CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE PROCEDURE	Proc. QAP-014 Revision 0 Page 1 of 4

Title

QAP-014 DOCUMENTATION AND VERIFICATION OF ROUTINE CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 0 of this procedure became effective on 5/31/91. This procedure consists of the pages and changes listed below.

Page No.	Change	Date Effective
All	0	5/31/91

SUPERSEDED

Supersedes Procedure No. None

Approvals

Written By	Date	Technical Review	Date
Robert Brient	5/28/91		5/30/91
Quality Assurance	**Date**	**Cognizant Director**	**Date**
	5/30/91		5/31/91

CNWRA Form QAP-1

QAP-014 DOCUMENTATION AND VERIFICATION OF ROUTINE CALCULATIONS

1. PURPOSE

The purpose of this procedure is to provide the methods for documenting and verifying routine calculations, which include data reduction, statistical, and simple scientific or engineering computations. This procedure does not apply to activities involving Scientific and Engineering Software which contain complex mathematical or numerical models of physical processes or configurations. This procedure implements the requirements of CQAM Section 3.

2. RESPONSIBILITIES

(1) Personnel performing calculations are responsible for documenting data inputs, calculational methods, and verifications in accordance with this procedure.

(2) Technical Report reviewers are responsible for performing or confirming that calculation verifications are accomplished in accordance with this procedure.

3. PROCEDURE

3.1 Documentation of Data Inputs

(a) Existing data used in calculations shall be qualified in accordance with QAP-014.

(b) Data shall be documented by direct recording in a report or notebook, or may be identified by reference to its source, if it has been previously documented. If the source of the data would be obvious to a qualified technical reviewer, such as data from the Periodic Table of Elements or other universally accepted and recognized sources, the reference may be implied and the source need not be directly identified.

3.2 Documentation of Computational Methods

(a) Documentation of the calculational methods is not necessary for obvious (to the qualified reviewer) simple addition, subtraction, unit conversion, statistics, etc.

(b) Calculational methods more complex or less obvious than those described in the preceding paragraph shall be documented by direct recording of the mathematical formula or algorithm or by reference. Documentation by reference to the calculational method may be by title of the method, by reference to published technical work, or by identification of the computer program. Calculational methods shall be documented in the Scientific Notebook or Technical Report, as applicable, which identifies the input data.

3.3 Verification of Calculations

(a) A sample of at least 10% of hand (and simple hand calculator) calculations shall be checked during technical reviews of reports and the associated supporting documentation (such as Scientific Notebooks), as specified in QAP-002. The calculation checks shall be documented on or attached to the Document Review/Comment Resolution Sheet.

(b) Calculations performed by computer program (or programmable calculator) shall be verified by an alternate (i.e., hand) calculation of a sample of the data. The sample shall be of sufficient size to determine that the calculational method is correctly encoded for the ranges of each parameter employed, or:

(c) In lieu of individual verification of each application, the computer program shall be verified (by alternate calculation) to show that it produces correct solutions for the encoded algorithm within defined limits for each parameter employed and the encoded algorithm shall be shown to be appropriate for the particular application. The program verification shall become invalid with any change to the computer code.

(d) Verification of computer calculations and verification of computer programs shall be documented in Scientific Notebooks associated with the original calculations. These verifications need not be performed by an independent reviewer. For individual verification of calculations performed by computer programs, the verifications shall be documented along with the entries documenting the original computer calculations or as separate notebook entries. For computer program verification, the verification should be performed prior to performing calculations. Reference to the notebook entry documenting its verification shall be made for each use of a verified computer program.

4. RECORDS

Records identified in this procedure are generated as a result of implementing QAP-002, and shall be controlled in accordance that procedure and CQAM Section 17.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE PROCEDURE	Proc. QAP-014 Revision 1 Chg 0 Page 1 of 4

Title

QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 1 of this procedure became effective on 10/14/96 . This procedure consists of the pages and changes listed below.

