Department of Energy
Washington, DC 20585
January 29, 2004

The Honorable John T. Conway
Chairman
Defense Nuclear Facilities Safety Board
625 Indiana Avenue, NW
Washington, D.C. 20004-2941

Dear Mr. Chairman:

The Implementation Plan for Software Quality Assurance (SQA) in response to Defense Nuclear Facilities Safety Board (DNFSB) Recommendation 2002-1 requires the Office of Environment, Safety and Health (EH) to perform a gap analysis on the toolbox codes. Commitment 4.2.1.3 requires this analysis to determine the actions needed to bring the codes into compliance with SQA criteria and to develop a schedule with milestones to upgrade each code based on the gap analysis results.

This commitment was reported on December 3, 2003, as partially complete. At that time, three of the six gap analyses reports were submitted as interim reports for MACCS2, ALOHA, and EPICODE. The remaining three gap analysis interim reports for MELCOR, GENII, and CFAST have now been completed and are attached. The gap analysis evaluated the SQA attributes of the six codes against identified criteria to determine the actions needed to bring the specific software into compliance with established SQA criteria. Because the Department does not own the six toolbox codes, a firm schedule for upgrading each code cannot be developed. The gap analysis does however, include an estimate of the level of effort required to upgrade each code based on the gap analysis results; a total of eight full-time equivalent years is estimated to upgrade all six toolbox codes. We are working with Program Secretarial Offices and the code developers to evaluate the feasibility and schedule for completing the upgrades.

The gap analyses identify no software-induced errors in the codes that would have led to non-conservatisms at defense nuclear facilities. The attached interim reports document this finding, provide the opportunity for peer review, and promote discussion within the SQA community. Peer review is in progress and code developer review will be completed as soon as practical. We will keep your staff apprised of our progress and expected completion schedule. Completion of this commitment will not impact other ongoing SQA Implementation Plan activities.

Please contact me at (202) 586-6151, or have your staff contact Frank Russo at (301) 903-8008 if you have any questions concerning this commitment.

Sincerely,

Beverly A. Cook
Assistant Secretary
Environment, Safety and Health

Attachments (3)

cc: Mark Whitaker, DR-1
Frank Russo, EH-3
Chip Lagdon, EH-31

SEPARATION

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DOE-EH-4.2.1.3-Interim-MELCOR

Defense Nuclear Facilities Safety Board Recommendation 2002-1
Software Quality Assurance Implementation Plan
Commitment 4.2.1.3:

MELCOR Gap Analysis

Interim Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

January 2004

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FOREWORD

This report documents the outcome of an evaluation of the Software Quality Assurance (SQA) attributes of the MELCOR computer code for leak path factor applications, relative to established requirements. This evaluation, a "gap analysis," is performed to meet Commitment 4.2.1.3 of the Department of Energy's Implementation Plan to resolve SQA issues identified in Defense Nuclear Facilities Safety Board Recommendation 2002-1.

Suggestions for corrections or improvements to this document should be addressed to:

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Software Quality Assurance Implementation Plan: MELCOR Gap Analysis

EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board (DNFSB) issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002 (DNFSB 2002). The Recommendation identified a number of quality assurance issues for software used in Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major improvement actions discussed in the *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. A DOE safety analysis toolbox would contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications.

The Methods for Estimation of Leakages and Consequences of Releases (MELCOR) software is one of the codes designated for the toolbox. It is being evaluated for leak path factor (LPF) applications. To determine the actions needed to bring the MELCOR code into compliance with the SQA qualification criteria in the context of LPF applications and develop an estimate of the resources required to perform the upgrade, the Implementation Plan has committed to sponsoring a code-specific gap analysis document. The gap analysis evaluates the software quality assurance attributes of MELCOR against identified criteria.

The balance of this document provides the outcome of the gap analysis compliant with NQA-1-based requirements. Of the ten SQA requirements for existing software at the Level B classification ("important for safety analysis but whose output is not applied without further review"), five requirements are met at acceptable level, i.e., *Software Classification, Implementation Phase, User Instructions*, *Acceptance Test,* and *Configuration Control*; Requirements 1, 5, 7, 8, and 9 respectively. Remedial actions are recommended to meet SQA criteria for the remaining five requirements.

A new software baseline is recommended for MELCOR in the context of LPF applications. Suggested remedial actions for this software would warrant upgrading software documents that describe the new baseline. At a minimum, it is recommended that software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation
3. Providing training on a regular basis, and
4. Developing new software documentation.

The complete list of suggested, revised baseline documents includes the following:

- Updated Software Quality Assurance Plan
- Software Requirements Document (Specific to LPF)
- Software Design Document (Specific to LPF)

- Test Case Description and Report (Specific to LPF)
- Updated Software Configuration and Control
- Updated Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

Once these actions have been accomplished, MELCOR Version 1.8.5 will be qualified in the context of LPF applications for the DOE Safety Analysis Toolbox. Initially, approximately two full-time equivalent years is estimated to complete these actions. Thereafter, maintenance funding will be required for activities such as defect reporting, coordinated update testing as NRC makes changes, and minor SQA administrative duties.

While SQA improvement actions are recommended for MELCOR Version 1.8.5, no evidence has been found of software-induced errors in MELCOR that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

1.0 Introduction

This document reports the results of a gap analysis for Version 1.8.5 of the MELCOR computer code in the context of LPF applications. The intent of the gap analysis is to determine the actions needed to bring the specific software into compliance with established SQA criteria. A secondary aspect of this report is to develop an estimate of the level of effort required to upgrade each code based on the gap analysis results.

1.1 Background: Overview of Designated Toolbox Software in the Context of 10 CFR 830

In January 2000, the DNFSB issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding computer SQA in the Department of Energy (DOE) Complex for software used to make safety-related decisions, or software that controls safety-related systems. Instances were noted of computer codes that were either inappropriately applied, or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, from facility to facility, and the variability in guidance and training in the appropriate use of accident analysis software.

While progress was made in resolving several of the issues raised in TECH-25, the DNFSB issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software. The Recommendation identified a number of quality assurance issues for software used in the DOE facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, SQA-compliant safety analysis codes is one of the major commitments contained in the March, 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities* (IP). In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications.

Six computer codes, including ALOHA (chemical release dispersion/consequence analysis), CFAST (fire analysis), EPIcode (chemical release dispersion/consequence analysis), GENII (radiological dispersion/consequence analysis), MACCS2 (radiological dispersion/consequence analysis), and MELCOR (LPF analysis) were designated by DOE for the toolbox (DOE/EH, 2003). It is found that this software provides generally recognized and acceptable approaches for modeling source term and consequence phenomenology, and can be applied as appropriate to support accident analysis in Documented Safety Analyses (DSAs).

As one of the designated toolbox codes, MELCOR Version 1.8.5 will likely require some degree of quality assurance improvement before meeting current SQA standards. The analysis documented herein is an evaluation of MELCOR, in the context of LPF applications, relative to current SQA criteria. It assesses the margin of the deficiencies, or gaps, to provide DOE and the software developer the extent to which minimum upgrades are needed. The overall assessment is therefore termed a "gap" analysis.

1.2 Evaluation of Toolbox Codes

The quality assurance criteria identified in later sections of this report are defined as the set of established requirements, or bases, by which to evaluate each designated toolbox code. This gap analysis evaluation is Commitment 4.2.1.3 in the IP:

> Perform a gap analysis of the "toolbox" codes to determine the actions needed to bring the codes into compliance with the SQA qualification criteria, and develop a schedule with milestones to upgrade each code based on the gap analysis results.

This process is a prerequisite step for software improvement. It will allow DOE to determine the current limitations and vulnerabilities of each code as well as help define and prioritize the steps required for improvement.

Ideally, each toolbox code owner will provide input information on the SQA programs, processes, and procedures used to develop their software. However, the gap analysis itself will be performed by a SQA evaluator. The SQA evaluator is independent of the code developer, but knowledgeable in the use of the software for accident analysis applications and current software development standards.

1.3 Uses of the Gap Analysis

The gap analysis will provide information to DOE, code developers, and code users.

DOE will see the following benefits:

- Estimates of the resources required to perform modifications to designated toolbox codes
- Basis for schedule and prioritization to upgrade each designated toolbox code.

Each code developer will be provided the following:

- Information on areas where SQA improvements are needed to comply with industry SQA standards and practices
- Specific areas for improvement for guiding development of new versions of the software.

DOE safety analysts and code users will benefit from the following:

- Improved awareness of the strengths, limits, and vulnerable areas of each computer code
- Recommendations for code use in safety analysis application areas.

1.4 Scope

This analysis is applicable to the MELCOR code, one of the six designated toolbox codes for safety analysis, for applications of LPF analysis. While the MELCOR code is the subject of the current report, other safety analysis software considered for the toolbox in the future may be evaluated with the same process applied here. The template outlined in this document is applicable for any analytical software as long as the primary criteria are ASME NQA-1, 10 CFR 830, and related DOE directives discussed in DOE (2003e).

1.5 Purpose

The purpose of this report is to document the gap analysis performed on the MELCOR code for LPF applications as part of DOE's implementation plan on SQA improvements.

1.6 Methodology for Gap Analysis

The gap analysis for MELCOR (LPF applications) is based on the plan and criteria described in *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes* (DOE 2003e). The overall methodology for the gap analysis is summarized in Table 1-1. The gap analysis utilizes ten of the fourteen topical areas listed in DOE (2003e) related to SQA to assess the quality of the MELCOR code in the context of LPF applications. The four areas eliminated in this gap analysis are dedication, evaluation, operation and maintenance, and access control. These areas focus on software intended to control hardware or focus on the end user SQA for the software. Therefore, the remaining ten areas are assessed individually in Section 4.

An information template was transmitted to the Safety Analysis Software Developers on 20 October 2003 to provide basic information as input to the gap analysis process. It is noted that, no written response to the information template has been provided by the MELCOR software developers. Instead, SNL personnel were interviewed in January 2004 to obtain needed information to perform this analysis.

Table 1-1 — Plan for SQA Evaluation of Existing Safety Analysis Software[1]

Phase	**Procedure**
1. Prerequisites	a. Determine that sufficient information is provided by the software developer to allow it to be properly classified for its intended end-use. b. Review SQAP per applicable requirements in Table 3-3 of DOE (2003e).
2. Software Engineering Process Requirements	a. Review SQAP for: • Required activities, documents, and deliverables • Level and extent of reviews and approvals, including internal and independent review. Confirm that actions and deliverables (as specified in the SQAP) have been completed and are adequate. b. Review engineering documentation identified in the SQAP, e.g., • Software Requirements Document • Software Design Document • Test Case Description and Report • Software Configuration and Control Document • Error Notification and Corrective Action Report, and • User's Instructions (alternatively, a User's Manual), Model Description (if this information has not already been covered). c. Identify documents that are acceptable from SQA perspective. Note inadequate documents as appropriate.
3. Software Product Technical/ Functional Requirements	a. Review requirements documentation to determine if requirements support intended use in Safety Analysis. Document this determination in gap analysis document. b. Review previously conducted software testing to verify that it sufficiently demonstrated software performance required by the Software Requirements Document. Document this determination in the gap analysis document.
4. Testing	a. Determine whether past software testing for the software being evaluated provides adequate assurance that software product/technical requirements have been met. Obtain documentation of this determination. Document this determination in the gap analysis report. b. (Optional) Recommend test plans/cases/acceptance criteria as needed per the SQAP if testing not performed or incomplete.
5. New Software Baseline	a. Recommend remedial actions for upgrading software documents that constitute baseline for software. Recommendations can include complete revision or providing new documentation. A complete list of baseline documents includes: • SQA Plan • Software Requirements Document • Software Design Document • Test Case Description and Report • Software Configuration and Control • Error Notification and Corrective Action Report, and • User's Instructions (alternatively, a User's Manual) b. Provide recommendation for central registry as to minimum set of SQA documents to constitute new baseline per the SQAP.

[1] Originally documented as Table 2-2 in DOE (2003e).

Table 1-1 – Plan for SQA Evaluation of Existing Safety Analysis Software (continued)

Phase	Procedure
6. Training	a. Identify current training programs provided by developer. b. Determine applicability of training for DOE facility safety analysis.
7. Software Engineering Planning	a. Identify planned improvements of software to comply with SQA requirements. b. Determine software modifications planned by developer. c. Provide recommendations from user community. d. Estimate resources required to upgrade software.

1.7 Summary Description of Software Being Reviewed

The gap analysis was performed on Version 1.8.5 of the MELCOR code in the context of LPF applications. MELCOR (Gauntt, 2000a) is a generalized mass transport and thermal hydraulic computer program. MELCOR is available for the UNIX workstation platform as well as the PC platform.

MELCOR is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. MELCOR estimates fission product source terms and their sensitivities and uncertainties in a variety of applications. The MELCOR code is composed of a number of major modules, or packages, that together model the major systems of a reactor plant and its generally coupled interactions.

MELCOR was initially developed at the Sandia National Laboratories (SNL) under the sponsorship of the USNRC to assess reactor severe accident conditions. MELCOR was developed as a "research" code by the NRC and SNL. It was intended to be used to perform parametric studies, scoping studies, and studies to check the results of other models. For the last several years, MELCOR has been used in the DOE complex to model release of radioactive airborne material from nuclear facilities and structures. The amount released is termed leakage and is usually expressed as a fraction of the amount considered available for release. This fraction released is referred to as the Leak Path Factor, LPF.

Although the MELCOR computer code was developed to model the progression of accidents in light water reactor nuclear power plants, the modeling capabilities of MELCOR are sufficiently flexible that it can be applied to the analysis of nonreactor problems. When performing LPF studies for nuclear facilities the modules used are reduced (through input specification) to those which will enable the modeling of the release and transport of aerosolized materials – the code activates modules based on the input card identification field. The most common modules used for Leak Path Factor analyses are:

- Executive Package (EXEC)
- Non-Condensable Gas Package (NCG)
- Control Volume Hydrodynamics Package (CVH)
- Flow Path Package (FL)
- Heat Structures Package (HS)
- Radio-Nuclide Package (RN)
- Control Function Package (CF)
- Tabular Function Package (TF)

Both NRC and the DOE have sponsored changes to the code, with NRC being the primary sponsor. For example, modifications were made to a version of MELCOR to model K reactor severe accidents at the DOE operated Savannah River Site. Some of this work factored into later updates of the code.

Figure 1-1 depicts a basic flowchart showing the steps required to successfully execute MELCOR.

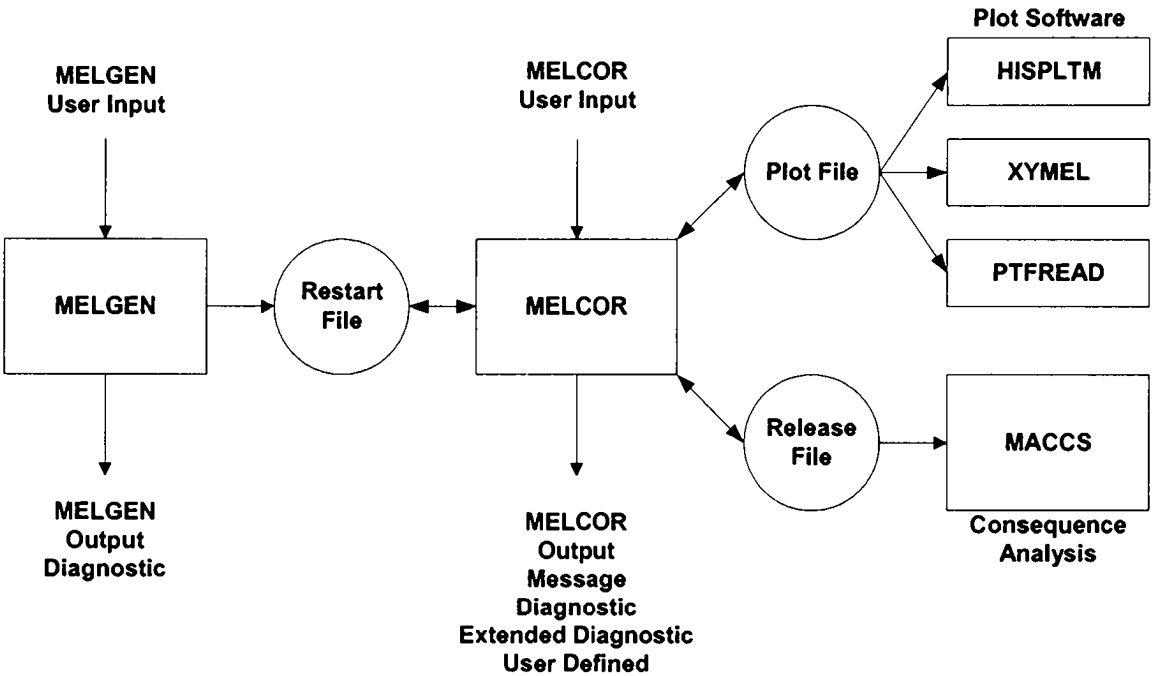

Figure 1-1 MELCOR Execution Flowchart

A brief summary of MELCOR is contained in Table 1-2.

The documents reviewed as part of the gap analysis are listed in Table 1-3.

Table 1-2 — Summary Description of the MELCOR Software in the Context of LPF Analysis

Type	Specific Information
Code Name	MELCOR - Methods for Estimation of Leakages and Consequences of Releases
Developing Organization and Sponsor	Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (primary), International Cooperative Severe Accident Research Program (CSARP) and U.S. Department of Energy (minor contribution)
Version of the Code	Version 1.8.5
Auxiliary Codes	AUXILIARY CODES: The plotting software distributed with MELCOR includes HISPLTM, XYMEL, and PTFREAD. The output from MELCOR can be input into the MACCS2 (or earlier version MACCS) code to perform consequence analysis. MELCOR INSTALL Installs software.
Software Platform/Portability	FORTRAN 77/90, PC based some system dependencies. Also runs on Unix (not tested for every platform), source code is available for HP, SUN and others.
Coding and Computer	Fortran 77, PC based 80486 or Pentium processor (C00652/PC486/00).
Technical Support	R. O. Gauntt Sandia National Laboratories P.O. Box 5800 Albuquerque, NM 87185-0748 (505) 284-3989 rogaunt@sandia.gov;
Code Procurement	The MELCOR program and comprehensive set of MELCOR documentation is available through SNL. MELCOR has a website: http://melcor.sandia.gov/. Permission from NRC is needed to acquire the code.
Code Package	Included are the references cited below. Also included are the Fortran source code and an executable file. Training slides and a sample input deck are also available on the web site.

Table 1-2 — Summary Description of MELCOR Software in the Context of LPF Analysis (Continued)

Documentation Supplied with Code Transmittal	1. Gauntt, 2000a, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 1: Primer and Users' Guide*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/1, May 2000. 2. Gauntt, 2000b, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 2: Reference Manuals*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/2, May 2000. 3. Gauntt, 2001, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 3: Demonstration Problems*, Version 1.8.5, NUREG/CR-6119 Rev. 0, SAND2001-0929P, May 2001. (Available upon request) 4. File of electronic input decks. 5. MELCOR INSTALLER. 6. Instructions for installing MELCOR for use with Digital Fortran 5/6 and Developer Studio.
Nature of Problem	MELCOR is a fully integrated, relatively fast-running code that models the progression of severe accidents in nuclear power plants. An entire spectrum of severe accident phenomena is modeled in MELCOR. Characteristics of severe accident progression that can be treated with MELCOR include the thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings; core heatup and degradation; radionuclide release and transport; hydrogen production, transport, and combustion; core-concrete attack; heat structure response; and the impact of engineering safety features on thermal-hydraulic and radionuclide behavior. For applications in non-reactor facilities of the DOE complex, MELCOR has been used primarily to model in-facility transport of the release of radioactive airborne material. Deposition inside the building is calculated and the leakage to the outside environment is expressed as a fraction of the amount considered available for release and is termed the LPF.
Method of Solution	MELCOR can be used to model in-facility transport that involves the two broad areas of mixing/transport of a hazardous gas and/or aerosol transport of a hazardous material. MELCOR employs the control volume approach with lumped parameter models. MELCOR has detailed mechanistic aerosol dynamics models for the transport, deposition, and agglomeration of aerosols. Major assumptions in MELCOR include: • Each control volume gas space is well mixed, except each cell does allow for a pool covered by a gas volume. • Each gas species has the same velocity in the flow path connections. • No condensable gases are assumed to be ideal. • Turbulence and species diffusion within a control volume are not modeled, except in the aerosol model and condensation/evaporation on surfaces.

Table **1-2 — Summary Description of MELCOR Software in the Context of LPF Analysis (Continued)**

Restrictions or Limitations	The control-volume, lumped-parameter approach of MELCOR does not model multi-dimensional effects, such as stratification of gases within a room. (To overcome this, one approach is to break the room into more volumes sometimes coupling the approach with computational fluid dynamics (CFD) code results.)
Run Time	The typical execution time depends on machine, detail of the model, and the length of the transient. Runtimes on the CRAY vary from 0.1 s to on the order of 1 h.[2] Runtimes for the Marviken-V Aerosol Transport Tests ATT varied from 3442 cpu(s) on a CRAY XMP-24, to 26,700 cpu(s) on a SUN Sparc2. Detailed code calculation of 24-h LaSalle Station Blackout calculation was 2 h on an HP. Simplified code calculation runtime for a 4-h sample problem transient was 15 min on an HP. The ratio of real time to runtime can vary from 0.5 to 100, depending on the nodalization.
Computer Hardware Requirements	Memory requirement is 5 MB. Depending on the model application Gigabytes of storage for output files may be required.[2]
Computer Software Requirements	MELCOR is available for the UNIX workstation platform as well as the PC platform. The execution of MELCOR on a PC is very efficient and user friendly. While either platform may be used, simply because of ease of use the latter is recommended. (A benefit of running on a PC is the ease with which output data can be processed in spreadsheet or text file programs.)
Other Versions Available	No other versions are available from SNL. INEEL and SRS both have developed specialized versions, but these are not supported by SNL and the sponsors.

[2] The data in this paragraph is dated by about 10 years. Typical run times on today's computers would be a few minutes. The most complicated models run approximately one week. Storage (output file size) is often more of limit today than run time. Actual conditions will depend on the hardware and the type of problem being executed.

