditions used to develop grid documented in project files
 Initial temperature conditions used to develop grid documented in project files

Yes No
 Final grid developed with computer-aided-design (CAD) software

Name of CAD software used to develop final grid _____

Yes No
 Name of computer, filename, and date generated included in footer on hard-copy of final grid
 Hard-copy of final grid in project files
 Hard-copy of final grid submitted to client for review
 Hard-copy of final grid submitted to surveying contractor for review

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 5
DESIGN OF SITE-SPECIFIC MODEL (Section 5.4)

INPUT PARAMETERS

- | Yes | No | |
|--------------------------|--------------------------|---|
| <input type="checkbox"/> | <input type="checkbox"/> | Site-specific data used for boundary conditions |
| <input type="checkbox"/> | <input type="checkbox"/> | Site-specific data used for initial conditions |
| <input type="checkbox"/> | <input type="checkbox"/> | Site-specific data used for media properties |
| <input type="checkbox"/> | <input type="checkbox"/> | Site-specific data used for media stresses |

General comments regarding use of site-specific data to define values of input parameters

- | Yes | No | |
|--------------------------|--------------------------|--|
| <input type="checkbox"/> | <input type="checkbox"/> | Source(s) of site-specific data used for boundary conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Source(s) of site-specific data used for initial conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Source(s) of site-specific data used for media properties documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Source(s) of site-specific data used for media stresses documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Copies of field notes regarding boundary conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Copies of field notes regarding initial conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Copies of field notes regarding media properties documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Copies of field notes regarding media stresses documented in project files |

- | Yes | No | |
|--------------------------|--------------------------|---|
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding size of initial time-step documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding size of minimum and maximum time-step documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding minimum and maximum number of iterations documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding convergence criteria documented in project files |

If site-specific data are not used:

- | Yes | No | |
|--------------------------|--------------------------|--|
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding boundary conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding initial conditions documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding media properties documented in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Assumptions/calculations regarding media stresses documented in project files |

Signatures (Dated)

QA Manager _____
 Project Manager _____

CMQAP FORM 6

Page 1 of 2

DESIGN OF SITE-SPECIFIC MODEL (Section 5.4)

GENERAL SIMULATION NOTES

Name of input file #1 _____
 Name of input file #2 _____
 Name of input file #3 _____
 Date(s) finalized _____
 Purpose of simulation _____

Starting date of simulation _____
 Ending date of simulation _____
 Simulation run-time _____

Name of output file #1 _____
 Name of output file #2 _____
 Name of output file #3 _____

Name of screen dump file #1 _____
 Name of screen dump file #2 _____
 Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 6

Page 2 of 2

DESIGN OF SITE-SPECIFIC MODEL (Section 5.4)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Name of compressed file #1 _____

Name of compressed file #2 _____

Name of compressed file #3 _____

- | | | |
|--------------------------|--------------------------|---|
| Yes | No | |
| <input type="checkbox"/> | <input type="checkbox"/> | Catalog of contents of compressed file(s) contained in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of final input file(s) for site-specific model contained in project files |

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 7

Page 1 of 2

MODEL CALIBRATION (Section 5.5)

GENERAL SIMULATION NOTES

Name of input file #1 _____
 Name of input file #2 _____
 Name of input file #3 _____
 Date(s) finalized _____
 Purpose of simulation _____

Starting date of simulation _____
 Ending date of simulation _____
 Simulation run-time _____

Name of output file #1 _____
 Name of output file #2 _____
 Name of output file #3 _____

Name of screen dump file #1 _____
 Name of screen dump file #2 _____
 Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 7

Page 2 of 2

MODEL CALIBRATION (Section 5.5)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Multiple horizontal lines for entering general comments regarding discussions associated with simulation.

Name of compressed file #1 _____

Name of compressed file #2 _____

Name of compressed file #3 _____

Yes No

- Two rows of checkboxes for Yes/No responses regarding catalog of contents and hard-copy of final input file(s).