Page No.	Change	Date Effective
All	0	10/14/96

SUPERSEDED

Supersedes Procedure No. QAP-014, Rev. 0, Chg 0 dated 05/31/91.

Approvals

Written By Robert Brient	Date 10/14/96	Concurrence Review for Budhi Sagar B. Sagar	Date 10/14/96
Quality Assurance Bruce Mabrito	Date 10/14/96	Cognizant Director Henry Garcia for H.C.	Date 10/14/96

QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

1. PURPOSE

The purpose of this procedure is to specify the methods for documenting and verifying scientific and engineering calculations. This procedure applies to calculations performed by hand, hand calculator, and by computer software.

2. RESPONSIBILITIES

2.1 The investigator is responsible for documenting calculations in an appropriate Scientific Notebook as specified in this procedure.

2.2 Technical reviewers are responsible for verifying samples of calculations as specified in this procedure.

3. PROCEDURE

3.1 Documentation of Calculations

Calculations shall be documented in appropriate Scientific Notebooks sufficiently so that the calculation can be duplicated. Data inputs, the calculational methods, and data outputs shall be documented as follows:

3.1.1 Data inputs, including those used in (i) simple calculations (i.e., those that can be easily duplicated by a hand calculator); (ii) complex numerical analysis by uncontrolled software; and (iii) complex numerical analysis by software controlled under TOP-18, shall be documented by direct recording of the data or by reference. Any reference should identify the source of the data, such as (i) another calculation; (ii) a report; (iii) an engineering handbook, periodic table, or other accepted source; or (iv) a laboratory or field notebook.

3.1.2 Computational methods shall be documented according to the method of calculation.

(i) Simple Calculations — The algorithm used or reference to a standard method shall be recorded in the scientific notebook unless obvious to a qualified technical reviewer.

(ii) Uncontrolled Software — Software not under TOP-018 control shall be identified by name and version in the scientific notebook and in reports presenting the results of the calculation. To preserve the exact configuration of the software used in the calculation, a copy of the software shall be archived and submitted in the review package of the associated reports. The Scientific Notebook shall include a justification for the use of the software for the specific application. In addition, one or more test cases, appropriate for the specific application of the software, shall be run to demonstrate proper operation of the software, and shall be documented in the Scientific Notebook.

(iii) Controlled Software — Software which has been controlled and released in accordance with TOP-018 shall be identified by name and version number in the Scientific Notebook and in associated reports. Additionally, justification for the use of the software for the specific application shall be documented in the Scientific Notebook.

3.1.3 Output data for calculations shall be documented in the appropriate Scientific Notebook. If the output data consist of large files, the files may be copied to a disk and attached to the Scientific Notebook or the Scientific Notebook may reference a file location. Electronic output files should identify the software name and version and date of the calculation.

3.2 Verification of Calculations

In accordance with QAP-002, the Element Manager shall check the technical review criterion associated with QAP-014 for technical reports which involve scientific or engineering calculations. The designated Technical Reviewer shall identify data within the report that were or appear to have been derived through calculation (i.e., data not directly referenced to another source), and shall sample at least 10 percent of the data for verification or as required by contract. The Technical Reviewer shall obtain the appropriate Scientific Notebooks from the investigator(s), and with the assistance of the investigator, locate the sampled calculations.

3.2.1 The Technical Reviewer shall verify that the input data have been documented as required in paragraph 3.1.1.

3.2.2 The Technical Reviewer shall verify that the calculational methods have been documented as required in paragraph 3.1.2., sections (i), (ii), or (iii) as appropriate.

3.2.3 The Technical Reviewer shall verify that the output data have been documented, and that the calculations have been correctly performed, as follows:

(i) Simple Calculations — Simple calculations (originally performed by hand, hand calculator, spread sheet, or statistical software) within the sample shall be verified by duplicate calculations.

