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NNWSI-SOP-03-02			
Software Quality Assurance	0	2/28/86	44

Remarks Insert in NNWSI Quality Assurance Plan Section II, following SOP-03-01

WM Record File 102.2 WM Project 11

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NNWSI Nevada Nuclear Waste Storage Investigations PROJECT

Nevada Nuclear Waste Storage Investigations Project

NNWSI-SOP-03-02

REVISION 0

SOFTWARE QUALITY ASSURANCE

Nevada Operations Office

UNITED STATES DEPARTMENT OF ENERGY

Title	No. NNWSI-SOP-03-02 Rev. 0
SOFTWARE QUALITY ASSURANCE	Effective Date 2/28/86
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1.0 PURPOSE & SCOPE

The purpose of this Standard Operating Procedure (SOP) is to establish requirements for documenting and controlling the quality of software used to support a high-level nuclear waste repository license application.

This SOP applies to scientific and engineering (SES) software used in support of an NNWSI license application (Quality Assurance Level I). Assignment of quality assurance levels is covered by SOP-02-02. It does not apply to operating systems, compilers, standard libraries, auxiliary software, utilities, or data bases. Data generated by software before the effective date of this SOP may be qualified under SOP-03-03.

2.0 APPLICABILITY

This document defines the requirements to be met to satisfy the Nuclear Regulatory Commission of the quality of software used in a nuclear waste repository license application. It uses the guidance contained in NUREG-0856 and applies to Quality Assurance Level I as defined in NVO-196-17. This SOP also applies to Quality Assurance Level II to the extent appropriate as also defined in NVO-196-17. Furthermore, numerical methods are differentiated from analytic methods to be consistent with standard usage in the sciences and engineering and to allow appropriate application of the requirements to analytic software.

The requirements set forth below define the extent of the documentation and controls required. The development and implementation of procedures for this SOP are the responsibility and sole province of the participating organizations, and NTS Support Contractors are to be incorporated into their Quality Assurance Program Plans, and are to be approved by the Waste Management Project Office.

3.0 DEFINITIONS

Comparable terms defined in NUREG-0856 are given in parentheses.

Analytic Method - A direct transliteration of mathematical formulae into software, where no computational approximations are made other than those imposed by the word length of the computer.

Auxiliary Software - Software which is not scientific and engineering software. Auxiliary software includes but is not limited to simple statistics, coordinate transformations, trivial calculations, sorting, reformatting, data acquisition, and graphics.

APPROVALS

Originator	Director, WMPO	Director, DOE/NV QAD	Supersede N/A
James Blaylock	for		Rev. Initial
Date 1/31/86	Date 2/3/86	Date 2-3-86	Date Issue

Benchmarking - Comparison of the results of one item of software with the results of another item of software designed to solve a comparable problem to show that they produce similar results. The particular problem for which this comparison is made is called a benchmark problem.

Component - Any logically distinct subset of a model. Model is understood to include components. (component model)

Computer Program, Computer Code, Code - Synonyms for "software" or any type of software.

Configuration Management - A system of controls and authorizations which prevents ambiguity as to which version of software is used for a particular computation.

Independent Peer - A disinterested qualified peer. An independent peer may be a member of the participating organization of the NNWSI Project as long as the peer is not a member of both the participating organization and the NNWSI Project.

Loader - Any combination of utilities used to perform the tasks of linkage editing and loading, whether relocatably or not.

Mathematical Model - A mathematical representation of any model. (mathematical model)

Model - Synonym for any or all of the kinds of models defined.

NNWSI - Nevada Nuclear Waste Storage Investigations. A U.S. Department of Energy Project.

Numerical Method - An approximate computational method for solving a problem mainly by a sequence of arithmetic operations. (numerical method)

Numerical Model - A representation of a physical or mathematical model using numerical methods. (numerical model)

Peer - An individual or group with expertise comparable to that of the software creator(s).

Peer Review - A documented review, by an independent peer of items required by the relevant sections of this SOP, the process also includes the Technical Contact's documented response to questions raised by the reviewer.

Physical Model - Any representation of a physical system or process. (model)

Records Management System (RMS) - The system of record keeping defined in SOP-17-01.

RMS - Records management system.

Scientific and Engineering Software - Software which specifies operations according to a physical or mathematical model or which uses a numerical method.

SES - Scientific and engineering software.

Software - A set or sets of computer operations specified by any language(s) which can be translated unambiguously into machine language. Machine language is also software. (computer code)

SOP - Standard Operating Procedure. A document in the NNWSI Quality Assurance Plan,

Technical Contact - The technical professional identified on the software summary form (usually the author of or current expert on the software).

TPO - Technical Project Officer.

Trivial Calculations - computation which could be done on paper or with an unprogrammed calculator.