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 8

Page 1 of 2

UNCERTAINTY ANALYSIS (Section 5.6)

GENERAL SIMULATION NOTES

Name of input file #1 _____

Name of input file #2 _____

Name of input file #3 _____

Date(s) finalized _____

Purpose of simulation _____

Starting date of simulation _____

Ending date of simulation _____

Simulation run-time _____

Name of output file #1 _____

Name of output file #2 _____

Name of output file #3 _____

Name of screen dump file #1 _____

Name of screen dump file #2 _____

Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 8

Page 2 of 2

UNCERTAINTY ANALYSIS (Section 5.6)

General comments regarding discussions associated with simulation (include names, dates, and locations)

Name of compressed file #1 _____

Name of compressed file #2 _____

Name of compressed file #3 _____

- Yes No
- Catalog of contents of compressed file(s) contained in project files
- Hard-copy of final input file(s) for site-specific model contained in project files

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 9

Page 1 of 2

MODEL VERIFICATION (Section 5.7)

GENERAL SIMULATION NOTES

Name of input file #1 _____
 Name of input file #2 _____
 Name of input file #3 _____
 Date(s) finalized _____
 Purpose of simulation _____

Starting date of simulation _____
 Ending date of simulation _____
 Simulation run-time _____

Name of output file #1 _____
 Name of output file #2 _____
 Name of output file #3 _____

Name of screen dump file #1 _____
 Name of screen dump file #2 _____
 Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 9

Page 2 of 2

MODEL VERIFICATION (Section 5.7)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Multiple horizontal lines for handwritten input.

Name of compressed file #1 _____
Name of compressed file #2 _____
Name of compressed file #3 _____

- | | | |
|--------------------------|--------------------------|---|
| Yes | No | |
| <input type="checkbox"/> | <input type="checkbox"/> | Catalog of contents of compressed file(s) contained in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of final input file(s) for site-specific model contained in project files |

Signatures (Dated)

QA Manager _____
Project Manager _____

CMQAP FORM 10

Page 1 of 2

PREDICTIVE SIMULATIONS (Section 5.8)

GENERAL SIMULATION NOTES

Name of input file #1 _____

Name of input file #2 _____

Name of input file #3 _____

Date(s) finalized _____

Purpose of simulation _____

Starting date of simulation _____

Ending date of simulation _____

Simulation run-time _____

Name of output file #1 _____

Name of output file #2 _____

Name of output file #3 _____

Name of screen dump file #1 _____

Name of screen dump file #2 _____

Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 10

Page 2 of 2

PREDICTIVE SIMULATIONS (Section 5.8)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Multiple horizontal lines for writing general comments.

Name of compressed file #1 _____
Name of compressed file #2 _____
Name of compressed file #3 _____

- | | | |
|--------------------------|--------------------------|---|
| Yes | No | |
| <input type="checkbox"/> | <input type="checkbox"/> | Catalog of contents of compressed file(s) contained in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of final input file(s) for site-specific model contained in project files |

Signatures (Dated)

QA Manager _____
Project Manager _____

CMQAP FORM 11

Page 1 of 2

SENSITIVITY ANALYSIS (Section 3.9)

GENERAL SIMULATION NOTES

Name of input file #1 _____

Name of input file #2 _____

Name of input file #3 _____

Date(s) finalized _____

Purpose of simulation _____

Starting date of simulation _____

Ending date of simulation _____

Simulation run-time _____

Name of output file #1 _____

Name of output file #2 _____

Name of output file #3 _____

Name of screen dump file #1 _____

Name of screen dump file #2 _____

Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 11

Page 2 of 2

SENSITIVITY ANALYSIS (Section 3.9)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Multiple horizontal lines for handwritten notes.

Name of compressed file #1 _____

Name of compressed file #2 _____

Name of compressed file #3 _____

Yes No

- Checkboxes for 'Catalog of contents of compressed file(s) contained in project files' and 'Hard-copy of final input file(s) for site-specific model contained in project files'.

Signatures (Dated)

QA Manager _____

Project Manager _____

CMQAP FORM 12

Page 1 of 2

MODEL VALIDATION (Section 5.10)

GENERAL SIMULATION NOTES

Name of input file #1 _____

Name of input file #2 _____

Name of input file #3 _____

Date(s) finalized _____

Purpose of simulation _____

Starting date of simulation _____

Ending date of simulation _____

Simulation run-time _____

Name of output file #1 _____

Name of output file #2 _____

Name of output file #3 _____

Name of screen dump file #1 _____

Name of screen dump file #2 _____

Name of screen dump file #3 _____

General comments regarding results of simulation _____

CMQAP FORM 12

Page 2 of 2

MODEL VALIDATION (Section 5.10)

General comments regarding discussions associated with simulation (include names, dates, and locations) _____

Multiple horizontal lines for writing general comments.

Name of compressed file #1 _____
Name of compressed file #2 _____
Name of compressed file #3 _____

- | | | |
|--------------------------|--------------------------|---|
| Yes | No | |
| <input type="checkbox"/> | <input type="checkbox"/> | Catalog of contents of compressed file(s) contained in project files |
| <input type="checkbox"/> | <input type="checkbox"/> | Hard-copy of final input file(s) for site-specific model contained in project files |

Signatures (Dated)

QA Manager _____
Project Manager _____

8 RECORDS MANAGEMENT⁴

The requirements of this Standard set forth in this section pertain to hard copy and electronic (e.g., hard disk and floppy disk) files and documents.