(ii) Uncontrolled Software — Calculations performed by uncontrolled software within the sample shall be verified by checking that the input data have been correctly transferred (values, units, etc.) to the input data deck. The output data (including any post-processing of data) shall be evaluated for reasonableness considering the input data and calculation performed.

(iii) Controlled Software — Calculations performed by controlled software within the sample shall be verified by checking that the input data have been correctly transferred (values, units, etc.) to the input data deck. The output data (including any post-processing of data) shall be evaluated for reasonableness considering the input data and calculation performed.

3.2.4 Verifications shall be documented on the report comment resolution sheets (CNWRA Form TOP-3), identifying the location of the calculation by Scientific Notebook number and page. Any duplicate calculations [see paragraph 3.2.3(i)] shall be documented on or attached to the comment resolution sheet.

3.2.5 Any discrepancies between the calculation documentation and those required by this procedure shall be recorded as technical review comments requiring resolution. Resolution shall be by amending the calculation documentation so that the requirements of this procedure are met.

4. RECORDS

No records are generated as a result of this procedure. Technical review comment resolution sheets shall be retained as QA records in accordance with QAP-002.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE PROCEDURE	Proc. QAP-014 Revision 2 Chg 0 Page 1 of 4

Title: QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 2 of this procedure became effective on 8/30/2000. This procedure consists of the pages and changes listed below.

Page No.	Change	Date Effective
All	0	8/30/2000

SUPERSEDED

Supersedes Procedure No. QAP-014, Rev. 1, Chg 0 dated 10/14/96.

Approvals

Written By Budhi Sagar	Date 8/30/2000	Concurrence Review English Pearcy	Date 8/30/2000
Quality Assurance Bruce Mabrito	Date 8/30/2000	Cognizant Director Henry Garcia	Date 8/30/00

CNWRA Form QAP 1 (12/92)

QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

1. PURPOSE

The purpose of this procedure is to specify the methods for documenting and verifying scientific and engineering calculations. This procedure applies to calculations performed by hand, hand calculator, and by computer software.

2. RESPONSIBILITIES

2.1 The investigator is responsible for documenting calculations in an appropriate Scientific Notebook as specified in this procedure.

2.2 Technical reviewers are responsible for verifying samples of calculations as specified in this procedure.

3. PROCEDURE

3.1 Documentation of Calculations

Calculations shall be documented in appropriate Scientific Notebooks sufficiently so that the calculation can be duplicated.

3.1.1 Data inputs and computational methods shall be documented as follows:

(i) Calculations Performed Using Controlled Software – The name and version number of the controlled software and the input files will be documented and submitted as a part of the QA records.

(ii) Calculations Performed Using Uncontrolled Software – A source code and/or an executable copy of the uncontrolled software together with the input file will be documented and submitted as a part of the QA records.

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – The name and version number of the commercial-off-the-shelf software (e.g., spreadsheets, Mathematica, Mathcad) source code of any macros or formulae or script, and the input data will be documented and submitted as a part of the QA records.

(iv) Other Calculations – A description of the calculation method in detail sufficient for reapplication and the data used will be documented and submitted as a part of the QA records.

3.1.2 Output data from calculations shall be documented in the appropriate Scientific Notebook. If the output data consist of large files, the files may be copied to a disk and attached to the Scientific Notebook, or the Scientific Notebook may reference a file location. Electronic output files should identify the software name and version and date of the calculation. When complete input files are included in the QA records, it will be sufficient to document only a sample of the output files.