Validation - Assurance that the physical model as embodied in software is a correct representation of the intended physical system or process. (validation)

Verification - Assurance that the software correctly represents the model(s). (verification)

4.0 RESPONSIBILITIES

4.1 Participating organizations and NTS Support Contractors are responsible for implementing this SOP for software within the scope of their activities by developing and implementing appropriate written procedures and including them in their Quality Assurance Program Plans. The Technical Project Officer (TPO) is the responsible party within each participating organization. The TPO may delegate all or part of these responsibilities; any such delegation shall be documented in the Quality Assurance Program Plan.

4.2 Participating Organizations and NTS Support Contractors quality assurance is responsible for reviewing these procedures and auditing their implementation.

5.0 REQUIREMENTS

5.1 Format - This SOP shall not be construed to endorse any documentation format or software-portability requirements. The information called for is required but the format in which it is given may be varied.

5.2 Configuration Management Program - All Participating Organizations and NTS Support Contractors shall institute a software configuration management program appropriate to the projects they conduct and shall provide documentation of this program to the Records Management System (RMS).

5.2.1 The minimum requirements for this configuration management program shall be: the inclusion of a unique identification, including software version numbers, whenever feasible, in the output and listings of the software on all versions of SES under the scope of this SOP; and a brief chronology of the software versions under the scope of this SOP, including descriptions of the changes made between versions to ensure an audit trail of all changes made to a specific software program.

5.3 Software Summary Form - For each item of SES a software summary form shall be provided to the RMS. Standard Form 185 or its functional equivalent shall be used for this software summary.

5.3.1 The software summary shall be updated and the updated version provided to the RMS whenever a new version of the software is released, whenever, major modifications are made to the software, whenever the Technical Contact is changed, whenever an error is discovered in the software or documentation is reported, and whenever any change to the software summary is made.

5.4 Description of Models - Physical, mathematical, and numerical models used for the software shall be explained such that peers can understand the methods used. This documentation shall be detailed enough to stand alone as a basis for peer review of the methods used in the software, and it shall be reviewed by an independent peer. These documents, including peer reviews, shall be provided to the RMS (cf. 5.6.3).

5.4.1 The overall nature and purpose of the analysis of which the model is a part shall be described and the general aspects of this analysis addressed by the model shall be stated. Specific aspects of the analysis addressed by the model shall be stated by software users. The information that goes into and comes out of the software shall be stated in general terms.

5.4.2 The overall solution strategy shall be described with any appropriate combination of flowcharts, block diagrams, narratives, and pseudocode listings (cf 5.4.4.4). The locations of subroutines within this strategy shall be shown. Subdivisions of the software reflecting any model components shall be defined, and the location of each such component in the overall solution strategy shall be described.

5.4.3 To the extent it is known, the overall performance of the models shall be discussed and the conditions under which they are known to perform well or adversely shall be described. General rules or recommendations that should be followed when using the models shall be given if available.

5.4.4 For each physical or mathematical model or component thereof the following shall be described.

5.4.4.1 The purpose and scope of the model or component; its input, output, and solution strategy; and the circumstances under which it is used shall be described as in 5.4.1 and 5.4.2.

5.4.4.2 The final mathematical form of the physical model (i.e. the governing equations) shall be given and an appropriate combination of references or derivations from generally accepted principles shall be included to justify that mathematical model. Any assumptions made or known limitations to the physical or mathematical model shall be described. Major variables important to understanding the operation of the software, including all input and output variables and governing equation variables, shall be cross-referenced between this derivation and the software (cf. 5.5.1, 5.5.2.1, and 5.5.2.2).

5.4.4.3 If the model or component is empirical or semi-empirical, its derivation from experimental data and the range and type of data used shall be described or referenced.

5.4.4.4 Any numerical methods used shall be characterized and the derivation of the numerical model from the mathematical or physical model shall be described. Available references for the numerical method and numerical model shall be given. The input to and output from the numerical model, including boundary conditions and coefficients, and the origin and use of these data shall be stated. An appropriate combination of flowcharts, block diagrams, narratives, and pseudocode listings shall be used to describe the computational sequence and numerical solution strategy used (cf. 5.4.2). The location of the numerical model in the software shall be stated. The known stability and accuracy of the numerical model shall be stated, differentiating between proven and empirical effects. (The requirements of this section do not apply to any analytic methods used.)

5.4.4.5 Alternatives considered to the model or component and the reasons for choosing the one used shall be stated briefly.

5.5 User's Manual - A user's manual which allows a peer to understand the results produced by the software, to run the software, and to install it on an appropriately equipped computer shall be provided to the RMS. The software listing (cf. 5.7) and all comments given in that listing shall be considered part of the user's manual.