Table 1-3 — Software Documentation Reviewed for MELCOR (LPF Applications)

No.	Reference
1.	Gauntt, 2000a, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 1: Primer and Users' Guide*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/1, May 2000.
2.	Gauntt, 2000b, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 2: Reference Manuals*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/2, May 2000.
3.	Gauntt, 2001, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 3: Demonstration Problems*, Version 1.8.5, NUREG/CR-6119 Rev. 0, SAND2001-0929P, May 2001.
4.	SNL, 2001, Sandia National Laboratories. *5th MELCOR User's Workshop*, Bethesda, MD, May 10th – 15th, 2001.
5.	SNL 2003, Sandia National Laboratories. Nuclear Waste Management Procedure, NP 19-1, *Software Requirements*, Revision 10, Waste Isolation Pilot Plant, (May 2003).
6.	East, 1998, J.M. East and E.P. Hope, *Independent Evaluation of the MACCS2 Software Quality Assurance Program (U)*, WSRC-RP-98-00712, Westinghouse Savannah River Company, Aiken, SC (August 1998).
7.	DNFSB, 2000, Defense Nuclear Facilities Safety Board, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Technical Report DNFSB/TECH-25, (January 2000).
8.	DOE 2003f, U.S. Department of Energy. *MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis*, Interim Report, (September 2003).
9.	SNL 1992, Sandia National Laboratories. *Software Quality Assurance Procedures for MELCOR*, Revision 1.2, (August 1992).

2.0 Assessment Summary Results

2.1 Criteria Met

Of the 10 general topical quality areas assessed in the gap analysis, five satisfactorily met the criteria. The analysis found that the MELCOR SQA program (in the context of LPF applications) in general, met criteria for *Software Classification, Implementation Phase, User Instructions, Acceptance Test,* and *Configuration Control*, Requirements 1, 5, 7, 8, and 9 respectively. Five topical quality areas were not met satisfactorily. The major deficiency areas are covered below in Section 2.2 (Exceptions to Requirements). Detail on the evaluation process relative to the requirements and the criteria applied are found in Section 4.

2.2 Exceptions to Requirements

Some of the more important exceptions to criteria found for MELCOR are listed below in Table 2-1. The requirement is given, the reason the requirement was not met is provided, and remedial action(s) are listed to correct the exceptions.

Table 2-1 — Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion	Reason Not Met	Remedial Action(s)
1.	SQA Procedures/Plans (Section 4.2)	SQA Plan and Procedures for Version 1.8.5 of MELCOR software were lacking components to match present day requirements. Portions of the existing version are out of date or are not currently followed.	As part of the new software baseline, the SQA Plan covering version 1.8.5 and successor versions of MELCOR should be provided to the Central Registry. SQA procedures that provide prescriptive guidance to the MELCOR software developers should be made available to a SQA evaluator for confirmatory review.
			Establish a written and approved SQA plan eliminating draft or non-compliant informal processes of development.
			Upgrade SQA program documentation, especially those procedures used for new features added in MELCOR that have an effect on modules that are typically used in LPF applications. Ensure prompt defect/error reporting.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document for Version 1.8.5 of MELCOR is not available.	As part of the new software baseline for MELCOR, a Software Requirements Document should be prepared.
3.	Design Phase (Section 4.4)	A Software Design Document is not available. Thus, design information was not directly available. Instead, it was necessary to infer the intent of MELCOR design from model	As part of the new software baseline for MELCOR, a Software Design Document should be prepared.

No.	Criterion	Reason Not Met	Remedial Action(s)
		description and user guidance documents.	
4.	Testing Phase (Section 4.6)	A Software Testing Report Document has not been produced for MELCOR, and therefore, test process and methodology could not be evaluated directly. Thus, testing process and methods had to be inferred from other information. Isolated validation studies have been previously documented for various phenomenological areas, including aerosol transport, which is the key area for LPF applications. While these studies promote confidence in the models for LPF applications, the necessary formality is lacking to make a complete evaluation.	As part of the new software baseline for MELCOR, a test case report should be prepared. An important part of the new baseline set of documentation should specifically address aerosol transport phenomena and LPF applications.
5.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report process is in place at SNL, but limited documentation is available. Users are not necessarily notified of errors. Follow up with the notifying agent is not always guaranteed, and the impact is not always assessed and reported.	While a Software Problem Reporting system is in place at SNL, it requires revision to ensure affected users are notified, closure occurs with the originator, and impact determinations are completed promptly.

2.3 Areas Needing Improvement

The gap analysis, communications with DOE, oversight organizations, safety analysts, and inputs from the long-term MELCOR users have identified a few improvements that could be made related to the code and its quality assurance. The major areas to be addressed are described in this section.

The key recommendations for improvements to MELCOR are summarized in Table 2-2.

Table 2-2 — Summary of Important Recommendations for MELCOR for LPF Applications

No.	UI – User Interface Enhancements TM – Technical Model Upgrade	Recommendation
1.	UI	Expand selection of sample problems to include those problems and releases type that are often treated in LPF analysis for Documented Safety Analyses (DSAs).
2.	UI	Provide the user more control over the printed output by allowing only selected items to print. This will help avoid lengthy output files, and enhance post-processing. As an example, similar print options as used in MACCS would be useful. Consider adding in this same update an option to print summary information on the aerosol mass balance amongst volumes. This would consolidate information currently available that the user must manually extract at

No.	UI – User Interface Enhancements TM – Technical Model Upgrade	Recommendation
		present, and would lessen the likelihood of error.

Item 1 in the above table will serve at least two functions. First, it will serve to enhance training for LPF. Second, it will support the LPF testing and SQA changes identified in other areas of this report.

2.4 Conclusion Regarding Software's Ability to Meet Intended Function

The MELCOR code was evaluated to determine if the software, in its current state, meets the intended function in a safety analysis context as assessed in this gap analysis. When the code is run for the intended applications as detailed in the code guidance document, MELCOR *Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis*, (DOE 2003f), it is judged that it will meet the intended function. Current software concerns and issues can be avoided by understanding MELCOR limitations and capabilities, and applying the software in the appropriate types of scenarios for which precedents have been identified.

3.0 Lessons Learned

Table 3-1 provides a summary of the lessons learned during the performance of the MELCOR gap analysis.

Table 3-1 — Lessons Learned

No.	Lesson
1.	Use of NQA-1 or other SQA criteria could not be fully verified. It is obvious that many actions supporting SQA practices have been applied in developing MELCOR, but independent confirmation of the SQA program, practices, and procedures is not possible due to lack of documentation.
2.	Observance of SQA requirements in the development of safety analysis software has not been consistent. It appears to be sporadic in application, poorly funded, and performed as an add-on activity. (Note that this is consistent with the "research" specification as given to the code.) Funding level during program development has been a key factor in determining the level of attention to SQA and the adequacy of documentation.
3.	While some evidence of pre-development planning is found for the MELCOR software, documentation is not maintained as would be expected for compliance with Quality Assurance criteria in Subpart A to 10 CFR 830 (Nuclear Safety Management).
4.	A new software baseline can be produced with "modest" resources. Initial rough estimates are 2 full-time equivalent years and should be a high priority. As time passes, knowledgeable personnel may become unavailable and it will become more difficult and costly (if not impossible) to document the QA status of the code.
5.	Additional opportunities and venues should be sought for training and user qualification on safety analysis software. This is a long-term deficiency that needs to be addressed for MELCOR LPF applications and other designated software for the DOE toolbox.

4.0 Detailed Results of the Assessment Process

Ten topical areas, or requirements, are presented in the assessment as listed in Table 4.0-1. Training and Software Improvements (resource estimate) sections follow the 10 topical areas.

Table 4.0-1 — Cross-Reference of Requirements with Subsection and Entry from DOE (2003e)

Subsection (This Report)	Corresponding Entry Table 3-3 from DOE (2003e)	Requirement
4.1	1	Software Classification
4.2	2	SQA Procedures/Plans
4.3	5	Requirements Phase
4.4	6	Design Phase
4.5	7	Implementation Phase
4.6	8	Testing Phase
4.7	9	User Instructions
4.8	10	Acceptance Test
4.9	12	Configuration Control
4.10	13	Error Notification

The gap analysis utilizes ten of the fourteen topical areas listed in DOE (2003e) related to SQA to assess the quality of the MELCOR code in the context of LPF applications. The four areas eliminated in this gap
analysis are dedication, evaluation, operation and maintenance, and access control. These areas focus on software intended to control hardware or focus on the end user SQA for the software. Consequently, they were evaluated as not being sufficiently relevant to the safety analyses software or to this GAP analyses which focuses on the code prior to receipt by end users.

In the tables that follow, criteria and recommendations are labeled as (1.x, 2,x, ...10.x) with the first value (1., 2., ... 10) corresponding to the topical area and the second value (x), the sequential table order of each entry.

4.1 Topical Area 1 Assessment: Software Classification

This area corresponds to the requirement entitled Software Classification in Table 3-3 of DOE (2003e).

4.1.1 Criterion Specification and Result

Table 4.1-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Sufficient documentation is provided with the software on the MELCOR website (see Table 1-2, under "Documentation Supplied with Code Transmittal"), to make an informed determination of the classification of the software. A user of the MELCOR software for LPF calculations in safety analysis applications would be expected to interpret the information on the software in light of the requirements that are discussed in Appendix A to DOE-STD-3009-94 to decide on an appropriate safety classification. For most organizations, the safety class or safety significant classification, or Level B in the classification hierarchy discussed in DOE (2003e), would be selected. In the software requirements procedure provided by SNL, the MELCOR software would be deemed Compliance Decision (CD) software (SNL 2003).

Table 4.1-1 — Subset of Criteria for Software Classification Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
1.1	The code developer must provide sufficient information to allow the user to make an informed decision on the classification of the software.	Yes	Sufficient information is provided by the MELCOR users' manuals that are available from the software developer and the MELCOR website. Interpreted in light of Appendix A to DOE-STD-3009-94.

4.1.2 Sources and Method of Review

Documentation supplied with the MELCOR software package.

4.1.3 Software Quality-Related Issues or Concerns

There are no SQA issues or concerns relative to this requirement.

4.1.4 Recommendations

No recommendations are provided at this time.

4.2 Topical Area 2 Assessment: SQA Procedures and Plans

This area corresponds to the requirement entitled SQA Procedures and Plans in Table 3-3 of DOE (2003e).

Use is made of an earlier independent review of the MACCS2 SQA Program (East 1998) coupled with an interview of the Sandia National Laboratories authors to determine the level of compliance with this requirement.

While the (East 1998) review focused on the MACCS2 computer code, much information was obtained on the general SQA program that existed at SNL around the time that both MACCS2 and the MELCOR

software were being developed. The documented review was preceded by an in-depth review at Sandia National Laboratories in 1997. The following, based on the earlier review, provides a good synopsis of the SQA program that existed in the late 1980s and early 1990s.

SNL established a SQA program for Laboratory software in the late 1980s and early 1990s that was compliant with the IEEE Standard for SQA Plans. The final volume was put into place in 1995. The guidelines[3] are documented as shown:

Volume 1 – Software Quality Planning [SNL, 1987]
Volume 2 – Documentation [SNL, 1995]
Volume 3 – Standards, Practices, and Conventions [SNL, 1986]
Volume 4 – Configuration Management [SNL, 1992a]; and
Volume 5 –Tools, Techniques, and Methodologies [SNL, 1989].

The following is a list and description of the necessary documents required for a complete SNL SQA package [SNL, 1986]:

Project Plan: The project plan is a brief overview of the project. It defines the project, describes the organization, proposes schedules and milestones, and defines procedures to ensure the quality of the final product.

Software Requirements Specification (SRSp): The SRSp is a description of the external interfaces and essential requirements of the software in terms of functions, performance, constraints, and attributes. Requirements are objective and measurable. The SRSp is concerned with what is required, not how to achieve it. This document is reviewed by project members, users, and management. They verify that the intent of the SRSp is clear, the software proposed by the SRSp is what is desired, and that the project can proceed to the next development stage.

Design Description: A Design Description documents the design work accomplished during the design phase. Documenting the design prior to coding avoids (or reduces) any design misunderstandings and subsequent re-coding.

Design Review Results: The results of the Design Review are documented in a report, which identifies all deficiencies discovered during the review along with a plan and schedule for corrective actions. The updated design description document, when placed under configuration control, will establish the baseline for subsequent phases of the software life cycle.

Structured Source Code: Implementation is the translation of the detailed design into a computer language; a process commonly called *coding*.

Test Set: The Test Set includes "rich" test data and relevant test procedures and tools to adequately test the application's response to valid as well as invalid data.

Test Set Documentation: The Test Set Documentation (or Software Test Plan) describes the test data, procedures, tools, and overall plan.

Test Results: The results of the tests should be documented to identify all deficiencies discovered.

Maintenance Documentation: Well-documented code and the software design document provide the backbone of maintenance documentation and the starting point for determining training needs.

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[3] - The SNL documentation is clearly described as guidance. The management directing the project may choose not to follow any part, or all, of the recommendations outlined in the guidelines.

Training Plan: The preparation of a well thought out training plan is an essential part of bringing a system into smooth operation. If the people, documents, and training techniques are not considered in the early planning for a new system, resources may not be available and training will be haphazard.

User's Manual or Operating Procedures: A user's manual is organized to contain practical information for the individuals required to put the software into action. Depending on the size and type of system, operating procedures may be required as a separate document to cover management of the logical and physical components. Without a properly prepared user's guide or operator instructions, either the time of the user will be wasted determining what to do, or the system will be inappropriately used, or both.

Configuration Management Plan: The Configuration Management Plan lists all modules used by the project, module locations, personnel responsible for controlling changes, and change procedures.

Baseline Table: The Baseline Table lists modules and versions in the project's baselined system.

Change Table: The Change Table lists all changes and enhancements made to the modules. Additional update supporting documents reflect changes and enhancements made to the system.

During the interview conducted with SNL personnel in January 2004, the MELCOR SQA procedures document (SNL-1992b) was provided and reviewed. (SNL-1992b) provides SQA plan detailed information specific to MELCOR. It references (SNL 1986, SNL 1987, and SNL 1989) discussed above as primary documents. Topics covered include:

- Maintenance Procedures
  - Configuration Identification
  - Alternate Software Packages
- The DIR Process
  - Request Description
  - Diagnosis
  - Resolution Plan
  - Change/Testing
  - Update Implementation
- Documenting Actions Not Involving Code Changes
- Configuration Status Accounting
- Validation and Verification of MELCOR
- MELCOR User's Guides and Reference Manuals
- Testing and Review for Code Release
- Tools, Techniques and Methodologies
- Code Written by External Suppliers
- Special Purpose Code Modifications

This plan was followed during the 1990's as MELCOR was developed and modified. The authors continue to follow the plan today, with less rigidity and with some modification as funding allows.

4.2.1 Criterion Specification and Result

Table 4.2-1 lists the subset of criteria reviewed for this topical area and summarizes the findings. Based on the SQA Program review from 1997-1998 (J. East), and East (1998), it can be inferred from the general SNL SQA information and MACCS2-specific details that most elements of a compliant SQA plan and procedures were likely in place and followed during the development of MELCOR version 1.8.5. This was confirmed by meetings with the code authors in January 2004. However, definitive confirmation through written, approved documentation is not always available.

Table 4.2-1 — Subset of Criteria for SQA Procedures and Plans Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
2.1	Verify that procedures/plans for SQA (**SQA Plan**) have identified organizations responsible for performing work; independent reviews, etc.	Yes.	(SNL 1992b) outlines the MELCOR software assurance plan and the procedures in place when MELCOR was developed.
2.2	Verify that procedures/plans for SQA (**SQA Plan**) have identified software engineering methods.	Yes.	(SNL 1992b) provides coding guidelines as well as steps for modifying or adding code.
2.3	Verify that procedures/plans for SQA (**SQA Plan**) have identified documentation to be required as part of program.	Yes.	(SNL 1992b) Section 4.0 provides direct reference to and plans for user's guides and reference manuals
2.4	Verify that procedures/plans for SQA (**SQA Plan**) have identified standards, conventions, techniques, and/or methodologies that shall be used to guide the software development, methods to ensure compliance with the same.	Yes.	(SNL 1992b) provides standards for coding, techniques for modifying the coding and methods to be used in program development.
2.5	Verify that procedures/plans for SQA (**SQA Plan**) have identified software reviews and schedule.	Partial.	Elements of this existed based on discussions with the authors. Software reviews were conducted. Schedules for the reviews and evidence for the thoroughness of the reviews were not found in the available documentation. (SNL 1992b) discusses testing and review in Section 5.0.
2.6	Verify that procedures/plans for SQA (**SQA Plan**) have identified methods for error reporting and corrective actions.	Yes. (Recently less rigor)	(SNL-1992b) provides discussion of the DIR (Defect Investigation Report) process. Discussion with SNL in January 2004 indicates the DIR process was rigorously followed during the 90's. With decreasing funding, error reporting has continued, but is less rigorous,

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			with corrective actions requiring more time. Documentation and notification is less rigorous.

4.2.2 Sources and Method of Review

This review was based initially on the general SNL SQA information and the MACCS2-specific information from East (1998) and making inferences to the MELCOR code that was developed around the same timeframe as MACCS2 (MELCOR 1.8.0 released in March of 1989 and the current version 1.8.5 was released October 2000; development of MACCS2 began in 1992 with the release of the current version 1.12 occurring in 1997). This was later supported by meetings with SNL in January 2004 specifically to discuss SQA for MELCOR. The primary reference for the SQA plan was provided in this meeting as (SNL-1992b). This plan refers to the same governing SQA documents as used by MACCS2 and reported on by East.

4.2.3 Software Quality-Related Issues or Concerns

An SQA plan for MELCOR exists. The plan is dated and consideration should be given to revising it to conform to current practices being followed for MELCOR and current day SQA expectations.

The SQA plan lacks guidance for providing design requirements for modifications being made for the code.

The SQA plan lacks detailed guidance on testing of newly developed software or modifications. Guidance should concentrate on level of testing required, type of testing, and independent verification of coding. Documentation requirements for code testing appear to be lacking. Currently modifications are made and tested against experimental results. In fact, most recent modifications are planned specifically to match to a particular type of result or experiment. This gives a level of confidence in the overall results. Testing of the coding on a line-by-line basis and for quality was not evident in the available documentation for the SQA plan although it is known this was done with varying degrees of rigor during development.

The SQA plan should address prompt error and impact notification to users. Currently (SNL-1992b) requires users be notified if funding is available. Errors or deficiencies are usually reported via email. These are then logged and if code modifications are made, they are incorporated into a future version of the code. Recently no major errors have been discovered. It may take many months for modifications resulting from any given email to be incorporated into the code and released. Not all users are notified of code modifications being made due to these emails. Documentation of detailed closure with the original email author is lacking or not formalized.

4.2.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Develop an updated SQA plan for Version 1.8.5 of MELCOR (at least as the code relates to LPF analysis). (Revise as needed for future updates released for public distribution).
    - Ensure the update is consistent with the current technology and practices.
    - Ensure the plan provides specific guidance regarding design requirements and documentation of design requirements.
    - Ensure the plan addresses prompt defect/error notification to users. (At least as the errors relate to LPF analyses)

4.3 Topical Area 3 Assessment: Requirements Phase

This area corresponds to the requirement entitled Requirements Phase in Table 3-3 of DOE (2003e).

4.3.1 Criterion Specification and Results

Table 4.3-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.3-1 — Subset of Criteria for Requirements Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
3.1	Software requirements for the subject software have been established.	Partial	A verifiable, written set of software requirements is lacking. Requirements for modifications are given verbally/contractually with NRC.
3.2	Software requirements are specified, documented, reviewed and approved.	Partial.	In earlier MELCOR development efforts, written hypothetical coding plans were generated. In practice, this was found not to be beneficial and the plans would be completely rewritten or pitched. Current modifications do not generate comparable initial guidance. A verifiable, written set of software requirements is lacking.
3.3	Requirements define the functions to be performed by the software and provide detail and information necessary to design the software.	Partial.	A verifiable, written set of software requirements is lacking.
3.4	A **Software Requirements Document**, or equivalent defines requirements for functionality, performance, design inputs, design constraints, installation considerations, operating systems (if applicable), and external interfaces necessary to design the software.	Partial.	A verifiable, written set of software requirements is lacking. The contractual agreements for code development with NRC do lay out top-level direction year to year.
3.5	Acceptance criteria are established in the software requirements	No.	A verifiable, written set of software requirements is lacking. Judgment is

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	documentation for each of the identified requirements.		used as modeling progresses to discern the adequacy of model changes, usually against experiments.

4.3.2 Sources and Method of Review

This review was based on based on discussion with SNL in January 2004 and information contained in East (1998), Gauntt (2000a), Gauntt (2000b), Gauntt (2001), and (SNL 1992b).

4.3.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written Software Requirements Document for MELCOR should be addressed as part of the written SQA Plan and Procedures for this software.

4.3.4 Recommendations

Develop a Software Requirements Document for MELCOR. At a minimum, this document should address requirements related to LPF applications for meeting the prerequisites for the DOE toolbox. A broader approach would consider NRC-specified needs for the software as well and address the full capabilities of the code.

4.4 Topical Area 4 Assessment: Design Phase

This area corresponds to the requirement entitled Design Phase in Table 3-3 of DOE (2003e).

A Software Design Document has not been provided by the MELCOR software developers. To permit a limited evaluation, an alternative process was employed of reviewing MELCOR documentation for evidence that criterion requirements were met at least partially in an informal manner.