3.2 Verification of Calculations

The objective of the verification of calculations is to assure their arithmetic correctness. In consultation with the author(s), the Element Manager will determine whether a CNWRA product contains calculations and the extent to which these calculations require verification. The Element Manager will make this decision based on (i) potential importance of the calculations with respect to their intended use, (ii) extent of prior verification in related reports or papers, and (iii) complexity of calculation and potential for errors. For calculations performed using controlled software, verification of input data is generally sufficient. For calculations performed using uncontrolled software, a check of output using alternate software or hand calculations of a subset of the analysis will generally also be required. For calculations performed using commercial-off-the-shelf software (e.g., spread sheets, Mathematica, Mathcad), verification of a suitable number of formulae will generally be required in addition to the foregoing checks of input and output. The Element Manager will note on the QAP-002 review form (CNWRA Form TOP-3) the extent and type of verification required and obtain concurrence of the Technical Director for the same.

In verifying calculations, the assigned reviewer will obtain access to relevant scientific notebooks and records of input and output data files, as appropriate. The reviewer may require access to the software, if any, and exercise it as a part of the verification process.

3.2.1 The reviewer shall verify that the input data have been documented as required in paragraph 3.1.1.

3.2.2 The reviewer shall verify that the calculation methods have been documented as required in paragraph 3.1.2., sections (i), (ii), or (iii) as appropriate.

3.2.3 The reviewer shall verify the calculations to the extent determined by the Element Manager as follows.

(i) Calculations Performed Using Controlled Software – Check a sample of the input data to determine that data is correctly entered and that the input data are potentially free of errors (e.g., incorrect units, misplaced decimal, incorrect exponent, value in the wrong field, etc.). Check a sample of the output for reasonableness.

(ii) Calculations Performed Using Uncontrolled Software– In addition to checks in (i), verify sample results by alternate calculations either by hand or using alternate software, if available, or reviewing the basic logic of the uncontrolled software. The reviewer may ask the assistance of the author(s) to accomplish alternate calculations.

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – Check a sample of the formulae employed , the correctness of a sample of the input data, and the reasonableness of a sample of the output.

(iv) Other Calculations – Check correctness of a sample of the input data and verify sample results by alternate calculations.

3.2.4 Verification of calculations will be documented as part of the reviewer comments on the CNWRA TOP-3 Form. The reviewer shall indicate how the sample verification was accomplished and the conclusions regarding the correctness of calculations. For example, the reviewer may state that the report or paper under review used xxx software(s), which is controlled /uncontrolled, a sample of the input data recorded within the report or in Scientific Notebook No. yyy was checked, and an alternate calculation was/was not performed. The check determined that the calculations were/were not performed correctly.

3.2.5 In case errors are found, the author(s) must obtain resolution with the reviewer before the product can be released.

4. RECORDS

Technical review comment resolution sheets shall be retained as QA records in accordance with QAP-012, Quality Records Control.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

QUALITY ASSURANCE PROCEDURE

Proc. QAP-014
Revision 2 Chg 1

Title QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 2 of this procedure became effective on 8/30/2000. This procedure consists of the pages and changes listed below.

Page No.	Change	Date Effective
All	0	8/30/2000
1	1	2/28/2001
3	1	2/28/2001

Supersedes Procedure No. QAP-014, Rev. 1, Chg 0 dated 10/14/96.

Approvals

Written By Budhi Sagar	Date 2/28/01	Concurrence Review English Pearcy	Date 2/28/2001
Quality Assurance Bruce Mabrito	Date 2/28/2001	Cognizant Director Henry Garcia	Date 2/28/01

QAP-014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

1. PURPOSE

The purpose of this procedure is to specify the methods for documenting and verifying scientific and engineering calculations. This procedure applies to calculations performed by hand, hand calculator, and by computer software.

2. RESPONSIBILITIES

2.1 The investigator is responsible for documenting calculations in an appropriate Scientific Notebook as specified in this procedure.

2.2 Technical reviewers are responsible for verifying samples of calculations as specified in this procedure.

3. PROCEDURE

3.1 Documentation of Calculations

Calculations shall be documented in appropriate Scientific Notebooks sufficiently so that the calculation can be duplicated.

3.1.1 Data inputs and computational methods shall be documented as follows:

(i) Calculations Performed Using Controlled Software – The name and version number of the controlled software and the input files will be documented and submitted as a part of the QA records.

