

**GEOSCIENCES AND ENGINEERING DIVISION**

**QUALITY ASSURANCE PROCEDURE**

Proc. QAP-014

Revision 3 Chg 1

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

**EFFECTIVITY AND APPROVAL**

Revision 3 of this procedure became effective on 8/25/2005. This procedure consists of the pages and changes listed below.

<u>Page No.</u>	<u>Change</u>	<u>Date Effective</u>
1-5	1	05/03/2006

Change 1 clarifies how calculation documentation must be traceable to scientific notebook entries.

Supersedes Procedure No. QAP-014, Rev.3, Chg 0, dated 8/25/2005

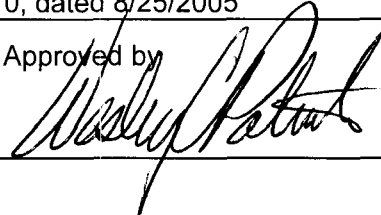
Prepared by



Date

4/21/2006

Approved by



Date

4/21/2006

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QAP-014 DOCUMENTATION AND VERIFICATION  
OF SCIENTIFIC AND ENGINEERING CALCULATIONS

1. PURPOSE

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

2. RESPONSIBILITIES

- 2.1 The investigator is responsible for documenting calculations as specified in this procedure.
- 2.2 Technical reviewers are responsible for verifying calculations as specified in this procedure.

3. PROCEDURE

3.1 Documenting Calculations

Calculations shall be documented in appropriate scientific notebooks or in the reviewed document (e.g., a technical report, journal article, or similar item) in sufficient detail so that the calculations and results can be reproduced.

- 3.1.1 The required documentation for various calculation methods is specified in Table 1.
- 3.1.2 Calculation documentation may be copied to electronic media and attached to the scientific notebook. The electronic media input and output files shall be identified such that traceability to the associated scientific notebook(s) entry is provided and maintained.

3.2 Verifying Calculations

- 3.2.1 The objective of verifying calculations is to assure their arithmetic correctness. When preparing a document for review in accordance with QAP-002, Review of Documents, Reports, and Papers, the manager responsible for the document will determine whether a product contains calculations and the extent to which these calculations require verification. The 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. By checking the appropriate blocks of the Instructions to Technical Reviewers (form QAP-12) the manager shall identify the extent and type of over-checks required

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based on the calculation methods used. Rationale shall be provided to justify when calculation over-checks are not required.

- 3.2.2 When calculation verification is required in the Instructions to Technical Reviewers form, the technical reviewer shall obtain access to relevant scientific notebooks and records of input and output data files, as necessary. As applicable, the technical reviewer may require access to the software used to perform the calculation and exercise the software as a part of the verification process.
- 3.2.3 The technical reviewer shall verify that input data, calculation methods (i.e., software identification and version), and output data have been documented as specified in Table 1.
- 3.2.4 The technical reviewer shall verify the calculations using the methods specified in Table 1 for the calculation method used.
- 3.2.5 Calculation verification shall be documented as part of the technical reviewer comments on the form TOP-3 Report Review/Comment Resolution Record. The technical reviewer shall indicate how the verification was accomplished and the conclusions regarding the correctness of calculations. The technical reviewer should identify the software used (when applicable), the software control and validation status, and the location of the calculation documentation (i.e., scientific notebook number).
- 3.2.6 If calculation errors are found during the technical review, the calculations and affected portions of the report shall be corrected before the review process is completed and the product is released.

#### 4. RECORDS

Report review/comment resolution sheets shall be retained as quality assurance records in accordance with QAP-012, Quality Assurance Records Control.

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**Table 1**

<b>Calculation Method</b>	<b>Required Documentation</b>	<b>Required Verification</b>
Using Controlled Software	Name and version number of the controlled software  Input files  User defined variables, parameters, and other information needed to perform the calculation  Output files  Documentation in electronic media shall be traceable to the associated scientific notebook entry.	Check a sample of the input data to determine that data are correctly entered and are 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.
Using Uncontrolled Software	Copy of the source code or executable code of the uncontrolled software (submitted in the quality assurance record package for the technical document).  Input files  User defined variables, parameters, and other information needed to perform the calculation  Output files  Documentation in electronic media shall be traceable to the associated scientific notebook entry.	Check a sample of the input data to determine that data are correctly entered and are free of errors (e.g., incorrect units, misplaced decimal, incorrect exponent, value in the wrong field, etc.).  Check a sample of results by alternate calculations either by hand, by using alternate software, or by reviewing the basic logic of the uncontrolled software. The reviewer may ask the assistance of the report author(s) in operating the software.

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**Table 1 (Continued)**

<b>Calculation Method</b>	<b>Required Documentation</b>	<b>Required Verification</b>
Using Commercial-Off-the-Shelf Software	<p>Name and version number of the commercial-off-the-shelf software (e.g., spreadsheets, Mathematica, Mathcad).</p> <p>Source code or description of any macros, formulae, or scripts, as applicable.</p> <p>Input data</p> <p>Output data</p> <p>Documentation in electronic media shall be traceable to the associated scientific notebook entry.</p>	<p>Check a sample of the input data to determine that data are correctly entered and are free of errors (e.g., incorrect units, misplaced decimal, incorrect exponent, value in the wrong field, etc.).</p> <p>Check a sample of the formulae employed.</p> <p>Check the reasonableness of a sample of the output.</p>
Other Calculations (Hand, Hand Calculator)	<p>Description of the calculation method in detail sufficient to reproduce the calculation and results.</p> <p>Input data</p> <p>Output data</p> <p>All documentation shall be traceable to the associated scientific notebook entry.</p>	<p>Check correctness of a sample of the input data.</p> <p>Check a sample of results by alternate calculations.</p>