4.4.1 Criterion Specification and Result

Table 4.4-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.4-1 — Subset of Criteria for Design Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
4.1	The software design was developed, documented, reviewed and controlled.	Partial.	Elements of this criterion may be inferred from code user documentation, reference manuals and discussions with SNL.
4.2	Code developer prescribed and documented the design activities to the	Partial.	(SNL 1992b) provides significant detail in some area

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	level of detail necessary to permit the design process to be carried out and to permit verification that the design met requirements.		on code design and modeling constraints. Similar constraints were understood by the developers when not documented on paper. Documented design requirements were lacking, therefore, documentation of having met requirements is lacking.
4.3	The following design should be present and documented: the design should specify the interfaces, overall structure (control and data flow) and the reduction of the overall structure into physical solutions (algorithms, equations, control logic, and data structures).	Yes.	Inferred from MELCOR documentation.
4.4	The following design should be present and documented: that computer programs were designed as an integral part of an overall system. Therefore, evidence should be present that the software design considered the computer program's operating environment.	Yes.	Inferred from MELCOR documentation.
4.5	The following design should be present and documented: evidence of measures to mitigate the consequences of software design problems. These potential problems include external and internal abnormal conditions and events that can affect the computer program.	Partial.	The documentation of a systematic effort in this area is lacking. Practical steps were taken by the code developers to handle abnormal conditions. For example, the code developers do not let the code stop execution without a message log. Bugs and problems have been corrected over the years when found.
4.6	A Software Design Document, or equivalent, is available and contains a description of the major components of the software design as they relate to the software requirements.	No.	While there is some evidence of the design relating back to requirements as set out for the code contractually with the sponsor, there was no formal documentation available and little evidence of a systematic effort to tie final design to a set of initial requirements.
4.7	A Software Design Document, or equivalent, is available and contains a technical description of the software with respect to the theoretical basis,	Partial.	A set of the listed elements is addressed in documentation (see Section 4.4.2 of this report). Most of the models,

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	mathematical model, control flow, data flow, control logic, data structure, numerical methods, physical models, process flow, process structures, and applicable relationship between data structure and process standards.		etc. are described in detail. A formal design document was not initially generated as a part of each modification process. The authors would informally sketch out the modifications to be made. Final models as developed would normally be incorporated in the User's Manual or Reference Manuals, for major changes.
4.8	A Software Design Document, or equivalent, is available and contains a description of the allowable or prescribed ranges for inputs and outputs.	Partial	Formal design documents are lacking. However, with the supplied documentation and some experience it is possible to understand if inputs/outputs are logical and within range.
4.9	A Software Design Document, or equivalent, is available and contains the design described in a manner that can be translated into code.	Yes.	Formal design documents are lacking. However, with the supplied documentation and some experience, it is possible to translate the models and theories as described to code.
4.10	A Software Design Document, or equivalent, is available and contains a description of the approach to be taken for intended test activities based on the requirements and design that specify the hardware and software configuration to be used during test execution.	Partial.	Documentation is lacking. Most modifications are initiated as part of a project to compare to test data or experiment.
4.11	The organization responsible for the design identified and documented the particular verification methods to be used and assured that an Independent Review was performed and documented. This review evaluated the technical adequacy of the design approach; assured internal completeness, consistency, clarity, and correctness of the software design; and verified that the software design is traceable to the requirements.	Partial.	Evidence of substantial peer review exists. Documentation of completeness is difficult to corroborate. Documentation of pre-planning in software design documents is lacking.
4.12	The organization responsible for the design assured that the test results adequately demonstrated the requirements were met.	Partial.	A verifiable, written set of documentation of software design requirements is lacking. Evidence exists that substantial testing was performed.
4.13	The Independent Review was performed	Partial.	Significant independent

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	by competent individual(s) other than those who developed and documented the original design, but who may have been from the same organization.		review has been performed. Documentation of reviewer qualifications and independence is lacking. For example, there is evidence of peer review during the 1990-91 timeframe from training slide material that is available from the MELCOR website (SNL, 2001). The NRC reviews code modules when completed by SNL.
4.14	The results of the Independent Review are documented with the identification of the verifier indicated.	Partial.	Significant independent review has been performed. Complete documentation is lacking.
4.15	If review alone was not adequate to determine if requirements are met, alternate calculations were used, or tests were developed and integrated into the appropriate activities of the software development cycle.	Partial.	A verifiable, written set of documentation of software design requirements is lacking. Significant independent review has been performed. The code has been modified over the years and tested to provide reasonable assurance the models are adequate.
4.16	Software design documentation was completed prior to finalizing the Independent Review.	Partial.	Some review was known to have been conducted in parallel with design documentation preparation or before preparation of its equivalent.
4.17	The extent of the Independent Review and the methods chosen are shown to be a function of: the importance to safety, the complexity of the software, the degree of standardization, and the similarity with previously proven software.	Partial.	Integrated documentation of the design requirements is lacking, as is documentation of the review detail and its bases. Judgment was used by the code developers to determine what would be reviewed and when. MELCOR has undergone many man-years of independent review and is believed to be robust. Elements of this activity have been documented by various organizations at various times for varying applications and models.

4.4.2 Sources and Method of Review

SNL personnel were interviewed in January 2004. Design requirements were evaluated through review of the following documents:

Gauntt, 2000a, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 1: Primer and Users' Guide*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/1, May 2000.

Gauntt, 2000b, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 2: Reference Manuals*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/2, May 2000.

Gauntt, 2001, Gauntt et al., *MELCOR Computer Code Manuals, Vol. 3: Demonstration Problems*, Version 1.8.5, NUREG/CR-6119 Rev. 0, SAND2001-0929P, May 2001.

SNL, 2001, Sandia National Laboratories. *5th MELCOR User's Workshop*, Bethesda, MD, May 10th – 15th, 2001.

SNL 2003, Sandia National Laboratories. Nuclear Waste Management Procedure, NP 19-1, *Software Requirements*, Revision 10, Waste Isolation Pilot Plant, (May 2003).

SNL (1992b). *Software Quality Assurance Procedures for MELCOR*. Sandia National Laboratories

4.4.3 Software Quality-Related Issues or Concerns

A verifiable, written Software Design Document for MELCOR should be part of the written SQA Plan and Procedures for this software. Upgrades to the Model Description and other documentation can meet the intent of the Software Design Document for an interim period. However, in reconstituting the baseline for MELCOR, it is highly desirable that a new Software Design Document be developed. At a minimum, the Software Design Document should cover those modules that are used in LPF calculations.

4.4.4 Recommendations

Model descriptions in the MELCOR reference manual and other documentation and undocumented practices followed meet the intent of the software design document for the time being. Internal and independent testing of the existing code modules is believed to be robust. However, a software design report addressing the above table elements should be prepared. It is recommended that existing information on aerosol transport (theory, models, model results, tests, experiments, etc.) be gathered and consolidated and that the MELCOR LPF models be verified and validated against these within the context of the elements in Table 4.4-1.

4.5 Topical Area 5 Assessment: Implementation Phase

This area corresponds to the requirement entitled Implementation Phase in Table 3-3 of DOE (2003e).

4.5.1 Criterion Specification and Result

Table 4.5-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.5-1 — Subset of Criteria for Implementation Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
5.1	The implementation process resulted in software products such as computer program listings and instructions for computer program use.	Yes.	User guide, model description, and code listing from the MELCOR transmittal confirm that the essential features of this criterion are met.
5.2	Implemented software was analyzed to identify and correct errors.	Yes.	Test problems exercising the model components are run prior to each release.
5.3	The source code finalized during verification (this phase) was placed under configuration control.	Yes.	(SNL-1992b) is followed and configuration control is maintained on beta versions as well as release versions.
5.4	Documentation during verification included a copy of the software, test case description and associated criteria that are traceable to the software requirements and design documentation.	Yes.	Copy of software and test case description are available. Not possible to trace to requirements and design documents which are lacking documentation.

4.5.2 Sources and Method of Review

Documentation listed in Table 1-3 was reviewed to complete review of this criterion. The code listing is available from SNL with transmittal of MELCOR to requesting user groups.

4.5.3 Software Quality-Related Issues or Concerns

Not all criteria can be confirmed due to the lack of written records on implementation. However, based on available information, it is inferred that most of these requirements were met.

4.5.4 Recommendations

No recommendations related to this topical area are made.

4.6 Topical Area 6 Assessment: Testing Phase

This area corresponds to the requirement entitled Testing Phase in Table 3-3 of DOE (2003e). A Software Test Report has not been provided by the MELCOR software developers. Instead, a limited

evaluation is performed applying Gauntt (2001), and the related documents listed in Table 1-3 as a basis to address the criteria in Table 4.6-1.

4.6.1 Criterion Specification and Result

Table 4.6-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.6-1 — Subset of Criteria for Testing Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
6.1	The software was validated by executing test cases.	Yes.	Documentation, especially Gauntt (2001), supports the satisfaction of this criterion.
6.2	Testing demonstrated the capability of the software to produce valid results for test cases encompassing the range of permitted usage defined by the program documentation. Such activities ensured that the software adequately and correctly performed all intended functions.	Yes.	A series of test cases are run prior to release exercising most of the modules. Other testing is performed ad-hoc by the code authors.
6.3	Testing demonstrated that the computer program properly handles abnormal conditions and events as well as credible failures	Yes.	A series of test cases are run prior to release exercising most of the modules. Other testing is performed ad-hoc by the code authors.
6.4	Testing demonstrated that the computer program does not perform adverse unintended functions.	Yes.	A series of test cases are run prior to release exercising most of the modules. Other testing is performed ad-hoc by the code authors.
6.5	Test Phase activities were performed to assure adherence to requirements, and to assure that the software produces correct results for the test case specified. Acceptable methods for evaluating adequacy of software test case results included: (1) analysis with computer assistance; (2) other validated computer programs; (3) experiments and tests; (4) standard problems with known solutions; (5) confirmed published data and correlations.	Partial	A series of test cases are run prior to release exercising most of the modules. Other testing is performed ad-hoc by the code authors. Significant work has been performed to compare results to experiment. Current suite of test cases (Volume III) supplied with software includes commercial reactor and experimental facility examples. Documentation of requirements is lacking.
6.6	Test Phase documentation includes test procedures or plans and the results of the execution of test cases. The test results documentation demonstrates successful completion of all test cases or the resolution of unsuccessful test cases and provides direct traceability between the test results and specified software requirements.	Partial.	Only partial record of testing is available. It is known that testing was conducted on MELCOR, and it is judged that the final version (1.8.5) performs as intended. However, resolution of unsuccessful cases is not possible to check, nor is

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			traceability between test results and software requirements.
6.7	Test procedures or plans specify the following, as applicable: (1) Required tests and test sequence, (2) Required range of input parameters, (3) Identification of the stages at which testing is required, (4) Requirements for testing logic branches, (5) Requirements for hardware integration, (6) Anticipated output values, (7) Acceptance criteria, (8) Reports, records, standard formatting, and conventions, (9) Identification of operating environment, support software, software tools or system software, hardware operating system(s) and/or limitations.	Partial.	A series of test cases are run prior to release exercising most of the modules. Other testing is performed ad-hoc by the code authors. No comprehensive detailed record of test procedures and plans was available. It can be inferred that this criterion was partially met. Complete verification was not possible due to lack of documentation.

4.6.2 Sources and Method of Review

SNL personnel were interviewed and documentation listed in Table 1-3 was reviewed.

4.6.3 Software Quality-Related Issues or Concerns

Lack of a test report for MELCOR forces the review to infer test case program results and outcome based on limited information. Volume 3 of the MELCOR 1.8.5 code manual (Gauntt, 2001) contains a portfolio of sample demonstration problems. These problems are a combination of experiment analyses, which illustrate code model performance against data, and full plant analyses showing MELCOR's performance on larger realistic problems. A few of these problems address, at least partially, aerosol transport, which is a key phenomenological area for LPF applications. While these studies promote confidence in the models for LPF applications, the documentation of these tests lack the necessary formality and comprehensiveness to address all components of the testing phase criterion.

4.6.4 Recommendations

A verifiable, written Test Report Document for MELCOR should be part of the written SQA Plan and Procedures for this software. Upgrades to the MELCOR software baseline will require that a Test Case Description and Report be completed. Test cases should include one or more example types that serve to demonstrate adequacy of the MELCOR software for LPF calculations that are representative of applications for DOE safety analysis. The Test Report and test phase documentation should address each of the above table elements.

4.7 Topical Area 7 Assessment: User Instructions

This area corresponds to the requirement entitled User Instructions in Table 3-3 of DOE (2003e).

User instructions for MELCOR have been documented (Gauntt, 2000a; Gauntt, 2000b). Considered along with DOE-specific input preparation guidance in DOE (2003f), there is sufficient information to evaluate compliance to this requirement.

4.7.1 Criterion Specification and Result

Table 4.7-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.7-1 — Subset of Criteria for User Instructions Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
7.1	A description of the model is documented.	Yes.	MELCOR models are described sufficiently (Gauntt, 2000a; Gauntt, 2000b).
7.2	User's manual or guide includes approved operating systems (for cases where source code is provided, applicable compilers should be noted).	Yes.	(Gauntt, 2000a; Gauntt, 2000b)
7.3	User's manual or guide includes description of the user's interaction with the software.	Yes.	(Gauntt, 2000a; Gauntt, 2000b)
7.4	User's manual or guide includes a description of any required training necessary to use the software.	Partial.	The MELCOR primer document discusses an approach a new user might take to become familiar with the code.
7.5	User's manual or guide includes input and output specifications.	Yes.	The User's manual (Gauntt, 200a, Gauntt 2000b)
7.6	User's manual or guide includes a description of software and hardware limitations.	Yes.	The Reference Manual discusses the physics and models.
7.7	User's manual or guide includes a description of user messages initiated as a result of improper input and how the user can respond.	Yes.	The code and manuals provide adequate diagnostics.
7.8	User's manual or guide includes information for obtaining user and maintenance support.	Yes.	The MELCOR website contains email and phone contact information.

4.7.2 Sources and Method of Review

Compliance with this requirement was evaluated by review of documentation listed in Table 1.3. SNL personnel were interviewed in January 2004.

4.7.3 Software Quality-Related Issues or Concerns

User instruction documentation is good. No substantive issues or concerns have surfaced.

4.7.4 Recommendations

Recommendations related to this topical area are as follows:

- A simple training program would be useful. This could take several forms including a training manual, or interactive course. The novice user could be tasked with two to three simple problem types and walked through them with output information and explanation. The current sample case file could take on this function with expansion and concentration on LPF related elements.
- MELCOR limitations should be made more explicit in the User's Guide. Specific attention to limitations should be a focused topic and to the extent practical collected in one location.

4.8 Topical Area 8 Assessment: Acceptance Test

This area corresponds to the requirement entitled Acceptance Test Table 3-3 of DOE (2003e). During this phase of the software development, the software becomes part of a system incorporating applicable software components, hardware, and data, and then is accepted for use. Much of the testing is the burden of the user organization, but the developing organization assumes some responsibility.

4.8.1 Criterion Specification and Result

Table 4.8-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.8-1 — Subset of Criteria for Acceptance Test Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
8.1	To the extent applicable to the developer, acceptance testing includes a comprehensive test in the operating environment(s).	Yes.	Volume III (Gauntt 2001) and the electronic files provided allow the user to run a thorough test of the software. The sample problems should expand to provide one or more LPF specific cases.
8.2	To the extent applicable to the developer, acceptance testing was performed prior to approval of the computer program for use.	Yes.	Sample problem sets are run prior to release and checked. Errors or problems are corrected before release.

Criterion Number	Criterion Specification	Compliant	Summary Remarks
8.3	To the extent applicable to the developer, software validation was performed to ensure that the installed software product satisfies the specified software requirements. The engineering function (i.e., an engineering operation an item is required to perform to meet the component or system design basis) determines the acceptance testing to be performed prior to approval of the computer program for use.	Yes.	While documentation of requirements and comprehensive testing is lacking, the code is checked with a series of problems, and individual module testing is performed during development. Most new major modifications are compared against experiment and all are corrected before release.
8.4	Acceptance testing documentation includes results of the execution of test cases for system installation and integration, user instructions (Refer to Requirement 7 above), and documentation of the acceptance of the software for operational use.	Yes.	Volume III (Gauntt 2001) and the electronic files provided allow the user to run a thorough test of the software. Output for comparison is provided. Instructions are provided for installation.

4.8.2 Sources and Method of Review

Software package for code transmittal and documentation listed in Table 1.3 were reviewed. SNL personnel were interviewed in January 2004.

4.8.3 Software Quality-Related Issues or Concerns

There are no software quality issues or concerns for this requirement.

4.8.4 Recommendations

No recommendations are made for this topical area.

4.9 Topical Area 9 Assessment: Configuration Control

This area corresponds to the requirement entitled Configuration Control in Table 3-3 of (DOE 2003e).

4.9.1 Criterion Specification and Result

Table 4.9-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.9-1 — Subset of Criteria for Configuration Control Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks

Criterion Number	Criterion Specification	Compliant	Summary Remarks
9.1	For the developers the methods used to control, uniquely identify, describe, and document the configuration of each version or update of a computer program (for example, source, object, back-up files) and its related documentation (for example, software design requirements, instructions for computer program use, test plans, and results) are described in implementing procedures.	Yes.	(SNL –1992b) provides details of required configuration control of the code and its related documentation.
9.2	Implementing procedures meet applicable criteria for configuration identification, change control and configuration status accounting.	Yes.	(SNL-1992b) provides details.

4.9.2 Sources and Method of Review

SNL personnel were interviewed in January 2004. (SNL-1992b) was reviewed and discussed.

4.9.3 Software Quality-Related Issues or Concerns

There are no software quality issues or concerns for this requirement.

4.9.4 Recommendations

No recommendations are made for this topical area.

4.10 Topical Area 10 Assessment: Error Impact

This area corresponds to the requirement entitled Error Impact in Table 3-3 of DOE (2003e).

4.10.1 Criterion Specification and Result

Table 4.10-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.10-1 — Subset of Criteria for Error Impact Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
10.1	The problem reporting and corrective action process used by the software developing organization addresses the appropriate requirements of the developing organization's corrective action system, and are documented in implementing procedures.	Yes.	The process used for monitoring errors and user feedback on MELCOR is defined in (SNL-1992b). This was formerly strictly followed. It continues to be followed, but less rigidly than before, in part, because of funding considerations.
10.2	Method(s) for documenting (Error Notification and Corrective Action Report), evaluating, and correcting software problems describe the evaluation process for determining whether a reported problem is an error.	Partial.	Some guidance is given in (SNL-1992b). Judgment is used by the authors to determine the severity of the error. Formal specifications to help with this judgment are lacking.
10.3	Method(s) for documenting (Error Notification and Corrective Action Report), evaluating, and correcting software problems define the responsibilities for disposition of the problem reports, including notification to the originator of the results of the evaluation.	Partial.	Guidance is given in (SNL-1992b) Errors and defects are handled by logging them and including updates in the next release. Notification is lacking formality usually associated with a safety related code. Procedures state notification depends on funding. NRC as the current sponsor and SNL define MELCOR as a research code. The reporting scheme currently conforms to this definition.
10.4	When a problem is determined to be an error, then action to document, evaluate and correct, as appropriate, is provided for handling how the error relates to appropriate software engineering elements.	Yes.	Guidance is given in (SNL-1992b).
10.5	When a problem is determined to be an error, then action to document, evaluate and correct, as appropriate, is provided for handling how the error impacts past and present use of the computer program	Partial.	Some guidance is given in (SNL-1992b). In practice, this may be accomplished but is not automatic and is left to the judgment of the authors.
10.6	When a problem is determined to be an error, then action to document, evaluate and correct, as appropriate, is provided	No.	No information was available to support that this occurs formally. Rather consistency

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	for handling how the corrective action impacts previous development activities		of personnel and experience are used to the extent this is accomplished.
10.7	When a problem is determined to be an error, then action to document, evaluate and correct, as appropriate, is provided for handling how the users are notified of the identified error, its impact; and how to avoid the error, pending implementation of corrective actions.	No.	Errors and defects are handled by logging them and including updates in the next release. Notification is lacking formality. Procedures state notification depends on funding. NRC as the current sponsor and SNL define MELCOR as a research code. The reporting scheme conforms to this definition.

4.10.2 Sources and Method of Review

SNL personnel were interviewed in January 2004. SNL has an informal Software Reporting system. The MELCOR website has a link to send an e-mail to MELCOR technical staff. Staff indicated that email is the primary means by which defects are reported. Through the FAQ link on the MELCOR website, users can read about problems other users have reported and see the response of the MELCOR technical staff. The effectiveness or timeliness of this system, however, is difficult to judge. Under the FAQ link, the MELCOR technical staff relays user-reported problems, discuss the causes of error messages, and provide tips to avoid discovered problems until a patch or new version is distributed. As of January 2004, six problems were addressed at the FAQ link. None have been identified as having any significant impact on LPF results.

4.10.3 Software Quality-Related Issues or Concerns

While an informal Software Reporting system process is institutionalized at SNL, its effectiveness can not be established. The authors make concerted effort to record emails they receive, and log the information as it comes in internally. Notification to users of defects on a timely basis, close out with the defect reporter, and formal impact determination are in need of improvement.

4.10.4 Recommendations

As part of the new software baseline for MELCOR, a comprehensive Software Error Notification and Corrective Action process should be provided. Expanded use of the MELCOR website or its equivalent is suggested to provide timely reporting of user issues, errors and defects. It may also provide software news, suggested strategies for resolving software problems, and general communications. Timely, formal user notification of errors or defects should be addressed.

4.11 Training Program Assessment

Current MELCOR training opportunities are limited and not well publicized. Comprehensive training on a more frequent basis would be beneficial.

The Energy Facility Contractors Group (EFCOG) Workshops provide two annual opportunities to give training to the DOE users. The winter session is during the Safety Basis Subgroup meeting and the summer session is organized for the larger Safety Analysis Working Group. Multi-day MELCOR training at these two workshops would potentially reach 300 DOE MELCOR users, managers, regulators, and oversight groups.

In May 2004 the MELCOR Code Application Program (MCAP) group is planning to meet near Washington DC. The first day of this meeting is closed to non-members. Potential exists to add training for MELCOR, both general, or specific to LPF, at the end of this meeting.

Training could result in MELCOR LPF certification. This level of user proficiency could be measured by demonstrating competency through a written exam and software execution of a set of test cases. Ideally, this could be accomplished through formal course attendance or through a self directed (self-study) process.

4.12 Software Improvements and New Baseline

The minimum remedial program required to yield the new software baseline for MELCOR was discussed earlier as part of Table 1.1. Included are upgrades to software documents that constitute the baseline for software, including:

- Updated Software Quality Assurance Plan
- Software Requirements Document (Specific to LPF)
- Software Design Document (Specific to LPF)
- Test Case Description and Report (Specific to LPF)
- Updated Software Configuration and Control
- Updated Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

The SNL procedural guide NP-19 implements an earlier version of Subpart 2.7 to NQA-1, specifically NQA-2a-1990. Application of this procedure was assessed for the SNL MACCS2 code with the result being the minimum set of actions as documented in Bixler (2000) and shown below in Table 4.12-1. Column "SNL NP 19-1 (Bixler)". Application of this procedure to MELCOR can be expected to result in a similar set of actions as specified in the column labeled "Corresponding Recommended Steps from this GAP analysis".

While not exactly matching up with the recommendations proposed in this GAP analysis, the SNL proposed program is similar to the requirements outlined in this report. Furthermore, the estimates are based on SNL resources, and as such, are taken as more accurate resource estimates than could be provided otherwise. The overall SQA upgrade program in the SNL program was estimated to require 1.5 full-time equivalent years to complete. The requirements are matched against the requirements earlier, in Table 4.12-1. The overall level of effort, 1.5 FTE-years is rounded up to approximately 2 FTE-years as

the final estimate for resource allocation to perform the upgrades required to compensate for MELCOR's known SQA gaps. This is a very rough estimate based on this comparison, extrapolating from MACCS to MELCOR and considering the differences. It assumes there would not be major defects found as the program is completed and that existing information would be adequate to complete verification and validation of the LPF models. Long term, maintenance funding will be required for activities such as defect reporting, coordinated update testing as NRC makes changes in the future, and minor SQA administrative duties.