(ii) Calculations Performed Using Uncontrolled Software – A source code and/or an executable copy of the uncontrolled software together with the input file will be documented and submitted as a part of the QA records.

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – The name and version number of the commercial-off-the-shelf software (e.g., spreadsheets, Mathematica, Mathcad) source code of any macros or formulae or script, and the input data will be documented and submitted as a part of the QA records.

(iv) Other Calculations – A description of the calculation method in detail sufficient for reapplication and the data used will be documented and submitted as a part of the QA records.

3.1.2 Output data from calculations shall be documented in the appropriate Scientific Notebook. If the output data consist of large files, the files may be copied to a disk and attached to the Scientific Notebook, or the Scientific Notebook may reference a file location. Electronic output files should identify the software name and version and date of the calculation. When complete input files are included in the QA records, it will be sufficient to document only a sample of the output files.

3.2 Verification of Calculations

The objective of the verification of calculations is to assure their arithmetic correctness. In consultation with the author(s), the Element Manager will determine whether a CNWRA product contains calculations and the extent to which these calculations require verification. The Element Manager will make this decision based on (i) potential importance of the calculations with respect to their intended use, (ii) extent of prior verification in related reports or papers, and (iii) complexity of calculation and potential for errors. For calculations performed using controlled software, verification of input data is generally sufficient. For calculations performed using uncontrolled software, a check of output using alternate software or hand calculations of a subset of the analysis will generally also be required. For calculations performed using commercial-off-the-shelf software (e.g., spread sheets, Mathematica, Mathcad), verification of a suitable number of formulae will generally be required in addition to the foregoing checks of input and output. The Element Manager will note on the Instructions to Technical Reviewers (CNWRA QAP-12-4 Form) the extent and type of over checks required and obtain concurrence of the Technical Director for the same. When calculation over checks are not performed, there shall be a rationale clearly stated.

In verifying calculations, the assigned reviewer will obtain access to relevant scientific notebooks and records of input and output data files, as appropriate. The reviewer may require access to the software, if any, and exercise it as a part of the verification process.

3.2.1 The reviewer shall verify that the input data have been documented as required in paragraph 3.1.1.

3.2.2 The reviewer shall verify that the calculation methods have been documented as required in paragraph 3.1.2., sections (i), (ii), or (iii) as appropriate.

3.2.3 The reviewer shall verify the calculations to the extent determined by the Element Manager as follows.

(i) Calculations Performed Using Controlled Software – Check a sample of the input data to determine that data is correctly entered and that the input data are potentially free of errors (e.g., incorrect units, misplaced decimal, incorrect exponent, value in the wrong field, etc.). Check a sample of the output for reasonableness.

(ii) Calculations Performed Using Uncontrolled Software – In addition to checks in (i), verify sample results by alternate calculations either by hand or using alternate software, if available, or reviewing the basic logic of the uncontrolled software. The reviewer may ask the assistance of the author(s) to accomplish alternate calculations.

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – Check a sample of the formulae employed , the correctness of a sample of the input data, and the reasonableness of a sample of the output.

(iv) Other Calculations – Check correctness of a sample of the input data and verify sample results by alternate calculations.

3.2.4 Verification of calculations will be documented as part of the reviewer comments on the CNWRA TOP-3 Form. The reviewer shall indicate how the sample verification was accomplished and the conclusions regarding the correctness of calculations. For example, the reviewer may state that the report or paper under review used xxx software(s), which is controlled/uncontrolled, a sample of the input data recorded within the report or in Scientific Notebook No. yyy was checked, and an alternate calculation was/was not performed. The check determined that the calculations were/were not performed correctly.

3.2.5 In case errors are found, the author(s) must obtain resolution with the reviewer before the product can be released.

4. RECORDS

Technical review comment resolution sheets shall be retained as QA records in accordance with QAP-012, Quality Records Control.