5.5.1 The function and invocation of each major option and any recondite effects of combining options shall be described. Initial values of input, output, and governing-equation variables, where they are initialized, whether they are fixed or default values, and their units, if any, shall be described. Any restart and consecutive-case capabilities of the software and their use shall be described. Error processing,, including the location and likely causes of all major errors returns, shall be described unless the error messages returned contain such information (cf. 5.4.4.2).

5.5.2 The general content, purpose and organization of each data file used, and the location(s) in the software where these files are read or written shall be described. Known auxiliary software which uses or affects these files shall be referenced.

5.5.2.1 The input data, including formats of individual records and the structure and format of the overall input data, any record and field identifiers and delimiters, names of variables into which the data are read any any units of these data, and any known limits of the input data values, shall be described. Any optional data and defaults shall be described (cf. 5.4.4.2).

5.5.2.2 The output data, including any normalization, units, output variable names, graphical capabilities of the software, and the effects of input options on output formats shall be described (cf. 5.4.4.2).

5.5.2.3 Sample problems, including input and output listings, which exercise the major options shall be given. Computer-readable copies of the sample problem input shall also be given (cf. 5.7).

5.5.3 The interface between the software and the computer system shall be described. Any system-dependent features (e.g. external references), the compiler and loader and compiler- and load-options used, any special hardware requirements, the memory required, and any command cards or files used and interactive commands issued shall be described. Sample commands cards or files and interactive commands shall be listed, and any application-dependence of these command structures shall be described (cf. 5.5.1).

5.6 Verification and Validation - The correctness of the software shall be verified, and the applicability of the software to the problem shall be validated, both to the extent appropriate. Validation may be done by the software user with a peer review. The methods used to verify the software and validate the model shall be stated. Records of these verification and validation activities, including the peer review and the conclusions drawn from the peer reviews, shall be provided to the RMS.

5.6.1 The physical models, mathematical models, and any numerical models used, shall be reviewed by an independent peer, and any changes made or planned as a result of this review shall be described.

5.6.2 The correctness of the models' translation into software shall be verified to the extent appropriate by the software developer or Technical Contact and by an independent peer.

5.6.2.1 One acceptable form of verification is the documented wide use of the software by peers. Similarly, documented benchmarking and other documented comparisons to independently-derived results are acceptable forms of verification.

5.6.3 The applicability to and adequacy of the software for the problem shall be validated to the extent appropriate by the software developer, Technical Contact, or software user; and by an independent peer (cf 5.4).

5.6.3.1 The applicability of the model or component to the geologic repository, including any extrapolations, restrictions, and effects of unusual or extreme conditions peculiar to the repository, shall be described by the user.

5.7 Software Listings - Computer-readable and hard-copy listings of all versions of the software under the scope of this SOP shall be provided to the RMS (cf. 5.5 and 5.5.2.3).

5.7.1 Accessible copies of any software libraries used shall be referenced, including version numbers, or the parts of these libraries used shall be included in the listings described in 5.7.

5.8 Errors - Any errors discovered in either the software or any model used for the software, any effects of these errors on data used in the license application, and remedial actions taken to correct the errors and their effects shall be documented and these documents shall be provided to the RMS. Participating Organizations and NTS Support Contractors shall have provision for reporting such errors and change to the code users.

5.9 Documentation Changes - Any changes to the required documentation, due to changes made in the software, errors discovered in the documentation, new limitations discovered for the models, new results from the verification and validation program (cf. 5.6), or for any other reason, shall be provided to the RMS.

6.0 REFERENCES

NUREG-0856, Final Technical Position on Documentation of Computer Codes for High-Level Waste Management, Division of Waste Management, Office of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commission, Washington, D.C. 20555, June, 1983.

NVO-196-17, Nevada Nuclear Waste Storage Investigations Quality Assurance Plan, NNWSI, Nevada Operations Office, U.S. Department of Energy, Las Vegas, Nevada.

SOP-02-02, Assignment of Quality Assurance Levels to NNWSI Activities and Items, NNWSI, Nevada Operations Office, U.S. Department of Energy, Las Vegas, Nevada.

SOP-02-03, Verification of Data Generated Pre-NNWSI Project QAP, NNWSI, Nevada Operations Office, U.S. Department of Energy, Las Vegas, Nevada.

SOP-17-01, Records Management Plan, NNWSI, Nevada Operations Office, U.S. Department of Energy, Las Vegas, Nevada.

Standard Form 185, Federal Information Processing Standard Software Summary, Federal Information Processing Standard Publication 30 (FIPS. PUB 30), U.S. Department of Commerce, National Bureau of Standards, 1974. Available from: Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, July, 1974; or the General Services Administrations as Federal Supply Stock Item 7540-00-111-8541.