Table 4.12-1 — Comparison of SQA Upgrade Steps Discussed in Bixler (2000) with the Approach Discussed in DOE (2003e)

Topic No.	Topic: ASME NQA-1-2000 Require-ments	Level B Existing Software (Topic Applied?)	GAP Report Section No.	SNL NP 19-1 Steps (Bixler)	Compliance Steps in this GAP Document, DOE (2003e)
1	Software Classifi-cation	Yes	4.1	None	None
2	SQA Proce-dures/ Plans	Yes	4.2	Create a Primitive Baseline (PB) document to establish the SQA status of the existing code	Update SQA plan
3	Dedica-tion	No[4]	–	–	–
4	Evalua-tion	No[4]	–	–	–
5	Require-ments	Yes	4.3	Write a Software Requirements Document (SRD)	Write a Software Requirements Document (SRD)
6	Design Phase	Yes	4.4	None	Write a Design Document
7	Imple-menta-tion Phase	Yes	4.5	Create an Implementation Document (ID) to describe the process of generating the executable software modules	Create an Implementation Document (ID) to describe the process of generating the executable software modules

[4] Topic evaluated as not significantly relevant to safety analysis toolbox codes.

8	Testing Phase	Yes	4.6	Establish a Verification and Validation Plan (VVP) based on the SRD; Generate a Validation Document (VD), to measure the performance of the software against the criteria specified in the VVP	Establish a Verification and Validation Plan (VVP) based on the SRD; Generate a Validation Document (VD), to measure the performance of the software against the criteria specified in the VVP
9	User Instruc-tions	Yes	4.7	Update, the User's Manual (UM)	Update, the User's Manual (UM)
10	Accept-ance Test	Yes	4.8	Perform Installation and Checkout (I&C) to verify correct installation on all supported platforms	None (normally done for MELCOR))
11	Opera-tion and Mainten-ance	No[4]	–	–	–
12	Config-uration Control	Yes	4.9	Implement a Software Configuration Control System (CC)	Update Software Configuration Control System (CC)
13	Error Impact	Yes	4.10	Implement a Software Problem Reporting System (SPR)	Update Software Problem Reporting System (SPR)
14	Access Control	No[4]	–	–	–

5.0 Conclusions

The gap analysis for Version 1.8.5 of the MELCOR software, based on a set of requirements and criteria compliant with NQA-1, has been completed. Of the 10 general topical quality areas assessed, five satisfactorily met the criteria. In general, the gap analysis found that the MELCOR SQA program (in the context of LPF applications), met criteria for *Software Classification, Implementation Phase, User Instructions, Acceptance Test,* and *Configuration Control*, Requirements 1, 5, 7, 8, and 9 respectively. Five topical quality areas were not met satisfactorily. Remedial actions are recommended before MELCOR meets SQA criteria for the remaining five requirements.

A new software baseline is recommended for MELCOR. Suggested remedial actions for this software would warrant upgrading software documents that describe the new baseline. At a minimum, it is recommended that software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation
3. Providing training on a regular basis, and
4. Developing new software documentation.

The complete list of revised baseline documents includes:

- Updated Software Quality Assurance Plan
- Software Requirements Document (Specific to LPF)
- Software Design Document (Specific to LPF)
- Test Case Description and Report (Specific to LPF)
- Updated Software Configuration and Control
- Updated Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

Once these actions have been accomplished, MELCOR version 1.8.5 would be considered SQA compliant. It is estimated, approximately two full-time equivalent years is needed to complete these initial actions.

The MELCOR code was evaluated to determine if the software, in its current state, meets the intended function in a safety analysis context as assessed in this gap analysis. When the code is run for the intended applications as detailed in the code guidance document, MELCOR *Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis*, (DOE 2003f), it is judged that it will meet the intended function.

Current software concerns and issues can be avoided by understanding MELCOR limitations and capabilities, and applying the software in the appropriate types of scenarios for which precedents have been identified. While SQA improvement actions are recommended for MELCOR Version 1.8.5, no evidence has been found of software-induced errors in MELCOR that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

6.0 Acronyms and Definitions

ACRONYMS:

ANS	American Nuclear Society
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
CD	Compliance Decision
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CSARP	Cooperative Severe Accident Research Program
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
IEEE	Institute of Electrical and Electronics Engineers
INEEL	Idaho National Engineering and Environmental Laboratory
IP	Implementation Plan
ISO	International Organization for Standardization
LPF	Leak Path Factor
MCAP	MELCOR Code Applications Program
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (code)
NRC	Nuclear Regulatory Commission
QAP	Quality Assurance Program (alternatively, Plan)
SNL	Sandia National Laboratories
SQA	Software Quality Assurance
SRS	Savannah River Site
V&V	Verification and Validation
WSRC	Westinghouse Savannah River Company

DEFINITIONS:

The following definitions are taken from the Implementation Plan. References in brackets following definitions indicate the original source, when not the Implementation Plan.

Central Registry — An organization designated to be responsible for the storage, control, and long-term maintenance of the Department's safety analysis "toolbox codes." The central registry may also perform this function for other codes if the Department determines that this is appropriate.

Firmware — The combination of a hardware device and computer instructions and data that reside as read-only software on that device. [IEEE Standard 610.12-1990, IEEE Standard Glossary of Software Engineering Terminology]

Gap Analysis — Evaluation of the Software Quality Assurance attributes of specific computer software against identified criteria.

Nuclear Facility — A reactor or a nonreactor nuclear facility where an activity is conducted for or on behalf of DOE and includes any related area, structure, facility, or activity to the extent necessary to ensure proper implementation of the requirements established by 10 CFR 830. [10 CFR 830]

Safety Analysis and Design Software — Computer software that is not part of a structure, system, or component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure proper accident analysis of nuclear facilities; proper analysis and design of safety SSCs; and proper identification, maintenance, and operation of safety SSCs.

Safety Analysis Software Group (SASG) — A group of technical experts formed by the Deputy Secretary in October 2000 in response to Technical Report 25 issued by the Defense Nuclear Facilities Safety Board (DNFSB). This group was responsible for determining the safety analysis and instrument and control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment as appropriate.

Safety-Class Structures, Systems, and Components (SC SSCs) — SSCs, including portions of process systems, whose preventive and mitigative function is necessary to limit radioactive hazardous material exposure to the public, as determined from the safety analyses. [10 CFR 830]

Safety-Significant Structures, Systems, and Components (SS SSCs) — SSCs which are not designated as safety-class SSCs, but whose preventive or mitigative function is a major contributor to defense in depth and/or worker safety as determined from safety analyses. [10 CFR 830] As a general rule of thumb, SS SSC designations based on worker safety are limited to those systems, structures, or components whose failure is estimated to result in prompt worker fatalities, serious injuries, or significant radiological or chemical exposure to workers. The term serious injuries, as used in this definition, refers to medical treatment for immediately life-threatening or permanently disabling injuries

(e.g., loss of eye, loss of limb). The general rule of thumb cited above is neither an evaluation guideline nor a quantitative criterion. It represents a lower threshold of concern for which an SS SSC designation may be warranted. Estimates of worker consequences for the purpose of SS SSC designation are not intended to require detailed analytical modeling. Consideration should be based on engineering judgment of possible effects and the potential added value of SS SSC designation. [DOE G 420.1-1]

Safety Software — Includes both safety system software, and safety analysis and design software. [DOE O 414.1B]

Safety Structures, Systems, and Components (SSCs) — The set of safety-class SSCs and safety-significant SSCs for a given facility. [10 CFR 830]

Safety System Software — Computer software and firmware that performs a safety system function as part of a structure, system, or component (SSC) that has been functionally classified as Safety Class (SC) or Safety Significant (SS). This also includes computer software such as human-machine interface software, network interface software, programmable logic controller (PLC) programming language software, and safety management databases that are not part of an SSC but whose operation or malfunction can directly affect SS and SC SSC function. [DOE O 414.1B]

Safety Analysis and Design Software – Computer software that is not part of a structure, system, or component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure the proper accident analysis of nuclear facilities; the proper analysis and design of safety SSCs; and, the proper identification, maintenance, and operation of safety SSCs. [DOE O 414.1B]

Software — Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Standard 610.12-1990, IEEE Standard Glossary of Software Engineering Terminology]

Toolbox Codes — A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and of appropriate qualification that are maintained, managed, and distributed by a central source. Toolbox codes meet minimum quality assurance criteria. They may be applied to support 10 CFR 830 DSAs provided the application domain and input parameters are valid. In addition to public domain software, commercial or proprietary software may also be considered. In addition to safety analysis software, design codes may also be included if there is a benefit to maintain centralized control of the codes. [modified from DOE N 411.1]

Validation — 1) The process of testing a computer program and evaluating the results to ensure compliance with specified requirements. [ANSI/ANS-10.4-1987]
2) The process of determining the degree to which a model is an accurate representation of the real-world from the perspective of the intended uses of the model. [Department of Defense Directive 5000.59, DoD Modeling and Simulation (M&S) Management]

Verification — 1) The process of evaluating the products of a software development phase to provide assurance that they meet the requirements defined for them by the previous phase. [ANSI/ANS-10.4-1987]

2) The process of determining that a model implementation accurately represents the developer's conceptual description and specifications. [Department of Defense Directive 5000.59, DoD Modeling and Simulation (M&S) Management]

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SEPARATION

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Defense Nuclear Facilities Safety Board Recommendation 2002-1
Software Quality Assurance Implementation Plan
Commitment 4.2.1.3:

CFAST Gap Analysis

Interim Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

January 2004

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FOREWORD

This report documents the outcome of an evaluation of the Software Quality Assurance (SQA) attributes of the CFAST computer code for accident analysis applications, relative to established requirements. This evaluation, a "gap analysis," is performed to meet Commitment 4.2.1.3 of the Department of Energy's Implementation Plan to resolve SQA issues identified in Defense Nuclear Facilities Safety Board Recommendation 2002-1

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Software Quality Assurance Implementation Plan: CFAST Gap Analysis

EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002 (DNFSB 2002). The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major improvement actions discussed in the *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities* (DOE, 2003a). A DOE safety analysis toolbox would contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications.

The fire modeling software *Consolidated Model of Fire Growth and Smoke Transport* (CFAST), both versions 3.1.7 and 5.0.1, is one of the codes designated for the toolbox. To determine the actions needed to bring the CFAST software into compliance with the SQA qualification criteria, and develop an estimate of the resources required to perform the upgrade, the Implementation Plan has committed to sponsoring a code-specific gap analysis document. The gap analysis evaluates the software quality assurance attributes of CFAST against identified criteria.

The balance of this document provides the outcome of the CFAST gap analysis compliant with NQA-1-based requirements. Of the ten SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two requirements are met at acceptable level, i.e., *Classification* (1) and *Configuration Control* (9). Remedial actions are recommended to meet SQA criteria for the remaining eight requirements.

The code developer of CFAST, the National Institute of Standards and Technology, should address the most significant SQA shortcomings, which are related to error reporting, user training and user instructions. It is estimated that approximately 0.5 full-time equivalent year (FTE) would be required to address these three SQA areas. Approximately, one FTE-month per year would be needed to maintain a formal error notification and corrective action process (Section 4.10). However, such a process has not been defined in depth.

While SQA improvement actions are recommended for both versions of CFAST, no evidence has been found of software-induced errors that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

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1.0 Introduction

This document reports the results of a gap analysis for versions 3.1.7 and 5.0.1 of the CFAST computer code. The intent of the gap analysis is to determine the actions needed to bring the specific software into compliance with established Software Quality Assurance (SQA) criteria. A secondary aspect of this report is to develop an estimate of the level of effort required to upgrade each code based on the gap analysis results.

1.1 Background: Overview of Designated Toolbox Software in the Context of 10 CFR 830

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding computer software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety-related decisions, or software that controls safety-related systems. Instances were noted of computer codes that were either inappropriately applied, or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and the variability in guidance and training in the appropriate use of accident analysis software.

While progress was made in resolving several of the issues raised in TECH-25, the DNFSB issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002 (DNFSB, 2002). The DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software. The Recommendation identified a number of quality assurance issues for software used in the DOE facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, SQA-compliant safety analysis codes is one of the major commitments contained in the March 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities* (DOE, 2003a). In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications.

Six computer codes, including ALOHA (chemical release dispersion/consequence analysis), CFAST (fire analysis), EPIcode (chemical release dispersion/consequence analysis), GENII (radiological dispersion/consequence analysis), MACCS2 (radiological dispersion/consequence analysis), and MELCOR (leak path factor analysis), were designated by DOE for the toolbox (DOE, 2003b). It is found that this software provides generally recognized and acceptable approaches for modeling source term and consequence phenomenology, and can be applied as appropriate to support accident analysis in Documented Safety Analyses (DSAs).

As one of the designated toolbox codes, CFAST versions 3.1.7 and 5.0.1, will require some degree of quality assurance improvement before meeting current DOE SQA standards. The analysis documented herein is an evaluation of CFAST relative to current DOE software quality assurance criteria. It assesses the margin of the deficiencies, or gaps, to provide DOE and the software developer the extent to which minimum upgrades are needed. The overall assessment is therefore termed a "gap" analysis.

1.2 Evaluation of Toolbox Codes

The quality assurance criteria identified in later sections of this report are defined as the set of established requirements, or bases, by which to evaluate each designated toolbox code. This gap analysis evaluation, is commitment 4.2.1.3 in the Implementation Plan (DOE, 2003a):

> Perform a gap analysis of the "toolbox" codes to determine the actions needed to bring the codes into compliance with the SQA qualification criteria, and develop a schedule with milestones to upgrade each code based on the gap analysis results.

This process is a prerequisite step for software improvement. It will allow DOE to determine the current limitations and vulnerabilities of each code as well as help define and prioritize the steps required for improvement.

Ideally, each toolbox code owner will provide input information on the SQA programs, processes, and procedures used to develop their software. However, the gap analysis itself will be performed by a SQA evaluator. The SQA evaluator is independent of the code developer, but knowledgeable in the use of the software for accident analysis applications and current software development standards.

1.3 Uses of the Gap Analysis

The gap analysis will provide information to DOE, code developers, and code users.

DOE will see the following benefits:

- Estimates of the resources required to perform modifications to designated toolbox codes
- Basis for schedule and prioritization to upgrade each designated toolbox code.

Each code developer will be provided:

- Information on areas where software quality assurance improvements are needed to comply with industry SQA standards and practices
- Specific areas for improvement for guiding development of new versions of the software.

DOE safety analysts and code users will benefit from:

- Improved awareness of the strengths, limits, and vulnerable areas of each computer code
- Recommendations for code use in safety analysis application areas.

1.4 Scope

This analysis is applicable to the CFAST code, one of the six designated toolbox codes for safety analysis. While CFAST is the subject of the current report, other safety analysis software considered for the toolbox in the future may be evaluated with the same process applied here. The template outlined in this document is applicable for any analytical software as long as the primary criteria are ASME NQA-1, 10 CFR 830, and related DOE directives discussed in DOE (DOE, 2003e).

1.5 Purpose

The purpose of this report is to document the gap analysis performed on the CFAST code as part of DOE's implementation plan on SQA improvements.

1.6 Methodology for Gap Analysis

The gap analysis for CFAST is based on the plan and criteria described in *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes* (DOE, 2003e). The overall methodology for the gap analysis is summarized in Table 1-1. The gap analysis utilizes ten of the fourteen topical areas listed in DOE, 2003e, related to software quality assurance to assess the quality of the CFAST code. The ten areas are assessed individually in Section 4.

An information template was transmitted to the Safety Analysis Software Developers on 20 October 2003 to provide basic information as input to the gap analysis process. The core section of the template is attached as Appendix A to the present report. NIST has provided a positive preliminary response to this request and this input is included in this interim report.

1.7 Summary Description of Software Being Reviewed

The gap analysis was performed on both versions 3.1.7 and 5.0.1 of the CFAST code. CFAST was initially developed in 1990 and (http://cfast.nist.gov/versionhistory.html) is written in FORTRAN. This software is maintained by the National Institute of Standards and Technology and is in widespread use in the fire protection industry to evaluate the safety of exiting buildings, perform post-fire reconstructions and to evaluate performance based designs. Since the issuance of DOE-STD-3009-94 for nuclear facility accident analysis, CFAST has been used for DOE applications primarily as a tool for establishing compartment temperature profiles and target temperature predictions. The output of CFAST is used to support decision-making on control selection in nuclear facilities, specifically identification of safety structures, systems, and components (SSCs).

CFAST is a fire "model used to calculate the evolving distribution of smoke, fire gases and temperature throughout a constructed facility during a fire. In CFAST, each compartment is divided into two layers. [Models based on this simplification are referred to as zone models in the fire protection industry.] The modeling equations used in CFAST take the mathematical form of an initial value problem for a system of ordinary differential equations (ODE). These equations are derived using the conservation of mass, the conservation of energy (equivalently the first law of thermodynamics), the ideal gas law and relations for density and internal energy. These equations predict as functions of time quantities such as pressure, layer heights and temperatures given the accumulation of mass and enthalpy in the two layers. The CFAST model then consists of a set of ODEs to compute the environment in each compartment and a collection of algorithms to compute the mass and enthalpy source terms required by the ODEs." (Jones, 2003)

A brief summary of CFAST is contained in Table 1-2.

The set of documents reviewed as part of the gap analysis are listed in Table 1-3. All of this material is available at the NIST website www.cfast.nist.gov.

Table 1-1. – Plan for SQA Evaluation of Existing Safety Analysis Software[1]

Phase	Procedure
1. Prerequisites	a. Determine that sufficient information is provided by the software developer to allow it to be properly classified for its intended end-use. b. Review SQAP per applicable requirements in Table 3-3 [DOE, 2003e].
2. Software Engineering Process Requirements	a. Review SQAP for: • Required activities, documents, and deliverables • Level and extent of reviews and approvals, including internal and independent review. Confirm that actions and deliverables (as specified in the SQAP) have been completed and are adequate. b. Review engineering documentation identified in the SQAP, e.g., • Software Requirements Document • Software Design Document • Test Case Description and Report • Software Configuration and Control Document • Error Notification and Corrective Action Report, and • User's Instructions (alternatively, a User's Manual), Model Description (if this information has not already been covered). c. Identify documents that are acceptable from SQA perspective. Note inadequate documents as appropriate.
3. Software Product Technical/ Functional Requirements	a. Review requirements documentation to determine if requirements support intended use in Safety Analysis. Document this determination in gap analysis document. b. Review previously conducted software testing to verify that it sufficiently demonstrated software performance required by the Software Requirements Document. Document this determination in the gap analysis document.
4. Testing	a. Determine whether past software testing for the software being evaluated provides adequate assurance that software product/technical requirements have been met. Obtain documentation of this determination. Document this determination in the gap analysis report. b. (Optional) Recommend test plans/cases/acceptance criteria as needed per the SQAP if testing not performed or incomplete.
5. New Software Baseline	a. Recommend remedial actions for upgrading software documents that constitute baseline for software. Recommendations can include complete revision or providing new documentation. A complete list of baseline documents includes: • Software Quality Assurance Plan • Software Requirements Document • Software Design Document • Test Case Description and Report • Software Configuration and Control • Error Notification and Corrective Action Report, and • User's Instructions (alternatively, a User's Manual) b. Provide recommendation for central registry as to minimum set of SQA documents to constitute new baseline per the SQAP.
6. Training	a. Identify current training programs provided by developer. b. Determine applicability of training for DOE facility safety analysis.
7. Software Engineering Planning	a. Identify planned improvements of software to comply with SQA requirements. b. Determine software modifications planned by developer. c. Provide recommendations from user community. d. Estimate resources required to upgrade software.

[1] From Table 2-2 in DOE (DOE, 2003e).

Table 1-2. – Summary Description of CFAST Software

Type	Specific Information
Code Name	*Consolidated Model of Fire Growth and Smoke Transport* (CFAST),
Versions of the Code	Versions 3.1.7 and 5.0.1
Developing Organization and Sponsor	National Institute of Standards and Technology 100 Bureau Drive, MS 8883, Gaithersburg, MD 20899
Auxiliary Codes	FAST: Graphical User Interface that supports CFAST 3.1.7 CPLOT: Post-processor for use with CFAST history files
Software Platform/ Portability	PC (Windows 95 and later), IRIX (6.3)
Coding and Computer	FORTRAN, C
Technical Support	Walter W. Jones National Institute of Standards and Technology 301.975.6887 wwj@nist.gov
Code Procurement Point of Contact	Freeware available from: http://cfast.nist.gov/
Documentation Supplied with Code Transmittal	See Table 1-3.
Nature of Problem Addressed by Software	Fire growth and smoke spread
Significant Strengths of Software	Very fast; it has been verified and validated.
Known Restrictions or Limitations	Cannot calculate deflagration or detonation scenarios.
Preprocessing (set-up) time for Typical Safety Analysis Calculation	Problem dependent. Simple calculations take only a few minutes to set up and run
Execution Time	Run time will vary with the computer platform and the complexity of the model. Six compartment cases run faster than real time with a 2.6 gHz processor.
Computer Hardware Requirements	Disk space for version 5.0.1 is about 5 MB and requires about 10 MB of memory for large cases. History files (*.HI) can be up to 10 MB for complex cases.
Computer Software Requirements	The GUI uses Microsoft Office .ocx dialog boxes.
Contributing Organization(s)	Naval Research Laboratory, Nuclear Regulatory Commission, Concrete Masonry Institute

Table 1-3.— Software Documentation Reviewed for CFAST

No.	Reference purpose	Reference
1.	Users Guide for versions 3.1.7 and 5.0.1	Peacock, R. D., Paul A. Reneke, Walter W. Jones, Richard W. Bukowski, and Glenn P. Forney. 2000. *A User's Guide for FAST: Engineering Tools for Estimating Fire Growth and Smoke Transport.* Gaithersburg: MD. National Institute of Standards and Technology. (January) NIST Special Publication 921, 2000 edition (Peacock, 2000).
2.	Technical reference for version 3.1.7	Peacock, R. D., Paul A. Reneke, Walter W. Jones, Rebecca M. Portier, and Glenn P. Forney. 1993. *CFAST, the Consolidated Model of Fire Growth and Smoke Transport.* Gaithersburg: MD. National Institute of Standards and Technology. (February) NIST Technical Note 1299 (Peacock, 1993).
3.	Technical reference for version 5.0.1	Jones, Walter W., Glenn P. Forney, Richard D. Peacock and Paul A. Reneke. 2003. *A Technical Reference for CFAST: An Engineering Tool for Estimating Fire and Smoke Transport.* Gaithersburg: MD. National Institute of Standards and Technology. (April) NIST TN 1431 (Jones, 2003).