- 8.1.1. Records shall be legible, identifiable, retrievable, and protected against damage, deterioration, or loss.
- 8.1.2. Requirements and responsibilities for record transmittal, distribution, retention, maintenance, and disposition (e.g., classified and unclassified) shall be established and documented.
- 8.1.3. Electronic files shall be logged per the requirements set forth in Section 5.
- 8.1.4. Controls shall be maintained for the following:
 - 1. Records systems;
 - 2. Identification of documents designated to become records;
 - 3. Record validation;
 - 4. Records indexing (including revision number) and identification of record to item(s);
 - 5. Distribution and control;
 - 6. Classification as Lifetime or Nonpermanent;
 - 7. Record retention;
 - 8. Correction of information in records;
 - 9. Record receipt;
 - 10. Record storage, preservation, and safekeeping; and
 - 11. Record retrieval.

⁴Adapted from REECo (1990); page C-17-1.

9 TRAINING⁵

- 9.1.1. Personnel selected for performing the procedures set forth in this Standard shall have the experience and training commensurate with the scope, complexity, or special nature of the activities.
- 9.1.2. Provisions shall be made for the indoctrination of personnel as to the technical objectives and requirements of the applicable elements of the Standard that are to be employed.
- 9.1.3. The need for formal training shall be determined, and such activities shall be conducted as required to qualify personnel who perform the applicable procedures.
- 9.1.4. If needed, formal training shall be provided to achieve initial proficiency, maintain proficiency, and adapt to changes in technology and methods.
- 9.1.5. The capabilities of personnel shall be initially determined by a suitable evaluation of the candidate's education, experience, training, and capability demonstration.

⁵Adapted from ASME NQA-1 (1989a), and REECo (1990) ("Company Implementing Procedure" QA-2.4).

10 DOCUMENTATION AND VALIDATION⁶

- 10.1.1. Documentation and records which provide evidence that the procedures set forth in this Standard were performed, reviewed, and validated by responsible personnel shall be prepared and maintained.
- 10.1.2. Personnel responsible for preparing, reviewing, approving, and issuing documents and revisions shall be specified for all computer modeling projects.
- 10.1.3. Responsible personnel shall review all documents associated with modeling tasks for adequacy, completeness, and corrections prior to approval and issuance.

⁶Adapted from REECo (1990), page C-6-1.

11 PRECAUTIONS AND LIMITATIONS

- 11.1.1. Hard copies of computer codes as well as input and output files known to be defective or otherwise corrupted shall be labeled clearly as such and maintained in a separate file within the project files.
- 11.1.2. Access to electronic copies of computer codes as well as input and output files known to be defective or otherwise corrupted shall be limited through the use of passwords and other permission-limiting methods. Such files shall also be compressed to further minimize the likelihood of inadvertent use.
- 11.1.3. A text file (e.g., README.DOC or HISTORY.DOC) describing the contents of each subdirectory related to the modeling effort shall be maintained and updated daily. This procedure will ensure that all involved personnel have a complete and up-to-date record regarding the contents of files within the subdirectory.
- 11.1.4. Subdirectories and files related to the modeling effort shall be password-protected to ensure that only those personnel associated with the project are permitted access. "Read", "write", and "execution" permissions may be changed on an as-needed basis at the discretion of the project manager and/or computer system manager.

12 FORMULAS AND CALCULATIONS

- 12.1.1. Supporting references for all formulas and/or calculation methods used to determine values of parameters related to the modeling effort shall be documented in the project files. If feasible, a copy of the reference shall be kept in the project files.
- 12.1.2. Formulas used and hand calculations performed (e.g., those used for calculation of input parameters or conversion of output parameters) shall be reviewed by responsible personnel.
- 12.1.3. Documentation associated with the review, including a hard copy of the original worksheets signed and/or initialed by the originator and the reviewer, shall be maintained in project files.
- 12.1.4. Documentation associated with the review shall be dated.

13 STANDARDS⁷

- 13.1.1. Modeling personnel shall assure the use of appropriate voluntary standards where such standards are adequate and appropriate for the intended application, except when mandatory government standards apply; shall encourage participation in voluntary standards-developing activities; and shall submit nominations of individuals eligible to participate in voluntary standards-developing bodies to the appropriate personnel.

⁷Adapted from REECo (1990); page E-1.