2.0 Assessment Summary Results

2.1 Criteria Met

Of the ten general topical quality areas assessed in the gap analysis, two satisfactorily met the criteria. The analysis found that the CFAST SQA program, in general, met criteria for *Software Classification* and *User Instructions*, Requirements 1 and 9, respectively. Eight topical quality areas were not met satisfactorily. The major deficiency areas are covered below in Section 2.2 (Exceptions to Requirements). Detail on the evaluation process relative to the requirements and the criteria applied are found in Section 4.

2.2 Exceptions to Requirements

Some of the more important exceptions to criteria found for CFAST are listed in Table 2-1. The requirement is given, the reason the requirement was not met is provided, and remedial action(s) are listed to correct the exceptions. The most significant exceptions are:

- The CFAST Users Manual does not provide a comprehensive description of the software output (Section 4.7).
- A description of the training necessary to use the software is not available (Section 4.7)
- An acceptance test protocol to be used to assure that the installed version of CFAST is working properly is not documented (Section 4.8)
- There is no formal error notification and corrective action process (Section 4.10).

These exceptions are the most significant since they can directly affect the successful use of CFAST. All of the CFAST gap analysis recommendations are summarized in Table 2-2.

2.3 Other Areas Needing Improvement

The Graphical User Interface to support version 5.0.1 needs to be released. The presently available version is considered an alpha release and has limited capabilities.

CFAST does not explicitly calculate leak path factors (LPFs). It appears that it should be capable of this function, however instructions to accomplish this are not provided. Since fire is often a dominate risk in nuclear facilities, a software that should estimate LPFs would be very beneficial.

2.4 CFAST Issues Cited in TECH-25 and Recommended Approaches for Resolutions

One technical issue was noted in TECH-25 that explicitly related CFAST software. This section discusses the issue and recommended dispositioning.

TECH-25 noted, "no formal SQA plan was documented for this code [DOE, 2003d]. Some validation documentation is referenced. The SQA/V&V status of this code is not commensurate with current industry standards." Completion of this gap analysis and the development of an action plan will address this comment.

Table 2-1.— Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion	Reason Not Met	Remedial Action(s)
1.	SQA Procedures/ Plans (Section 4.2)	SQA Plan and Procedures for CFAST were not available for the gap analysis.	Contact NIST to obtain the presently available SQA documentation, review this documentation and develop an action plan.
2.	Requirements Phase (Section 4.3)	Requirements phase documentation for CFAST was not available for the gap analysis.	Contact NIST to obtain the presently available documentation, review this documentation and develop an action plan.
3.	Design Phase (Section 4.4)	Design phase documentation for CFAST was not available for the gap analysis.	Contact NIST to obtain the presently available documentation, review this documentation and develop an action plan.
4.	Implementation Phase (Section 4.5)	Implementation phase documentation for CFAST was not available for the gap analysis.	Contact NIST to obtain the presently available documentation, review this documentation and develop an action plan.
5.	Testing Phase (Section 4.6)	NIST has recently prepared a verification and validation report for CFAST. The report was not readily available to be included in this interim report.	Contact NIST to obtain the presently available documentation, review this documentation and develop an action plan.
6.	User Instructions (Section 4.7)	The user's manual does not list approved operating systems, a description of training necessary to use the software, a comprehensive description of the software outputs, a description of software and hardware limitations and a description on user messages.	Develop a training description with input from NIST. Work with NIST to establish a comprehensive description of CFAST outputs.
7.	Acceptance Test (Section 4.8)	An Acceptance Test protocol is not available. There is no known formal procedure to assure that an installed version of CFAST is working properly.	Work with NIST to document the existing Acceptance Test protocol.
8.	Error Impact (Section 4.10)	There is no formal Error Notification and Corrective Action Report process for CFAST. A version history is maintained on the CFAST web site that describes software updates.	DOE should establish a formal Error Notification and Correction Action Report process for CFAST.

Table 2-2.— Summary of Recommendations for CFAST

No.	Type*	Recommendation
2.1	OI	Contact NIST to establish the present available documentation on the SQA plan and procedures for CFAST.
2.2	OI	Review existing SQA documentation when it becomes available and establish a plan to identify gaps as appropriate.
3.1	OI	Contact NIST to establish the present available documentation on the Requirements Phase for CFAST.
3.2	OI	Review existing Requirements Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.
4.1	OI	Contact NIST to establish the present available documentation on the Design Phase for CFAST.
4.2	OI	Review existing Design Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.
5.1	OI	Contact NIST to establish the present available documentation on the Implementation Phase for CFAST.
5.2	OI	Review existing Implementation Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.
6.1	OI	Contact NIST to obtain a copy of the verification and validation report.
6.2	OI	Review recently prepared verification and validation report when it becomes available and establish a plan to identify gaps as appropriate.
7.1	UI	The user's manual should be updated to reflect the minimum operating system requirements.
7.2	PI	DOE should establish the minimum qualification for personnel who are expected to prepare safety analyses using CFAST. (Two levels of qualification may be appropriate. The lower tier would be to operate the software and produce results, the higher tier would be to interpret the results.)
7.3	UI	A description of output files should be prepared and included in the user's manual.
7.4	UI	Sample problems that include the input data files, output data files and a discussion of the results should be provided.
7.5	UI	The user's manual should be updated to include a description of software and hardware limitations.
8.1	OI	Work with NIST to document the existing acceptance tests and their use.
9.1	OI	Contact NIST to obtain a copy of the NIST internal report documenting the version update process.
9.2	OI	Review the existing NIST report documenting the version update process when it becomes available and establish a plan to identify gaps as appropriate.
10.1	OI	Establish an Error Impact Management Process plan.
12.1	UI	Support the development of a GUI for CFAST 5.0.1 by contributing to CFAST users groups.
12.2	TM	Determine if it is possible to utilize the contaminate term (CT keyword) to establish LPF values.

*OI – Open Item in gap analysis, PI – DOE Procedure Improvement, UI – User Interface Enhancements, TM – Technical Model Upgrade

2.5 Conclusion Regarding Software's Ability to Meet Intended Function

The CFAST code was evaluated to determine if the software, in its current state, meets the intended function in a safety analysis context as assessed in this gap analysis. When the code is run for the intended applications as detailed in the code guidance document, *The CFAST Computer Code Application Guidance for Documented Safety Analysis*, (DOE, 2003d), it is judged that it will meet the intended function. Current software concerns and issues can be avoided by understanding CFAST limitations and capabilities, and applying the software in the appropriate types of scenarios for which precedents have been identified.

3.0 Lessons Learned

Table 3-1 provides a summary of the lessons learned during the performance of the CFAST gap analysis.

Table 3-1.— Lessons Learned

No.	Lesson
1.	Use of NQA-1 or other SQA criteria could not be fully verified. It is known that significant effort has been expended in demonstrating the ability of CFAST to successfully predict fire behavior, however the documentation supporting this is not readily available.
2.	Non-DOE sponsored software that is used to support safety analysis is unlikely to explicitly meet the requirements of ASME NQA-1. To demonstrate compliance with Quality Assurance criteria in Subpart A to 10 CFR 830 (Nuclear Safety Management) will require resources beyond that applied for public-domain codes such as CFAST. A backfit approach to address the quality assurance requirements associated with the use of such software should be considered.
3.	Additional opportunities and venues should be sought for training and user qualification on safety analysis software. This is a long-term deficiency that needs to be addressed for CFAST and other designated software for the DOE toolbox.

4.0 Detailed Results of the Assessment Process

Ten topical areas, or requirements are presented in the assessment as listed in Table 4-0. Training and Software Improvements (resource estimate) sections follow the ten topical areas.

In the tables that follow criteria and recommendations are labeled as (1.x, 2,x, ...10.x) with the first value (1., 2., ...) corresponding to the topical area and the second value (x), the sequential table order.

Table 4-0.— Cross-Reference of Requirements with Subsection and Entry from (DOE, 2003e)

Subsection (This Report)	Corresponding Entry Table 3-2 from DOE, 2003e	Requirement
4.1	1	Software Classification
4.2	2	SQA Procedures/Plans
4.3	5	Requirements Phase
4.4	6	Design Phase
4.5	7	Implementation Phase
4.6	8	Testing Phase
4.7	9	User Instructions
4.8	10	Acceptance Test
4.9	12	Configuration Control
4.10	13	Error Impact [Notification]

4.1 Topical Area 1 Assessment: Software Classification

This area corresponds to the requirement entitled Software Classification in Table 3-3 of (DOE, 2003e).

4.1.1 Criterion Specification and Result

Table 4-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Sufficient documentation is provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, to make an informed determination of the classification of the software. A user of the CFAST software for safety analysis applications would be expected to interpret the information on the software in light of the requirements for atmospheric dispersion and consequence analysis discussed in Appendix A to DOE-STD-3009-94 to decide on an appropriate safety classification. For most organizations, the safety class or safety significant classification, or Level B in the classification hierarchy discussed in (DOE, 2003e), would be selected, which by definition relates to applications:

- Whose failure to properly function may have an indirect effect on nuclear safety protection systems or toxic materials hazard systems, that are used to keep nuclear or toxic material hazard exposure to the general public and workers below regulatory or evaluation guidelines, or
- Whose results are used to make decisions that could result in death or serious injury or are part of the evaluation in accident analyses.

Table 4-1.— Subset of Criteria for Software Classification Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
1.1	The code developer must provide sufficient information to allow the user to make an informed decision on the classification of the software.	Yes	It is concluded that sufficient information is provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, for the user to make an informed determination of the classification of the software.

4.1.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, was used as the basis for establishing the responses for this requirement.

4.1.3 Software Quality-Related Issues or Concerns

There are no SQA issues or concerns relative to this requirement.

4.1.4 Recommendations

No recommendations are provided at this time.

4.2 Topical Area 2 Assessment: SQA Procedures and Plans

This area corresponds to the requirement entitled SQA Procedures / Plans in Table 3-3 of (DOE, 2003e).

When this report was prepared no information on the SQA procedures and plans had been made available from the software developer.

4.2.1 Criterion Specification and Result

Table 4-2 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-2.— Subset of Criteria for SQA Procedures and Plans Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
2.1	Procedures/plans for SQA have identified organizations responsible for performing work; independent reviews, etc.	No	A verifiable, written set of SQA plans and procedures is lacking for CFAST.
2.2	Procedures/plans for SQA have identified software engineering methods.	No	See Criterion 2.1 summary remarks.
2.3	Procedures/plans for SQA have identified documentation to be required as part of program.	No	See Criterion 2.1 summary remarks.
2.4	Procedures/plans for SQA have identified standards, conventions, techniques, and/or methodologies which shall be used to guide the software development, methods to ensure compliance with the same.	No	See Criterion 2.1 summary remarks.
2.5	Procedures/plans for SQA have identified software reviews and schedule.	No	See Criterion 2.1 summary remarks.
2.6	Procedures/plans for SQA have identified methods for error reporting and corrective actions.	No	See Criterion 2.1 summary remarks.

4.2.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented with informal communications, was used as the basis for establishing the responses for this requirement.

4.2.3 Software Quality-Related Issues or Concerns

The unavailability of a verifiable, written set of SQA plan and procedures for CFAST should be addressed.

4.2.4 Recommendations

Recommendations related to this topical area are:

Recommendation 2.1 — Contact NIST to establish the present available documentation on the SQA plan and procedures for CFAST.

Recommendation 2.2 — Review existing SQA documentation when it becomes available and establish a plan to identify gaps as appropriate.

4.3 Topical Area 3 Assessment: Requirements Phase

This area corresponds to the requirement entitled Requirements Phase in Table 3-3 of (DOE, 2003e).

When this report was prepared no information on the Requirements Phase had been made available from the software developer.

4.3.1 Criterion Specification and Result

Table 4-3 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-3.— Subset of Criteria for Dedication Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
3.1	Software requirements for the subject software have been established.	Partial	See Summary Remark to 3.2.
3.2	Software requirements are specified, documented, reviewed and approved.	No	Improvements to CFAST are commonly developed using task orders. Most of this documentation is not generally available.
3.3	Requirements define the functions to be performed by the software and provide detail and information necessary to design the software.	Partial	See Summary Remark to 3.2.
3.4	A Software Requirements Document, or equivalent defines requirements for functionality, performance, design inputs, design constraints, installation considerations, operating systems (if applicable), and external interfaces necessary to design the software.	No	
3.5	Acceptance criteria are established in the software requirements documentation for each of the identified requirements.	Uncertain	No information on this topic has been identified.

4.3.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented with informal communications, was used as the basis for establishing the responses for this requirement.

4.3.3 Software Quality-Related Issues or Concerns

The unavailability of a written description of the Requirements Phase for CFAST should be addressed.

4.3.4 Recommendations

Recommendations related to this topical area are:

Recommendation 3.1 — Contact NIST to establish the present available documentation on the Requirements Phase for CFAST.

Recommendation 3.2 — Review existing Requirements Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.

4.4 Topical Area 4 Assessment: Design Phase

This area corresponds to the requirement entitled Design Phase in Table 3.3 of (DOE, 2003e).

When this report was prepared no information on the Design Phase had been made available from the software developer.

4.4.1 Criterion Specification and Result

Table 4-4 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-4.— Subset of Criteria for Design Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
4.1	The software design was developed, documented, reviewed and controlled.	Uncertain	
4.2	Code developer(s) prescribed and documented the design activities to the level of detail necessary to permit the design process to be carried out and to permit verification that the design met requirements.	Uncertain	
4.3	The following design should be present and documented: specification of interfaces, overall structure (control and data flow) and the reduction of the overall structure into physical solutions (algorithms, equations, control logic, and data structures).	Uncertain	
4.4	The following design should be present and documented: computer programs were designed as an integral part of an overall system. Therefore, evidence should be present that the software design considered the computer program's operating environment.	Uncertain	
4.5	The following design should be present and documented: evidence of measures to mitigate the consequences of software design problems. These potential problems include external and internal abnormal conditions and events that can affect the computer program.	Uncertain	
4.6	A Software Design Document, or equivalent, is available and contains a description of the major components of the software design as they relate to the software requirements.	No	

Criterion Number	Criterion Specification	Compliant	Summary Remarks
4.7	A Software Design Document, or equivalent, is available and contains a technical description of the software with respect to the theoretical basis, mathematical model, control flow, data flow, control logic, data structure, numerical methods, physical models, process flow, process structures, and applicable relationship between data structure and process standards.	No	
4.8	A Software Design Document, or equivalent, is available and contains a description of the allowable or prescribed ranges for inputs and outputs.	Partial	The limitations for many parameters are not fully described. Use of the software requires a working knowledge in fire modeling and severity analysis to judge if the inputs and output information is logical.
4.9	A Software Design Document, or equivalent, is available and contains the design described in a manner that can be translated into code.	No	
4.10	A Software Design Document, or equivalent, is available and contains a description of the approach to be taken for intended test activities based on the requirements and design that specify the hardware and software configuration to be used during test execution.	No	
4.11	The organization responsible for the design identified and documented the particular verification methods to be used and assured that an Independent Review was performed and documented. This review evaluated the technical adequacy of the design approach; assured internal completeness, consistency, clarity, and correctness of the software design; and verified that the software design is traceable to the requirements.	Uncertain	While some elements of this criterion may have been met informally per discussions with the software developer, there is no written documentation that allows confirmation.
4.12	The organization responsible for the design assured that the test results adequately demonstrated that the requirements were met.	Uncertain	
4.13	The Independent Review was performed by competent individual(s) other than those who developed and documented the original design, but who may have been from the same organization.	Uncertain	
4.14	The results of the Independent Review are documented with the identification of the verifier indicated.	Uncertain	

Criterion Number	Criterion Specification	Compliant	Summary Remarks
4.15	If review alone was not adequate to determine if requirements are met, alternate calculations were used, or tests were developed and integrated into the appropriate activities of the software development cycle.	Uncertain	
4.16	Software design documentation was completed prior to finalizing the Independent Review.	Uncertain	
4.17	The extent of the Independent Review and the methods chosen are shown to be a function of: ➢ The importance to safety, ➢ The complexity of the software, ➢ The degree of standardization, and ➢ The similarity with previously proven software.	Uncertain	

4.4.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, was used as the basis for establishing the responses for this requirement.

4.4.3 Software Quality-Related Issues or Concerns

The unavailability of a written description of the Requirements Phase for CFAST should be addressed.

4.4.4 Recommendations

Recommendations related to this topical area are:

Recommendation 4.1 — Contact NIST to establish the present available documentation on the Design Phase for CFAST.

Recommendation 4.2 — Review existing Design Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.

4.5 Topical Area 5 Assessment: Implementation Phase

This area corresponds to the requirement entitled Implementation Phase in Table 3-3 of (DOE, 2003e).

When this report was prepared no information on the Implementation Phase had been made available from the software developer.

4.5.1 Criterion Specification and Result

Table 4-5 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-5.— Subset of Criteria for Implementation Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
5.1	The implementation process resulted in software products such as computer program listings and instructions for computer program use.	Uncertain	Because SQA plans and procedures from the software developer are not available, a thorough evaluation was not possible.
5.2	Implemented software was analyzed to identify and correct errors.	Uncertain	
5.3	The source code finalized during verification (this phase) was placed under configuration control.	Uncertain	
5.4	Documentation during verification included a copy of the software, test case description and associated criteria that are traceable to the software requirements and design documentation.	No	

4.5.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, was used as the basis for establishing the responses for this requirement.

4.5.3 Software Quality-Related Issues or Concerns

The unavailability of a written description of the Implementation Phase for CFAST should be addressed.

4.5.4 Recommendations

Recommendations related to this topical area are:

Recommendation 5.1 — Contact NIST to establish the present available documentation on the Implementation Phase for CFAST.

Recommendation 5.2 — Review existing Implementation Phase documentation when it becomes available and establish a plan to identify gaps as appropriate.

4.6 Topical Area 6 Assessment: Testing Phase

This area corresponds to the requirement entitled Testing Phase in Table 3-3 of (DOE, 2003e).

NIST is about to publish *Verification and Validation of CFAST, a Model for Fire Growth and Smoke Transport*, (NIST IR 7080 - 2004). This report was not available to be reviewed as part of this gap analysis.

4.6.1 Criterion Specification and Result

Table 4-6 lists the subset of criteria reviewed for this topical area and summarizes the findings.

4.6.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented by informal communications, was used as the basis for establishing the responses for this requirement.

4.6.3 Software Quality-Related Issues or Concerns

NIST has recently documented a verification and validation of CFAST in an internal report. This efforts should be included in the gap analysis.

4.6.4 Recommendations

Recommendations related to this topical area are:

Recommendation 6.1 — Contact NIST to obtain a copy of the verification and validation report.

Recommendation 6.2 — Review recently prepared verification and validation report when it becomes available and establish a plan to identify gaps as appropriate.

Table 4-6.— Subset of Criteria for Testing Phase Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
6.1	The software was validated by executing test cases.	Yes	
6.2	Testing demonstrated the capability of the software to produce valid results for test cases encompassing the range of permitted usage defined by the program documentation. Such activities ensured that the software adequately and correctly performed all intended functions.	Uncertain	
6.3	Testing demonstrated that the compute program properly handles abnormal conditions and events as well as credible failures	Uncertain	
6.4	Testing demonstrated that the computer program does not perform adverse unintended functions.	Uncertain	
6.5	Test Phase activities were performed to assure adherence to requirements, and to assure that the software produces correct results for the test case specified. Acceptable methods for evaluating adequacy of software test case results included: (1) analysis with computer assistance; (2) other validated computer programs; (3) experiments and tests; (4) standard problems with known solutions; (5) confirmed published data and correlations.	Uncertain	
6.6	Test Phase documentation includes test procedures or plans and the results of the execution of test cases. The test results documentation demonstrates successful completion of all test cases or the resolution of unsuccessful test cases and provides direct traceability between the test results and specified software requirements.	Uncertain	
6.7	Test procedures or plans specify the following, as applicable: required tests and test sequence, required range of input parameters, identification of the stages at which testing is required, requirements for testing logic branches, requirements for hardware integration, anticipated output values, acceptance criteria, reports, records, standard formatting, and conventions, identification of operating environment, support software, software tools or system software, hardware operating system(s) and/or limitations.	Uncertain	

4.7 Topical Area 7 Assessment: User Instructions

This area corresponds to the requirement entitled User Instructions in Table 3-3 of (DOE, 2003e).

4.7.1 Criterion Specification and Result

Table 4-7 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-7.— Subset of Criteria for User Instructions Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
7.1	A description of the model is documented.	Yes	(Jones, 2003, Peacock, 1993, Peacock, 2000)
7.2	User's manual or guide includes approved operating systems (for cases where source code is provided, applicable compilers should be noted).	No	Approved operating systems are not established in the users documentation.
7.3	User's manual or guide includes description of the user's interaction with the software.	Yes	(Peacock, 2000)
7.4	User's manual or guide includes a description of any required training necessary to use the software.	No	
7.5	User's manual or guide includes input and output specifications.	Partially	(Jones, 2003, Peacock, 1993, Peacock, 2000) See Additional Details.
7.6	User's manual or guide includes a description of software and hardware limitations.	No	
7.7	User's manual or guide includes a description of user messages initiated as a result of improper input and how the user can respond.	No	
7.8	User's manual or guide includes information for obtaining user and maintenance support.	Yes	CFAST website contains an e-mail address to request assistance.

Additional Detail

Criterion 7.5. — There are three different output files that provide numerical output. These include the history file (*.HI), a comma delimited file (*.csv) and a text file (*.txt). The history file is accessed by the routine CPlot, which is executed from the DOS command prompt. This program is described in Appendix C of (Peacock, 2000). The methods to produce output in the other two formats is also described in (Peacock, 2000), however explicit descriptions for all of the available output information is not published.

4.7.2 Sources and Method of Review

There are two current technical references that the describe the algorithms and assumptions used in CFAST. There are (Peacock, 1993) and (Jones, 2003), which cover CFAST 3.1.7 and CFAST 5.0.1 respectively. There is one user's guide for both versions, (Peacock, 2000). These documents are available at the NIST sponsored web site http://cfast.nist.gov/ and were used as the basis for response to this requirement. Informal communications with NIST personnel provided additional information.

4.7.3 Software Quality-Related Issues or Concerns

As identified above, the description of the output files is limited. This can readily be addressed by preparing a description of each file type. In addition, NIST does not provide complete sample problems. While there are sample input data files provided with the initial installation, the output associated with these files are not available. An update to the user's guide is about to be published. This update has not been evaluated as part of this gap analysis.

4.7.4 Recommendations

Recommendations related to this topical area are provided as follows:

Recommendation 7.1 – The user's manual should be updated to reflect the minimum operating system requirements.

Recommendation 7.2 – DOE should establish the minimum qualification for personnel who are expected to prepare safety analyses using CFAST. (Two levels of qualification may be appropriate. The lower tier would be to operate the software and produce results, the higher tier would be to interpret the results.)

Recommendation 7.3 - A description of output files should be prepared and included in the user's manual.

Recommendation 7.4 - Sample problems that include the input data files, output data files and a discussion of the results should be provided.

Recommendation 7.5 – The user's manual should be updated to include a description of software and hardware limitations.

4.8 Topical Area 8 Assessment: Acceptance Test

This area corresponds to the requirement entitled Acceptance Test in Table 3-3 of (DOE, 2003e).

This section was prepared based on informal communication with NIST.

4.8.1 Criterion Specification and Result

Table 4-8 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-8.— Subset of Criteria for Acceptance Test Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
8.1	To the extent applicable to the developer, acceptance testing includes a comprehensive test in the operating environment(s).	No	CFAST is provided with a series of input data files that can be executed to establish if CFAST was installed successfully. Formal user instructions explaining the purpose of these files are not available.
8.2	To the extent applicable to the developer, acceptance testing was performed prior to approval of the computer program for use.	Uncertain	
8.3	To the extent applicable to the developer, software validation was performed to ensure that the installed software product satisfies the specified software requirements. The engineering function (i.e., an engineering operation an item is required to perform to meet the component or system design basis) determines the acceptance testing to be performed prior to approval of the computer program for use.	Uncertain	
8.4	Acceptance testing documentation includes results of the execution of test cases for system installation and integration, user instructions (Refer to Requirement 7 above), and documentation of the acceptance of the software for operational use.	Uncertain	

4.8.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented with informal communications, was used as the basis for establishing the responses for this requirement.

4.8.3 Software Quality-Related Issues or Concerns

As identified above, there is no publicly available acceptance testing protocol associated with CFAST. In addition, there is description of the output files is limited. This can readily be addressed by preparing a description of each file type. In addition, NIST does not provide complete sample problems. While there are sample input data files provided with the initial installation, the output associated with these files are not available.

4.8.4 Recommendations

Recommendations related to this topical area are:

Recommendation 8.1 — Work with NIST to document the existing acceptance tests and their use.

4.9 Topical Area 9 Assessment: Configuration Control

This area corresponds to the requirement entitled Configuration Control in Table 3-3 of (DOE, 2003e).

A NIST Internal Report (IR) has been prepared detailing the version update process.

4.9.1 Criterion Specification and Result

Table 4-9 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-9.— Subset of Criteria for Configuration Control Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
9.1	For the developers the methods used to control, uniquely identify, describe, and document the configuration of each version or update of a computer program (for example, source, object, back-up files) and its related documentation (for example, software design requirements, instructions for computer program use, test plans, and results) are described in implementing procedures.	Yes	CFAST is labeled and documented for release as Version 3.1.7 and 5.0.1. A NIST IR has been prepared detailing the version update process.
9.2	Implementing procedures meet applicable criteria for configuration identification, change control and configuration status accounting.	Yes	NIST IR has not been reviewed, however it is assumed to be adequate.

4.9.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented with informal communications, was used as the basis for establishing the responses for this requirement.

4.9.3 Software Quality-Related Issues or Concerns

There is no publicly available description of the configuration control process that is in place for CFAST.

4.9.4 Recommendations

Recommendations related to this topical area are:

Recommendation 9.1 — Contact NIST to obtain a copy of the NIST internal report documenting the version update process.

Recommendation 9.2 — Review the existing NIST report documenting the version update process when it becomes available and establish a plan to identify gaps as appropriate.

4.10 Topical Area 10 Assessment: Error Impact

This area corresponds to the requirement entitled Error Impact in Table 3-3 of (DOE, 2003e).

This section is based on informal communications with the software developer.

4.10.1 Criterion Specification and Result

Table 4-10 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4-10.— Subset of Criteria for Error Impact Topic and Results

Criterion Number	Criterion Specification	Compliant	Summary Remarks
10.1	The developing organization's problem reporting and corrective action process addresses the appropriate requirements of its corrective action system and is documented in implementing procedures.	No	NIST does not maintain a formal error notification system, however, NIST does gather comments, question, error reports and fix them as needed.
10.2	The process for evaluating, and documenting whether a reported problem is an error is documented and implemented.	No	See Criterion 10.1 summary remarks.
10.3	The process for disposition of the problem reports, including notification to the originator of the results of the evaluation, is documented and implemented.	No	See Criterion 10.1 summary remarks.
10.4	A documented process provides guidance on determining how identified errors relate to appropriate software engineering elements and is implemented.	No	See Criterion 10.1 summary remarks.
10.5	The process is documented and implemented for determining how an error impacts past and present use of the computer program.	No	See Criterion 10.1 summary remarks.
10.6	The process is documented and implemented for determining how an error and resulting corrective action impacts previous development activities.	No	See Criterion 10.1 summary remarks.
10.7	The process is documented and implemented describing how the users are notified of an identified error, its impact; and how to avoid the error, pending implementation of corrective actions.	Partial	A version history maintained on the CFAST web site.

4.10.2 Sources and Method of Review

Documentation provided at the NIST sponsored CFAST/FAST website, http://fast.nist.gov/, supplemented with informal communications, was used as the basis for establishing the responses for this requirement.

4.10.3 Software Quality-Related Issues or Concerns

There is no formal error reporting or notification system for CFAST.

4.10.4 Recommendations

Recommendations related to this topical area are provided as follows:

Recommendation 10.1 — Establish an Error Impact Management Process plan.

4.11 Training Program Assessment

NIST does not offer user training for CFAST, however the Society of Fire Protection Engineers (SFPE) has offered such training. While the course is not currently scheduled, SFPE will bring the course to clients when requested. A description of this training is presented in Appendix B. Training has also been offered through Worchester Polytechnical Institute. The link for information on this class is: http://www.wpi.edu/Academics/Depts/Fire/Courses/FP570/CFAST%20slides_files/frame.htm.

4.12 Software Improvements

A graphical user interface for version 5 is being developed to be compatible with Windows XP. The CFAST web site provides access to an Alpha version (0.9a).

CFAST appears to have the capability to track contaminate migration explicitly, however information on how to use this feature to support Leak Path Factor (LPF) analysis is not available.

Recommendation 12.1 — Support the development of a GUI for CFAST 5.0.1 by contributing to CFAST users groups.

Recommendation 12.2 — Determine if it is possible to utilize the contaminate term (CT keyword) to establish LPF values.

It is estimated that approximately 0.5 full-time equivalent year (FTE) would be required to fulfill the first three SQA recommendations described in Section 2.2, including

- The CFAST Users Manual does not provide a comprehensive description of the software output (Section 4.7).
- A description of the training necessary to use the software is not available (Section 4.7)
- An acceptance test protocol to be used to assure that the installed version of CFAST is working properly is not documented (Section 4.8).

Several more FTE-months is estimated to address other non-compliant areas discussed in Sections 4.1 through 4.10. Approximately, one FTE-month per year would be needed to maintain a formal error notification and corrective action process (Section 4.10). However, such a process has not been defined. It is likely to be applied to all toolbox codes collectively.

5.0 Conclusions

The gap analysis for Versions 3.1.7 and 5.0.1 of the CFAST software, based on a set of requirements and criteria compliant with NQA-1, has been completed. Of the ten SQA requirements for existing software classified as level B (important for safety analysis but whose output is not applied without further review), two requirements are met at acceptable level, i.e., *Classification* (1) and *Configuration Control* (9). Remedial actions are recommended before CFAST meets SQA criteria for the remaining eight requirements. These should be developed using a back-fit approach that focuses on the most important SQA features.

While SQA improvement actions are recommended for CFAST, no evidence has been found of software-induced errors that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

6.0 Acronyms and Definitions

6.1 Acronyms

ANS	American Nuclear Society
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
CFR	Code of Federal Regulations
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DSA	Documented Safety Analysis
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
NIST	National Institute of Standards and Technology
NRC	Nuclear Regulatory Commission
PSA	Probabilistic Safety Analysis (or Assessment)
SQA	Software Quality Assurance
SRS	Savannah River Site

6.2 Definitions

The following definitions are taken from the Implementation Plan. References in brackets following definitions indicate the original source, when not the Implementation Plan.

Acceptance Testing — [NQA-1] The process of exercising or evaluating a system or system component by manual or automated means to ensure that it satisfies the specified requirements and to identify differences between expected and actual results in the operating environment.

Central Registry — An organization designated to be responsible for the storage, control, and long-term maintenance of the Department's safety analysis "toolbox codes." The central registry may also perform this function for other codes if the Department determines that this is appropriate.

Configuration Management —The process that controls the activities, and interfaces, among design, construction, procurement, training, licensing, operations, and maintenance to ensure that the configuration of the facility is established, approved and maintained. (Software specific): The process of identifying and defining the configuration items in a system (i.e., software and hardware), controlling the release and change of these items throughout the system's life cycle, and recording and reporting the status of configuration items and change requests. [NQA-1]

Design Requirements — Description of the methodology, assumptions, functional requirements, and technical requirements for a software system.

Discrepancy — The failure of software to perform according to its documentation.

Error —A condition deviating from an established base line, including deviations from the current approved computer program and its baseline requirements. [NQA-1]

Executable Code — The user form of a computer code. For programs written in a compilable programming language, the compiled and loaded program. For programs written in an interpretable programming language, the source code.

Firmware — The combination of a hardware device and computer instructions and data that reside as read-only software on that device. [IEEE Standard 610.12-1990, IEEE Standard Glossary of Software Engineering Terminology]

Gap Analysis — Evaluation of the Software Quality Assurance attributes of specific computer software against identified criteria.

Independent Verification and Validation (IV&V) — Verification and validation performed by an organization that is technically, managerially, and financially independent of the development organization.

Nuclear Facility — A reactor or a nonreactor nuclear facility where an activity is conducted for or on behalf of DOE and includes any related area, structure, facility, or activity to the extent necessary to ensure proper implementation of the requirements established by 10 CFR 830. [10 CFR 830]

Operating Environment — A collection of software, firmware, and hardware elements that provide for the execution of computer programs. [NQA-1]

Safety Analysis and Design Software – Computer software that is not part of a structure, system, or component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure the proper accident analysis of nuclear facilities; the proper analysis and design of safety SSCs; and, the proper identification, maintenance, and operation of safety SSCs. [DOE O 414.1B]

Safety Analysis Software Group (SASG) — A group of technical experts formed by the Deputy Secretary in October 2000 in response to Technical Report 25 issued by the Defense Nuclear Facilities Safety Board (DNFSB). This group was responsible for determining the safety analysis and instrument and control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment as appropriate.

Safety Software — Includes both safety system software, and safety analysis and design software. [DOE O 414.1B]

Safety Structures, Systems, and Components (SSCs) — The set of safety-class SSCs and safety-significant SSCs for a given facility. [10 CFR 830]

Safety System Software — Computer software and firmware that performs a safety system function as part of a structure, system, or component (SSC) that has been functionally classified as Safety Class (SC) or Safety Significant (SS). This also includes computer software such as human-machine interface software, network interface software, programmable logic controller (PLC) programming language software, and safety management databases that are not part of an SSC but whose operation or malfunction can directly affect SS and SC SSC function. [DOE O 414.1B]

Safety-Class Structures, Systems, and Components (SC SSCs) — SSCs, including portions of process systems, whose preventive and mitigative function is necessary to limit radioactive hazardous material exposure to the public, as determined from the safety analyses. [10 CFR 830]

Safety-Significant Structures, Systems, and Components (SS SSCs) — SSCs which are not designated as safety-class SSCs, but whose preventive or mitigative function is a major contributor to defense in depth and/or worker safety as determined from safety analyses. [10 CFR 830] As a general rule of thumb, SS SSC designations based on worker safety are limited to those systems, structures, or components whose failure is estimated to result in prompt worker fatalities, serious injuries, or significant radiological or chemical exposure to workers. The term serious injuries, as used in this definition, refers to medical treatment for immediately life-threatening or permanently disabling injuries (e.g., loss of eye, loss of limb). The general rule of thumb cited above is neither an evaluation guideline nor a quantitative criterion. It represents a lower threshold of concern for which an SS SSC designation may be warranted. Estimates of worker consequences for the purpose of SS SSC designation are not intended to require detailed analytical modeling. Consideration should be based on engineering judgment of possible effects and the potential added value of SS SSC designation. [DOE G 420.1-1]

Sample Input — Input data for a designated sample problem that is maintained by the controlling organization for distribution to users.

Software — Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Standard 610.12-1990, IEEE Standard Glossary of Software Engineering Terminology]

Software Design Verification —The process of determining if the product of the software design activity fulfills the software design requirements. [NQA-1]

Software Development Cycle —The activities that begin with the decision to develop a software product and end when the software is delivered. The software development cycle typically includes the following activities:

Software Engineering — The application of a systematic, disciplined, quantifiable approach to the development, operation, and maintenance of software; that is, the application of engineering to software; also: the study of these applications. [NQA-1]

Software Life Cycle —The activities that comprise the evolution of software from conception to retirement. The software life cycle typically includes the software development cycle and the activities associated with operation, maintenance, and retirement. [NQA-1]

Source Code — A computer code in its originally coded form, typically in text file format. For programs written in a compilable programming language, the uncompiled program.

System Software —Software designed to enable the operation and maintenance of a computer system and its associated computer programs. [NQA-1]

Test Case —A set of test inputs, execution conditions, and expected results developed for a particular objective, such as to exercise a particular program path or to verify compliance with a specific requirement. [NQA-1]

Test Case Input — Input data for a test case used to verify a modification to a module or a data library.

Test Plan (Procedure) —A document that describes the approach to be followed for testing a system or component. Typical contents identify the items to be tested, tasks to be performed, and responsibilities for the testing activities. [NQA-1]

Testing —An element of verification for the determination of the capability of an item to meet specified requirements by subjecting the item to a set of physical, chemical, environmental, or operating conditions. [NQA-1]

Toolbox Codes — A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and of appropriate qualification that are maintained, managed, and distributed by a central source. Toolbox codes meet minimum quality assurance criteria. They may be applied to support 10 CFR 830 DSAs provided the application domain and input parameters are valid. In addition to public domain software, commercial or proprietary software may also be considered. In addition to safety analysis software, design codes may also be included if there is a benefit to maintain centralized control of the codes [modified from DOE N 411.1]..

User Manual — A document that presents the information necessary to employ a system or component to obtain desired results. Typically described are system or component capabilities, limitations, options, permitted inputs, expected outputs, possible error messages, and special instructions. Note: A user manual is distinguished from an operator manual when a distinction is made between those who operate a computer system (mounting tapes, etc.) and those who use the system for its intended purpose. Syn: User Guide. [IEEE 610-12]

Validation – 1. The process of testing a computer program and evaluating the results to ensure compliance with specified requirements [ANSI/ANS-10.4-1987].
2. The process of determining the degree to which a model is an accurate representation of the real-world from the perspective of the intended uses of the model [Department of Defense Directive 5000.59, *DoD Modeling and Simulation (M&S) Management*]
3. Assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended. This is usually accomplished by comparing code results to either physical data or a validated code designed to perform the same type of analysis. [IEEE-610.12]: The process of evaluating a system or component during or at the end of the development process to determine whether it satisfies specified requirements. Contrast with: **verification**.

Verification – 1. The process of evaluating the products of a software development phase to provide assurance that they meet the requirements defined for them by the previous phase [ANSI/ANS-10.4-1987].
2. The process of determining that a model implementation accurately represents the developer's conceptual description and specifications [Department of Defense Directive 5000.59, *DoD Modeling and Simulation (M&S) Management*].
3. Assurance that a computer code correctly performs the operations specified in a numerical model or the options specified in the user input. This is usually accomplished by comparing code results to a hand calculation or an analytical solution or approximation. [IEEE-610.12]: (1) The process of evaluating a system or component to determine whether the products of a given development phase satisfy the conditions

imposed at the start of that phase. Contrast with: **validation**. (2) Formal proof of program correctness.

7.0 References

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Appendices

Appendix	Subject
A	SOFTWARE INFORMATION TEMPLATE
B	SFPE TRAINING CLASS DESCRIPTIONS

APPENDIX A.— SOFTWARE INFORMATION TEMPLATE

Information Form

Development and Maintenance of Designated Safety Analysis Toolbox Codes

The following summary information in Table 2 should be completed to the level that is meaningful – enter N/A if not applicable. See Appendix A for an example of the input to the table prepared for the MACCS2 code.

Table 2. Summary Description of Subject Software

Table 2. Summary Description of Subject Software	
Type	**Specific Information**
Code Name	
Version of the Code	
Developing Organization and Sponsor Information	
Auxiliary Codes	
Software Platform/Portability	
Coding and Computer(s)	
Technical Support Point of Contact	
Code Procurement Point of Contact	
Code Package Label/Title	
Contributing Organization(s)	
Recommended Documentation - Supplied with Code Transmittal upon Distribution or Otherwise Available	1. 2. 3. 4. 5.

Table 2. Summary Description of Subject Software	
Type	**Specific Information**
Input Data/Parameter Requirements	
Summary of Output	
Nature of Problem Addressed by Software	
Significant Strengths of Software	
Known Restrictions or Limitations	
Preprocessing (set-up) time for Typical Safety Analysis Calculation	
Execution Time	
Computer Hardware Requirements	
Computer Software Requirements	
Other Versions Available	

Table 3. Point of Contact for Form Completion

Individual(s) completing this information form: Name: Organization: Telephone: Email: Fax:	

1. Software Quality Assurance Plan

The software quality assurance plan for your software may be either a standalone document, or embedded in other documents, related procedures, QA assessment reports, test reports, problem reports, corrective actions, supplier control, and training package.

1.a For this software, identify the governing Software Quality Assurance Plan (SQAP)?
[Please submit a PDF of the SQAP, or send hard copy of the SQAP[2]]

1.b What software quality assurance industry standards are met by the SQAP?

1.c What federal agency standards were used, if any, from the sponsoring organization?

1.d Has the SQAP been revised since the current version of the Subject Software was released? If so, what was the impact to the subject software?

1.e Is the SQAP proceduralized in your organization? If so, please list the primary procedures that provide guidance.

[2] Notify Kevin O'Kula of your intent to send hard copies of requested reports and shipping will be arranged.

Guidance for SQA Plans:

Requirement 2 – SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a)
ASME NQA-1 2000 Section 200
IEEE Standard 730, *IEEE Standard for Software Quality Assurance Plans.*
IEEE Standard 730.1, *IEEE Guide for Software Quality Assurance Planning.*

2. Software Requirements Description

The software requirements description (SRD) should contain functional and performance requirements for the subject software. It may be contained in a standalone document or embedded in another document, and should address functionality, performance, design constraints, attributes and external interfaces.

2.a For this software, was a software requirements description documented with the software sponsor? [If available, please submit a PDF of the Software Requirements Description, or include hard copy with transmittal of SQAP]

2.b If a SRD was not prepared, are there written communications that indicate agreement on requirements for the software? Please list other sources of this information if it is not available in one document.

Guidance for Software Requirements Documentation:

Requirement 5 – SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 401
IEEE Standard 830, *Software Requirements Specifications*

3. Software Design Documentation

The software design documentation (SDD) depicts how the software is structured to satisfy the requirements in the software requirements description. It should be defined and maintained to ensure that software will serve its intended function. The SDD for the subject software may be contained in a standalone document or embedded in another document.

The SDD should provide the following:

- Description of the major components of the software design as they relate to the software requirements,
- Technical description of the software with respect to the theoretical basis, mathematical model, control flow, data flow, control logic, and data structure,
- Description of the allowable or prescribed ranges of inputs and outputs,
- Design described in a manner suitable for translating into computer coding, and
- Computer program listings (or suitable references).

3.a For the subject software, was a software design document prepared, or were its constituents parts covered elsewhere? [If available, please submit a PDF of the Software Design Document, or include hard copy with transmittal of SQAP]

3.b If the intent of the SDD information is satisfied in other documents, provide the appropriate references (document number, section, and page number).

Guidance for Software Design Documentation:

Requirement 6 – SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 402
IEEE Standard 1016.1, *IEEE Guide for Software Design Descriptions* IEEE Standard 1016-1998, *IEEE Recommended Practice for Software Design Descriptions*
IEEE Standard 1012, *IEEE Standard for Software Verification and Validation;*
IEEE Standard 1012a, *IEEE Standard for Software Verification and Validation – Supplement to 1012*

4. Software User Documentation

Software User Documentation is necessary to assist the user in installing, operating, managing, and maintaining the software, and to ensure that the software satisfies user requirements. At minimum, the documentation should describe:

- The user's interaction with the software
- Any required training
- Input and output specifications and formats, options
- Software limitations
- Error message identification and description, including suggested corrective actions to be taken to correct those errors, and
- Other essential information for using the software.

4.a For the subject software, has Software User Documentation been prepared, or are its constituents parts covered elsewhere? [If available, please submit a PDF of the Software User Documentation, or include a hard copy with transmittal of SQAP]

4.b If the intent of the Software User Documentation information is satisfied in other documents, provide the appropriate references (document number, section, and page number).

4.c Training – How is training offered in correctly running the subject software? Complete the appropriate section in the following:

Type	Description	Frequency of training
Training Offered to User Groups as Needed		
Training Sessions Offered at Technical Meetings or Workshops		
Training Offered on Web or Through Video Conferencing		
Other Training Modes		
Training Not Provided		

Guidance for Software User Documentation:

Requirement 9 – SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 203
IEEE Standard 1063, *IEEE Standard for Software User Documentation*

5. Software Verification &Validation Documentation (Includes Test Reports)

Verification and Validation (*V&V*) documentation should confirm that a software V&V process has been defined, that V&V has been performed, and that related documentation is maintained to ensure that:

(a) The software adequately and correctly performs all intended functions, and
(b) The software does not perform any unintended function.

The software V&V documentation, either as a standalone document or embedded in other documents and should describe:

- The tasks and criteria for verifying the software in each development phase and validating it at completion,
- Specification of the hardware and software configurations pertaining to the software V&V
- Traceability to both software requirements and design
- Results of the V&V activities, including test plans, test results, and reviews (also see 5.b below)
- A summary of the status of the software's completeness
- Assurance that changes to software are subjected to appropriate V&V,
- V&V is complete, and all unintended conditions are dispositioned before software is approved for use, and
- V&V performed by individuals or organizations that are sufficiently independent.

5.a For the subject software, identify the V&V Documentation that has been prepared.
[If available, please submit a PDF of the Verification and Validation Documentation, or include a hard copy with transmittal of SQAP]

5.b If the intent of the V&V Documentation information is satisfied in one or more other documents, provide the appropriate references (document number, section, and page number). For example, a "Test Plan and Results" report, containing a plan for software testing, the test results, and associated reviews may be published separately.

5.c Testing of software: What has been used to test the subject software?

- ☐ Experimental data or observations
- ☐ Standalone calculations
- ☐ Another validated software
- ☐ Software is based on previously accepted solution technique

Provide any reports or written documentation substantiating the responses above.

Guidance for Software Verification & Validation, and Testing Documentation:

Requirement 6 – *Design Phase* - SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
Requirement 8 – *Testing Phase* - SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
Requirement 10 – *Acceptance Test* - SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 402 (Note: Some aspects of verification may be handled as part of the Design Phase).
ASME NQA-1 2000 Section 404 (Note: Aspects of validation may be handled as part of the Testing Phase).
IEEE Standard 1012, *IEEE Standard for Software Verification and Validation;*
IEEE Standard 1012a, *IEEE Standard for Software Verification and Validation – Supplement to 1012*
IEEE Standard 829, *IEEE Standard for Software Test Documentation.*
IEEE Standard 1008, *Software Unit Testing*

6. Software Configuration Management (SCM)

A process and related documentation for SCM should be defined, maintained, and controlled.

The appropriate documents, such as project procedures related to software change controls, should verify that a software configuration management process exists and is effective.

The following points should be covered in SCM document(s):

- A Software Configuration Management Plan, either in standalone form or embedded in another document,
- Configuration management data such as software source code components, calculational spreadsheets, operational data, run-time libraries, and operating systems,
- A configuration baseline with configuration items that have been placed under configuration control,
- Procedures governing change controls,
- Software change packages and work packages to demonstrate that (1) possible impacts of software modifications are evaluated before changes are made, (2) various software system products are examined for consistency after changes are made, and (3) software is tested according to established standards after changes have been made.

6.a For the subject software, has a Software Configuration Management Plan been prepared, or are its constituent parts covered elsewhere? [If available, please submit a PDF of the Software Configuration Management Plan and related procedures, or include hard copies with transmittal of SQAP].

6.b Identify the process and procedures governing control and distribution of the subject software with users.

6.c Do you currently interact with a software distribution organization such as the Radiation Safety Information Computational Center (RSICC)?

6.d A Central Registry organization, under the management and coordination of the Department of Energy's Office of Environment, Safety and Health (EH), will be responsible for the long-term maintenance and control of the safety analysis toolbox codes for DOE safety analysis applications. Indicate any questions, comments, or concerns on the Central Registry's role and the maintenance of the subject software.

Guidance for Software Configuration Management Plan Documentation:

Requirement 12 – *Configuration Control* - SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 203
IEEE Standard 828, *IEEE Standard for Software Configuration Management Plans.*

7. Software Problem Reporting and Corrective Action

Software problem reporting and corrective action documentation help ensure that a formal procedure for problem reporting and corrective action development for software errors and failures is established, maintained, and controlled.

A Software Error Notification and Corrective Action Report, procedure, or similar documentation, should be implemented to report, track, and resolve problems or issues identified in both software items, and in software development and maintenance processes. Documentation should note specific organizational responsibilities for implementation. Software problems should be promptly reported to affected organizations, along with corrective actions. Corrective actions taken ensure that:

- Problems are identified, evaluated, documented, and, if required, corrected,

- Problems are assessed for impact on past and present applications of the software by the responsible organization,
- Corrections and changes are executed according to established change control procedures, and
- Preventive actions and corrective actions results are provided to affected organizations.

Identify documentation specific to the subject software that controls the error notification and corrective actions. [If available, please submit a PDF of the Error Notification and Corrective Action Report documentation for the subject software (or related procedures). If this is not available, include hard copies with transmittal of SQAP].

7.aProvide examples of problem/error notification to users and the process followed to address the deficiency. Attach files as necessary.

7.bProvide an assessment of known errors or defects in the subject software and the planned action and time frame for correction.

Category of Error or Defect	Corrective Action	Planned schedule for correction
Major		
Minor		

7.cIdentify the process and procedures governing communication of errors/defects related to the subject software with users.

Guidance for Error/Defect Reporting and Corrective Action Documentation:

Requirement 13 – *Error Impact* - SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a))
ASME NQA-1 2000 Section 204
IEEE Standard 1063, *IEEE Standard for Software User Documentation*

8. Resource Estimates

If one or more plans, documents, or sets of procedures identified in parts one (1) through seven (7) do not exist, please provide estimates of the resources (full-time equivalent (40-hour) weeks, FTE-weeks) and the duration (months) needed to meet the specific SQA requirement.

Enter estimate in Table 4 only if specific document has not been prepared, or requires revision.

Table 4. Resource and Schedule for SQA Documentation

Plan/Document/Procedure	Resource Estimate (FTE-weeks)	Duration of Activity (months)
1. Software Quality Assurance Plan		
2. Software Requirements Document		
3. Software Design Document		
4. Test Case Description and Report		
5. Software Configuration and Control		
6. Error Notification and Corrective Action Report		
7. User's Instructions (User's Manual)		
8. Other SQA Documentation		

Comments or Questions:

9. Software Upgrades

Describe modifications planned for the subject software.

Technical Modifications

Priority	Description of Change	Resource Estimate (FTE-weeks)
1.		
2.		
3.		
4.		
5.		

User Interface Modifications

Priority	Description of Change	Resource Estimate (FTE-weeks)
1.		
2.		
3.		
4.		
5.		

Software Engineering Improvements

Priority	Description of Change	Resource Estimate (FTE-weeks)
1.		
2.		
3.		
4.		
5.		

Other Planned Modifications

Priority	Description of Change	Resource Estimate (FTE-weeks)
1.		
2.		
3.		
4.		
5.		

Thank you for your input to the SQA upgrade process. Your experience and insights are critical towards successfully resolving the issues identified in DNFSB Recommendation 2002-1.

APPENDIX B.— SFPE TRAINING CLASS DESCRIPTIONS

Introduction to Computer Fire Modeling

Intended for: This seminar is intended for fire protection engineers with a desire to develop a basic understanding of models used to predict the characteristics of compartment fire growth and the operation of fire protection systems. Attendees are expected to bring a laptop with a copy of FPEtool installed, details will be provided upon registration. Attendees will receive a set of class notes and selected reading and reference materials.

Seminar Description: This seminar provides an introduction to computer fire modeling and the underlying fire science. The fundamental driving force for fire modeling and design calculations is the heat release rate history of the burning objects. The basic fire science of compartment fire development is presented along with specific computer models or tools. Attendees will be given problems to solve independently to gain experience in use of the models. Problems will involve: detector and sprinkler activation, fire growth and spread, smoke and gas flow and an introduction to human behavior and egress. Limitations of the methodologies presented will be discussed. The seminar will employ case studies and conclude with demonstration of FASTlite. Participants will receive a detailed course notebook.

Seminar Outline:

- Introduction to Computer Modeling
- Heat Release Rate
- Ignition and Flame Spread
- Flow Through Cents
- Fire/Wind/Stack Forces on Doors
- Zone Fire Modeling Theory
- General Limitations of Zone Models
- Plume and Jet Temperatures
- Sprinkler and Detector Response
- Upper Layer Temperature
- ASET-B Room Fire
- Modeling the Occupants
- Modeling Sprinkler Suppression
- FASTlite

Advanced Computer Fire Modeling

Intended for: This seminar is intended for fire protection engineers who have a basic understanding of models used to predict the characteristics of compartment fire growth and the operation of fire protection systems and are seeking to apply these methods to fire protection engineering analysis and design. *Attendees are expected to bring a laptop with copies of FAST installed.* Other software may be used as well. Software and installation details will be provided upon registration. Attendees will receive a set of class notes and selected reading and reference materials.

Description: This seminar assumes a basic understanding of computer fire modeling and the underlying fire science. This seminar will expand on the methods introduced in *Introduction to Computer Fire Modeling,* providing alternative approaches and discussion of how to select the right model for the job. Limitations of the methodologies presented will be discussed. Computer fire modeling is the basis for predicting fire effects for performance-based design. Attendees

will be given problems to solve that will involve working from floor plans, setting design/performance criteria, developing design fires and selecting and evaluating design alternatives. The seminar will employ case studies and conclude with a discussion of computational fluid dynamics (CFD) fire modeling.

Outline:

- Introduction
- Toxic Species Modeling
- How to Select Your Model
- Performance-Based Design Criteria
- Plume and Jet Equations
- Design Application Case Studies
- Detection Issues
- Design Problems
- Modeling Effects of Suppression
- Overview of CFD
- Human Response Models
- Single & Multi-Compartment Modeling

SEPARATION

PAGE

DOE-EH-4.2.1.3-Interim-GENII

Defense Nuclear Facilities Safety Board Recommendation 2002-1
Software Quality Assurance Implementation Plan
Commitment 4.2.1.3:

GENII Gap Analysis

Interim Report

U.S. Department of Energy
Office of Environment, Safety, and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

January 2004

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FOREWORD

This document provides an evaluation of the Software Quality Assurance (SQA) attributes of the radiological dispersion computer code, GENII, relative to established requirements. The evaluation, a "gap analysis", is performed to meet commitment 4.2.1.3 of the Department of Energy's Implementation Plan to resolve SQA issues identified in the Defense Nuclear Facilities Safety Board Recommendation 2002-1. Both versions of the GENII code (1.485 and 2.0) are addressed.

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Software Quality Assurance Implementation Plan: GENII Gap Analysis

EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board (DNFSB) issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002 (DNFSB 2002). The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in the February 28, 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities* (DOE 2003a). A DOE safety analysis toolbox would contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed, and maintained for DOE-broad safety basis applications.

DOE has designated six computer codes for toolbox consideration. All six are accident and consequence analysis software, and include the following:

Fire Source Term:	CFAST
Leak Path Factor:	MELCOR
Chemical Release/Dispersion and Consequence:	ALOHA, EPIcode
Radiological Dispersion and Consequence:	MACCS2, GENII.

Each of the codes designated for the toolbox may require some degree of quality assurance improvement before meeting current SQA standards. In the interim period before these changes are completed, the designated toolbox codes are considered useful assets in the support of safety basis calculations. To determine the actions needed to bring the codes into compliance with the SQA qualification criteria and develop a schedule with milestones to upgrade each code based on the gap analysis results, the Implementation Plan has committed to sponsoring a set of code-specific gap analysis documents. Gap analysis evaluates each code's SQA attributes against identified criteria.

The balance of this document provides the GENII gap analysis documentation. Both versions of GENII, 1.485 and 2.0, have been evaluated. For GENII 1.485, of the ten general topical quality areas that were evaluated for software developers, nine met the criteria fully, and one failed to meet the criteria. For GENII 2.0, of the ten general topical quality areas, two met the criteria fully, five met the criteria partially, and three failed to meet the criteria. Recommendations are given for each of the topical areas in Section 4.0. The GENII code was evaluated to determine if the code, as it currently stands, meets the intended function for the code in the context as described in the scope of this gap analysis. When the code is run for the intended applications, as detailed in the code guidance document, *Computer Code Application Guidance for Documented Safety Analysis*,

(DOE 2003f), it is judged that GENII 1.485 will meet its intended function, but GENII 2.0 will not. Therefore, only GENII 1.485 can be recommended for DSA use at this time.

It is estimated that approximately ten full-time equivalent (FTE) months would be required to perform all SQA upgrade tasks identified in Section 4.0 of this report.

While completion of the GENII 2.0 development is encouraged, current DOE DSA support should be through the earlier code version, GENII 1.485. No evidence was found of software-induced errors in GENII 1.485 that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

1.0 Introduction

This document reports on the results of a gap analysis for the GENII computer code. Both versions of the code (1.485 and 2.0) are considered.

The intent of the gap analysis is to determine the actions needed to bring the toolbox codes into compliance with the SQA qualification criteria and develop a schedule with milestones to upgrade each code based on the gap analysis results. Gap analysis evaluates each code's SQA attributes against identified criteria.

1.1 Background: Overview of Designated Toolbox Software in the Context of 10 CFR 830

The DNFSB issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the DOE facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, SQA-compliant safety analysis codes is one of the major commitments contained in the March 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications.

Six computer codes, including ALOHA (chemical release dispersion/consequence analysis), CFAST (fire analysis), EPIcode (chemical release dispersion/consequence analysis), GENII (radiological dispersion/consequence analysis), MACCS2 (radiological dispersion/consequence analysis), and MELCOR (leak path factor analysis), were designated by DOE for the toolbox (DOE/EH, 2003). It is found that these codes provide generally recognized and acceptable approaches for modeling source term and consequence phenomenology, and can be applied as appropriate to support accident analysis in Documented Safety Analyses (DSAs).

As one of the designated toolbox codes, GENII, will likely require some degree of quality assurance improvement before meeting current SQA standards. The analysis documented herein is an evaluation of GENII, both versions 1.485 and 2.0, relative to current software quality assurance criteria. It assesses the margin of the deficiencies, or gaps, to provide DOE and the software developer the extent to which minimum upgrades are needed. The overall assessment is therefore termed a "gap" analysis.

1.2 Evaluation of Toolbox Codes

The quality assurance criteria identified in later sections of this report are defined as the set of established requirements, or bases, by which to evaluate each designated toolbox code. This gap analysis evaluation, is commitment 4.2.1.3 in the IP:

> Perform a SQA evaluation to the toolbox codes to determine the actions needed to bring the codes into compliance with the SQA qualification criteria, and develop a schedule with milestones to upgrade each code based on the SQA evaluation results.

This process is a prerequisite step for software improvement. It will allow DOE to determine the current limitations and vulnerabilities of each code as well as help define and prioritize the steps required for improvement.

Ideally, each toolbox code owner will provide input information on the SQA programs, processes, and procedures used to develop their software. However, the gap analysis itself will be performed by a SQA evaluator. The SQA evaluator is independent of the code developer, but knowledgeable in the use of the software for accident analysis applications and current software development standards.

1.3 Uses of the Gap Analysis

The gap analysis will provide information to DOE, code developers, and code users.

DOE will see the following benefits:

- Estimates of the resources required to perform modifications to designated toolbox codes
- Basis for schedule and prioritization to upgrade each designated toolbox code.

Each code developer will be provided:

- Information on areas where software quality assurance improvements are needed to comply with industry SQA standards and practices
- Specific areas for improvement for guiding development of new versions of the software.

DOE safety analysts and code users will benefit from:

- Improved awareness of the strengths, limits, and vulnerable areas of each computer code
- Recommendations for code use in safety analysis application areas.

1.4 Scope

This analysis is applicable to the GENII code, one of the six designated toolbox codes for safety analysis (Table 1-1). While GENII is the subject of the current report, other safety analysis software considered for the toolbox in the future may be evaluated with the same process applied here. The template outlined in this document is applicable to analytical software as long as the primary criteria are ASME NQA-1, 10 CFR 830, and related DOE directives discussed in DOE (2003e).

Table 1-1 — Software Designated for DOE Safety Analysis Toolbox

Code	Version or Revision
ALOHA	5.2.3
CFAST	3.1.6
EPIcode	7.0
GENII	1.485 and 2.0[1]
MACCS2	1.12[2]
MELCOR	1.8.5

1.5 Purpose

The purpose of this report is to document the gap analysis performed on the GENII code as part of DOE's implementation plan on SQA improvements.

1.6 Methodology for Gap Analysis

The gap analysis for GENII is based on the criteria as described in *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes* (DOE 2003e). In it, Table 3-2 lays out fourteen topical areas related to code quality assurance. The gap analysis as reported here utilizes ten of the fourteen areas to assess the quality of the GENII code. The ten areas are pertinent to software development, while the four not assessed are judged more applicable to software end user organizations or to different categories of software than is the subject of the current study. Section 4.0 gives the detail of each analysis for each of the ten areas in Subsections 4.1 to 4.10.

In general, fourteen requirement areas demonstrate compliance with NQA-1 2000. They are as follows:

1) Software Classification
2) SQA Procedures/Plans
3) Dedication
4) Evaluation

[1] In the interim period before quality assurance improvements are made to version 2.0 of GENII, version 1.485 is recommended.

[2] In the interim period before quality assurance improvements are made to MACCS2, either MACCS2 or its predecessor MACCS (version 1.5.11.1) may be applied to DSAs.

5) Requirements
6) Design
7) Implementation
8) Testing
9) User Instructions
10) Acceptance Test
11) Operation and Maintenance
12) Configuration Control
13) Error Impact
14) Access Control

Table 3-1 of *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes* (DOE 2003e)[3] provides the required versus graded breakdown per area for Class B software that is *existing* or *purchased* as well.

The gap analysis utilizes ten of the fourteen topical areas listed in DOE (2003e) related to SQA to assess the quality of the GENII code. The four areas eliminated in this gap analysis are dedication, evaluation, operation and maintenance, and access control. These areas focus on software intended to control hardware or focus on the end user SQA for the software. Therefore, the remaining ten areas are assessed individually in Section 4.

Each of the areas is broken down into one or more specific criteria. The requirements, as listed in Table 3-2 of the DOE SQA plan under the column 'software developer,' are refined, extracted, and listed separately in the tables that follow. NQA-1 2000 wording found in Table C-1 of the DOE SQA plan also aids this individual criterion development. Effort is made to preserve the exact wording of the requirements as much as possible.

No unique methodology related to the GENII was involved in this gap analysis.

1.7 Summary Description of Software Being Reviewed

The gap analysis was performed on both versions of the GENII code (i.e., Version 1.485 [Napier, 1988a, 1988b, 1988c] and Version 2.0 [Napier, 1995, 2002a, 2002b, 2003]). Although the earlier version (1.485) is the one recommended for use in current DSAs, the later version (2.0) is also evaluated, because the improvements recommended here, if implemented, would allow it to be used in DSAs in the future. In the following discussion, RSICC refers to the Radiation Safety Information Computational Center at Oak Ridge, TN.

The set of documents reviewed as part of the gap analysis are listed in Table 1-2.

[3] In the following discussion, this document (DOE, 2003e) is cited as "the DOE SQA plan."

Table 1-2 — Software Documentation Reviewed for GENII

No.	Information	
1.	Reference:	B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII – The Hanford Environmental Radiation Dosimetry Software System. Volume 1: Conceptual Representation.* PNL-6584, December 1988. (Napier, 1988a)
	Remarks:	Documentation provided by RSICC in .pdf format
2.	Reference:	B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII – The Hanford Environmental Radiation Dosimetry Software System. Volume 2: User's Manual,* PNL-6584, November 1988. (Napier, 1988b)
	Remarks:	Documentation provided by RSICC in .pdf format
3.	Reference:	B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII – The Hanford Environmental Radiation Dosimetry Software System. Volume 3: Code Maintenance Manual,* PNL-6584, September 1988. (Napier, 1988c) Only the table of contents is available (included as part of the .pdf file of Volumes 1 and 2). Bruce Napier has one of the few copies of the entire document (Volume 3), which is about 1,500 pages long, but a copy was not available for this gap analysis.
	Remarks:	Table of contents in .pdf format provided by RSICC.
4.	Reference:	B. A. Napier, J. V. Ramsdell, and D. L. Strenge, *Software Requirements Specifications for Hanford Environmental Dosimetry Coordination Project,* Draft Report, prepared for review by the EPA Office of Radiation and Indoor Air, May 1995. (Napier, 1995)
	Remarks:	Documentation provided by Bruce Napier.
5.	Reference:	B. A. Napier, *GENII Version 2 User's Guide* (Napier, 2002a)
	Remarks:	Downloaded from PNNL website

No.	Information	
6.	Reference:	B. A. Napier, D. L. Strenge, J. V. Ramsdell, Jr., P. W. Eslinger, and C. Fosmire, *GENII Version 2 Software Design Document* (Napier, 2002b)
	Remarks:	Downloaded from PNNL website
7.	Reference:	B. A. Napier, *GENII Version 2 Example Calculation Descriptions* (Napier, 1999a)
	Remarks:	Documentation on CD from EFCOG training class, June 1999
8.	Reference:	B. A. Napier and L. Staven, *GENII Version 2 Training Power Point Slides* (Napier, 1999b)
	Remarks:	Documentation on CD from EFCOG training class, June 1999
9.	Reference:	B. A. Napier, *Getting Started with GENII Version 2* (Napier, 2003)
	Remarks:	Downloaded from EPA/NESHAPs website
10.	Reference:	B. A. Napier, E-mail communications with K. R. O'Kula and Vern Peterson
	Remarks:	Provided in Appendix A
11.	Reference:	W. E. Joyce, Telephone conversation with V. L. Peterson
	Remarks:	Provided in Appendix A
12.	Reference:	Publications supporting GENII Benchmarking and V&V
	Remarks:	Provided in Appendix B

2.0 Assessment Summary Results

2.1 Criteria Met

For GENII 1.485, of the applicable ten general topical quality areas, nine met the criteria fully, and one failed to meet the criteria. An exception was found in the area of Error Impact. GENII 1.485 should create and follow a formal error reporting and corrective action process. For GENII 2.0, of the ten general topical quality areas, two met the criteria fully, five met the criteria partially, and three failed to meet the criteria. Exceptions were found in the areas of Testing Phase, Acceptance Test, Error Impact, and partially in the areas of SQA Procedures and Plans, Requirements Phase, Design Phase, Implementation Phase, and User Instructions.

2.2 Exceptions to Criteria

Some of the more important exceptions to criteria found are listed below in Table 2-1 for GENII 2.0. No similar list is needed for GENII 1.485. The criterion is given; the reason the criterion was judged not to be met is specified and action needed to remedy the exception is suggested.

Table 2-1 — Summary of Important Exceptions, Reasoning, and Suggested Remediation for GENII 2.0

No.	Criterion	Reason Not Met	Suggested remedial action(s)
1.	Testing Phase	Testing not yet complete	Document all testing of GENII 2.0
2.	Acceptance Test	Testing not yet complete	Develop and document acceptance criteria for GENII 2.0 and document acceptance testing.
4.	Error Impact	A formal error reporting and corrective action procedure is not followed.	Create and follow a formal error reporting and corrective action process (applies to GENII 1.485 as well)

2.3 Areas Needing Improvement

The gap analysis identified a number of improvements that could be made related to the code and its quality assurance. Some of the important ones are listed in Table 2-2.

Table 2-2 — Summary of Important Recommendations for GENII

N	Recommendation
1.	Establish and follow formal review schedules for GENII 2.0.
2.	Make GENII 2.0 code listings available upon completion and final testing of code.
3.	Correct the user documentation (see Section 4.7.4) and the bugs in the user interface for GENII 2.0 (see Criterion 9.6).
4.	Run a wide variety of scenarios using GENII 1.485 on both DOS and Windows based PCs to verify agreement in results. Memory management is different in Windows than in DOS (under which 1.485 was developed) and there is a potential for problems.
5.	Modify GENII 2.0 to make it easy for the user to determine 95th percentile consequences at the site boundary and at a user-selected collocated worker distance (for example, 100 m).
6.	Assemble the existing "software change packets" for GENII 1.485 into a document to verify that changes to the code followed a logical and verifiable process.

2.4 Areas Not Assessed and Any Limitations of Gap Analysis

All areas were assessed for this gap analysis. Some areas were found to be more difficult to assess than others, depending upon the level of detail provided in the documentation. However, no limitations were imposed on the gap analysis.

2.5 Conclusion Regarding Code's Ability to Meet Intended Function

The GENII code was evaluated to determine if the code, as it currently stands, meets the intended function for the code in the context as described in the scope of this gap analysis. When the code is run for the intended applications, as detailed in the code guidance document, *Computer Code Application Guidance for Documented Safety Analysis*, (DOE 2003f), it is judged that GENII 1.485 will meet its intended function, but GENII 2.0 will not. Therefore, only GENII 1.485 can be recommended for DSA use at this time.

The primary remedial actions required for GENII 2.0 include the following:

(1) Modify the software so that the user can determine the 95th percentile doses at the site boundary in all sectors
(2) Improve the user documentation
(3) Create an error-reporting and corrective action procedure, including its documentation
(4) Complete code testing and document it
(5) Create and implement a code maintenance procedure.

3.0 Lessons Learned

Table 3-1 provides a summary of the lessons learned during the performance of the GENII gap analysis.

Table 3-1 — Lessons Learned

No.	Lesson
1.	Changing criteria in SQA standards over the years can render codes non-compliant that were once compliant.
2.	Although the author of a code may intend the code to be compliant with SQA standards, the standards may present sufficient complexity so that some requirements are not met in total.
3.	Development of software that is compliant with SQA standards can be a costly and laborious endeavor, especially if it is back-fit to the software, instead of being a parallel requirement during software development. If funding for the project is meager, SQA will probably not be followed as closely as may have been intended originally. Completion of the code development may take precedence over SQA measures.
4.	Changing sponsors may impact the SQA pedigree of software. This situation can arise especially if more recent software development was driven by other, non-SQA requirements than were present originally. The current version of the code has been developed for Environmental Protection Agency (EPA)/National Emission Standards for Hazardous Air Pollutants (NESHAPS), while original versions of the code were funded out of the PNNL budget.

4.0 Assessment Detailed Results

Fourteen topical areas are presented. In the tables that follow, sub-criteria and recommendations are labeled as (1.x, 2.x, ..., 10.x) with the first value (1., 2., ...10) corresponding to the topical area and the second value (x), the sequential table order of each entry.

For both GENII 1.485 (Level B Existing) and GENII 2.0 (Level B Development), ten topical areas were considered. The ten subsections below discuss in detail the evaluation of each of the code versions relative to the ten topical areas.

4.1 Topical Area 1 Assessment: Software Classification

This area corresponds to the requirement entitled *Software Classification* in Table 3-2 of the DOE SQA plan. Because all of the designated toolbox codes are used in applications the results of which are part of an accident analysis evaluation, the most applicable classification is Level B. Level B is further broken down into "Development," "Existing," and "Purchased." Because GENII 1.485 has been in use for many years, it is considered "Level B Existing." However, GENII 2.0 is still in need of further testing and development (as shown below), and is, therefore, classified "Level B development" software.

4.1.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.1-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.1-1 — Subset of Criteria for Software Classification Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
1.1	The code developer must provide sufficient information to allow the user to make an informed decision on the classification of the software.	Yes for both	The documentation from the developer makes it clear that both GENII 1.485 and 2.0 are Level B software.

4.1.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Software Classification," except for Item 12 (see Appendix B).

4.1.3 Software Quality-Related Issues or Concerns

There are no other SQA-related issues or concerns in "Software Classification."

4.1.4 Other Areas for Improvement

No areas of improvement in "Software Classification" have been noted.

4.1.5 Recommendations

There are no recommendations related to this Topical Area.

4.2 Topical Area 2 Assessment: SQA Procedures and Plans

This area corresponds to the requirement entitled *SQA Procedures and Plans* in Table 3-2 of the DOE SQA plan (DOE 2003e). It deals with the planning efforts prior to code development.

4.2.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.2-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.2-1 — Subset of Criteria for SQA Procedures and Plans Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
2.1	Procedures/plans for SQA (SQA Plan) have identified organizations responsible for performing work, independent reviews, etc.	Yes for both	Pacific Northwest National Laboratory (PNNL) (formerly Pacific Northwest Laboratory [PNL]) is responsible for performing the work and providing for independent reviews (Napier, 1988a) and Napier (1995)
2.2	Procedures/plans for SQA (SQA Plan) have identified software engineering methods.	Yes for both	The software engineering methods are discussed in Napier (1988a) and Napier (1995)
2.3	Procedures/plans for SQA (SQA Plan) have identified documentation to be required as part of program.	Yes for both	Required documentation is discussed in Napier (1988a) and Napier (1995)
2.4	Procedures/plans for SQA (SQA Plan) have identified standards, conventions, techniques, and/or methodologies that shall be used to guide the software development, methods to ensure compliance with the same.	Yes for both	The standards, conventions, techniques, and/or methodologies that were used to guide code development are discussed in Napier (1988a) and Napier (1995).
2.5	Procedures/plans for SQA (SQA Plan)	Yes for	Napier (1988a) discusses two

Criterion Number	Criterion Specification	Met?	Summary Remarks
	have identified software reviews and schedule.	1.485. No for 2.0.	formal review periods for GENII 1.485. No similar discussion is in the GENII 2.0 documentation.
2.6	Procedures/plans for SQA (SQA Plan) have identified methods for error reporting and corrective actions.	Yes for 1.485. No for 2.0	Napier (1988b) discusses how to report errors and request upgrades. An informal method is used for GENII 2.0.

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

Criterion 2.1 — The GENII 1.485 system was developed under the direction of the DOE office at Hanford for use by nuclear safety analysts. Potential user groups were identified and representatives of these groups were then selected to form a committee to specify the software requirements. Other groups were identified to provide reviews of the design and perform independent testing. The documentation describes these groups by their functions and the names of individual members are given in the "Acknowledgements" section. The organization selected to perform the work was the PNL (now PNNL). The GENII 2.0 system was developed with funding from the EPA. It incorporates much of the code developed for GENII 1.485 but was developed for use by the EPA in Environmental Impact Statements (EISs). The various groups for review and testing are mentioned in Napier (1995), which is the SQA plan for GENII 2.0.

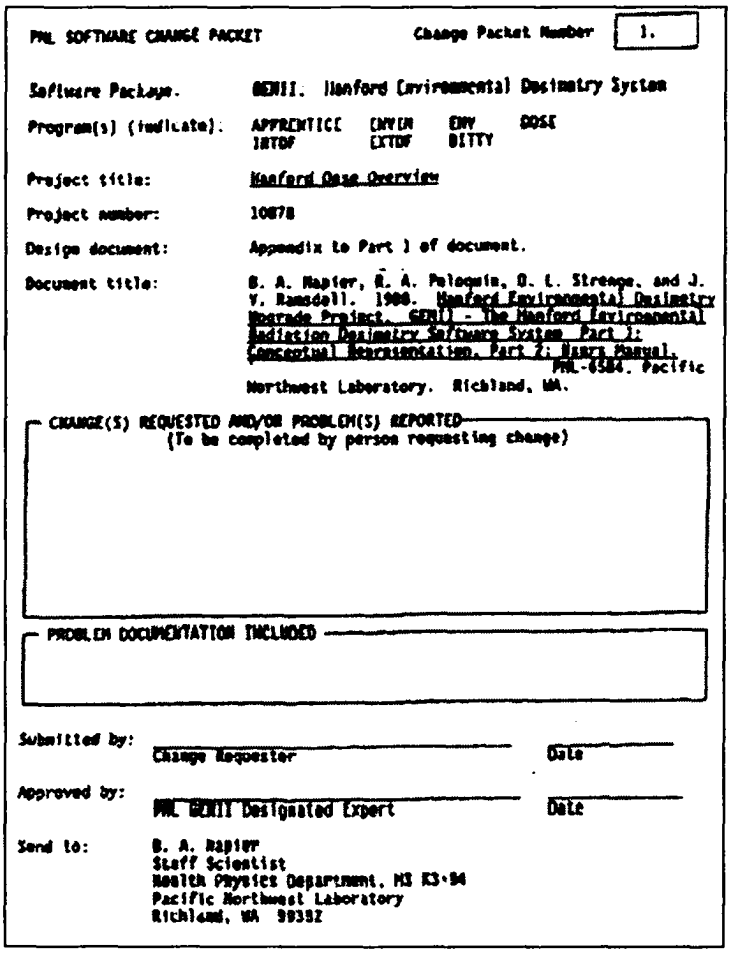
Criterion 2.2 — An appendix to the GENII 1.485 volume 1 (Napier, 1988a) is a detailed system-requirements document. In it, software engineering methods are discussed. For GENII 2.0, the system requirements are given in Napier (1995), which discusses software engineering. (However, the word "engineering" is not used in either document.)

Criterion 2.3 — The GENII 1.485 documentation (Napier, 1988a, 1988b) identified several required documents, including requirements for the overall system, design, implementation, testing, user manual, and maintenance. Likewise, Napier (1995) discusses the planned documentation for GENII 2.0.

Criterion 2.4 — Napier (1988a) and Napier (1995) discuss the standards, conventions, techniques, and/or methodologies to be used to guide code development. Napier (1988a) was prepared, during and after, the development of GENII 1.485 and is, thus, more detailed than Napier (1995), which was prepared before the development of GENII 2.0

Criterion 2.5 — External peer reviews of GENII 1.485 were conducted during the weeks beginning September 14, 1987 and February 1, 1988. This was followed by a formal acceptance of the code upon completion of the documentation packages for the user. Review schedules are not discussed in the GENII 2.0 documentation.

Criterion 2.6 — A formal error-reporting methodology was used for GENII 1.485. A copy of the reporting form is shown in Figure 4-1. For GENII 2.0, error reporting is informal, as evidenced by e-mail from Napier (see Appendix A) that includes the statement "I only have a few beta users; they let me know when it's broke and I fix it for them."



PNL SOFTWARE CHANGE PACKET Change Packet Number 1.

Software Package. GENII. Hanford Environmental Dosimetry System

Program(s) (indicate): APPRENTICE ENVIN ENV DOSE
INTDF EXTDF DITTY

Project title: Hanford Dose Overview

Project number: 10878

Design document: Appendix to Part 1 of document.

Document title: B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell. 1988. Hanford Environmental Dosimetry Upgrade Project. GENII - The Hanford Environmental Radiation Dosimetry Software System. Part 1: Conceptual Representation. Part 2: Users Manual. PNL-6584. Pacific Northwest Laboratory. Richland, WA.

CHANGE(S) REQUESTED AND/OR PROBLEM(S) REPORTED
(To be completed by person requesting change)

PROBLEM DOCUMENTATION INCLUDED

Submitted by: _____ Date _____
Change Requester

Approved by: _____ Date _____
PNL GENII Designated Expert

Send to: B. A. Napier
Staff Scientist
Health Physics Department, MS K3-54
Pacific Northwest Laboratory
Richland, WA 99352

Figure 4-1. Error reporting / update request form for GENII 1.485

4.2.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "SQA Procedures and Plans," except for Item 12 (see Appendix B).

4.2.3 Software Quality-Related Issues or Concerns

Review schedules and a formal error reporting and corrective action methodology needs to be implemented for GENII 2.0.

4.2.4 Other Areas for Improvement

No other areas of improvement are noted.

4.2.5 Recommendations

Recommendations related to this topical area are provide in Table 4.2-2.

Table 4.2-2 — Recommendations for SQA Procedures and Plans Topic

Recom-mendation Number	Relates to Table 4.2-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
2.1	2.6	Implement a Formal Error Report (FER) and handling methodology for GENII 2.0. This is not required for GENII 1.485.	One FTE week	Two weeks
2.2	2.5	Establish formal review schedules for GENII 2.0.	One FTE day	One week

4.3 Topical Area 3 Assessment: Requirements Phase

This area corresponds to the requirement entitled *Requirements* Phase in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.3.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.3-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.3-1 — Subset of Criteria for Requirements Phase Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
3.1	Software requirements for the subject software have been established.	Yes for both	Software Requirements are in: 1.485: Napier (1988a) appendix 2.0: Napier (1995)
3.2	Software requirements are specified, documented, reviewed, and approved.	Yes for both	1.485: Software specifications, review, and approval are in Napier (1988a) and its appendix. 2.0: Requirements in Napier (1995). Review and approval implied by Napier (2002b).
3.3	Requirements define the functions to be performed by the software and provide detail and information necessary to design the software.	Yes for both	Detailed functional requirements are defined in: 1.485: Napier (1988a) appendix 2.0: Napier (1995)
3.4	A **Software Requirements Document**, or equivalent, defines requirements for functionality, performance, design inputs, design constraints, installation considerations, operating systems (if applicable), and external interfaces necessary to design the software.	Yes for both	Detailed functional requirements are defined in the System Requirements documents: 1.485: Napier (1988a) appendix 2.0: Napier (1995)
3.5	Acceptance criteria are established in the software requirements documentation for each of the identified requirements.	Yes for 1.485. Partial for 2.0	1.485: Napier (1988b, 1988c) 2.0: Acceptance criteria are not specifically described but are implied by testing requirements

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table.

Criteria 3.1 and 3.2 — GENII 1.485 was developed by means of tasks designed to provide a state-of-the-art, technically peer-reviewed, and documented set of programs. The initial task resulted in a system design requirements report, based on input from potential Hanford users, providing general descriptions of the calculations that the final programs must perform. The recommendations of that report formed the basis for the remainder of the tasks, defining the elements that determined the equation formulation and parameter selection tasks (Napier, 1988a). The appendix to that document provides a discussion of SQA issues, including responsible organizations. Napier (1995) provides a similar discussion for GENII 2.0 and states the code was developed in a similar manner. The identified user groups are EPA analysts and contractors.

Criterion 3.5 — Napier (1988b, 1988c) discuss acceptance criteria and testing for GENII 1.485.

The GENII 2.0 documentation does not specifically address acceptance criteria but implies their existence by referring to code testing.

4.3.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Requirements," except for Item 12 (see Appendix B).

4.3.3 Software Quality-Related Issues or Concerns

The only SQA concern for GENII 2.0 was the lack of specific acceptance criteria. There are no similar concerns for GENII 1.485.

4.3.4 Other Areas for Improvement

No other areas of improvement were noted.

4.3.5 Recommendations

Recommendations related to this topical area are provide in Table 4.3-2.

Table 4.3-2 — Recommendations for Requirements Phase Topic

Recommendation Number	Relates to Table 4.5-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
5.1	5.5	Develop and document acceptance criteria for GENII 2.0.	One FTE week	One month

4.4 Topical Area 4 Assessment: Design Phase

This area corresponds to the requirement entitled *Design Phase* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.4.1 Criterion Specification and Result

This topical area is "graded" for GENII 1.485 and "required" for GENII 2.0. Table 4.4-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.4-1 — Subset of Criteria for Design Phase Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
4.1	The software design was developed, documented, reviewed, and controlled.	Yes for both	1.485: Napier (1988a) provides System Requirements as well as software design. 2.0: Napier (2002b) is the System Design Document
4.2	Code developer(s) prescribed and documented the design activities to the level of detail necessary to permit the design process to be carried out and to permit verification that the design met requirements.	Yes for both	1.485: Napier (1988a) provides System Requirements as well as software design activities. 2.0: Napier (2002b) is the System Design Document. Pseudo-code listings provided.
4.3	Design presents and documents specification of interfaces, overall structure (control and data flow) and the reduction of the overall structure into physical solutions (algorithms, equations, control logic, and data structures).	Yes for both	1.485: Napier (1988a, b, c) document overall structure, interfaces, control and data flow, and physical solutions. 2.0: Napier (1995, 2002b) document overall structure, interfaces, control and data flow, and physical solutions. Pseudo-code listings are provided. For both, diagrams show the flow of data and logic.

Criterion Number	Criterion Specification	Met?	Summary Remarks
4.4	Design presents and documents that computer programs were designed as an integral part of an overall system. Therefore, evidence should be present that the software design considered the computer program's operating environment.	Yes for both	1.485: Napier (1988ab,c) show that the overall system design accounted for hardware and software interfaces and limitations, including the O/S. 2.0: Napier (1,995, 2002b) provides similar features.
4.5	Design presents and documents that as an integral part of software design, problems are mitigated. These potential problems include external and internal abnormal conditions and events that can affect the computer program.	Yes for 1.485. Partial for 2.0.	1.485: Napier (1988b) provides error-reporting forms to testers and users so that errors can be fixed and users informed. 2.0: the error-reporting is less formal
4.6	A Software Design Document, or equivalent, is available and contains a description of the major components of the software design as they relate to the software requirements.	Yes for both	1.485: Napier (1988a) describes major components of design 2.0: Napier (2002b) is the System Design Document. Pseudo-code listings are provided.
4.7	A Software Design Document, or equivalent, is available and contains a technical description of the software with respect to the theoretical basis, mathematical model, control flow, data flow, control logic, data structure, numerical methods, physical models, process flow, process structures, and applicable relationship between data structure and process standards.	Yes for both	1.485: Napier (1988a) provides the theoretical basis, control logic and flow, data flow and structure, mathematical models, process flow and structure, physical models, and coupling between structure and standards. 2.0: Napier (2002b) provides similar information. Pseudo-code listings are provided.
4.8	A Software Design Document, or equivalent, is available and contains a description of the allowable or prescribed ranges for inputs and outputs.	Yes for both	1.485: Napier (1988a) discusses ranges of input variables and error message generated when out of range. 2.0: Napier (2002b) provides similar information.
4.9	A Software Design Document, or equivalent, is available and contains the design described in a manner that can be translated into code.	Yes for both	1.485: Napier (1988a) and its appendix provide enough detail that the design can be translated into code 2.0: Napier (2002b) provides similar information. Pseudo-

Criterion Number	Criterion Specification	Met?	Summary Remarks
			code listings are provided.
4.10	A Software Design Document, or equivalent, is available and contains a description of the approach to be taken for intended test activities based on the requirements and design that specify the hardware and software configuration to be used during test execution.	Yes for both	1.485: Napier (1988a, b, c) discuss testing and the H/W and S/W configurations 2.0: Napier (1995, 2002b) provides similar information.
4.11	The organization responsible for the design identified and documented the particular verification methods to be used and assured that an Independent Review was performed and documented. This review evaluated the technical adequacy of the design approach; assured internal completeness, consistency, clarity, and correctness of the software design; and verified that the software design is traceable to the requirements.	Yes for 1.495. No for 2.0	1.485: Napier (1988a, b, c) states that the code has been thoroughly tested and verified by independent reviewers according to NQA-1 standards. 2.0: Because this code has not been completed in all its aspects, the final testing has not yet been done.
4.12	The organization responsible for the design assured that the test results adequately demonstrated the requirements were met.	Yes for 1.495. No for 2.0	1.485: Napier (1988a, b, c) states that the code has been thoroughly tested and verified by independent reviewers according to NQA-1 standards. 2.0: Because this code has not been completed in all its aspects, the final testing has not yet been done.
4.13	The Independent Review was performed by competent individual(s) other than those who developed and documented the original design, but who may have been from the same organization.	Yes for 1.495. No for 2.0	1.485: Napier (1988a, b, c) states that the code has been thoroughly tested and verified by independent reviewers according to NQA-1 standards. This includes review by competent, independent individuals. 2.0: Because this code has not been completed in all its aspects, the final testing has not yet been done.

Criterion Number	Criterion Specification	Met?	Summary Remarks
4.14	The results of the Independent Review are documented with the identification of the verifier indicated.	Yes for 1.495. No for 2.0	1.485: The independent reviewers are identified by name in the Acknowledgements section of Napier (1988a,b) 2.0: Because this code has not been completed in all its aspects, the final testing has not yet been done.
4.15	If review alone was not adequate to determine if requirements are met, alternate calculations were used, or tests were developed and integrated into the appropriate activities of the software development cycle.	N/A	N/A
4.16	Software design documentation was completed prior to finalizing the Independent Review.	Yes for both	1.485: Napier (1988a) states that the code has been thoroughly tested and verified by independent reviewers according to NQA-1 standards. This includes completion of S/W design prior to finalizing independent review. 2.0: Napier (2002b), the design document, has been completed. The final independent review has not yet occurred.
4.17	The extent of the Independent Review and the methods chosen are shown to be a function of the following: The importance to safety The complexity of the software The degree of standardization The similarity with previously proven software	N/A	These issues are decided by the independent reviewers, not the code developers. Therefore they are not specifically addressed in the documentation of either version GENII.

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

Criterion 4.1 — The Napier (1988a) appendix, *Hanford Environmental Dosimetry Upgrade Project (HEDUP) Task 02 - System Design Requirements*, is the complete SQA requirements document for GENII 1.485. It includes the following:

1. General computational requirements
2. Computational facilities, hardware, and databases
3. Code language
4. Coding Standard and coding standard tools
5. Input parameters and format:
   - Release category and source term
   - Scenarios
   - Meteorology
   - Environmental transport
   - Exposure pathways
6. Dosimetry specifications
7. Risk assessment calculations
8. Integration of separate codes
9. Customized pathway requirements
10. Specialized scenario requirements
11. Output format
12. Graphics
13. Documentation and instructions
14. Error messages
15. Updates and revisions
16. Security
17. Quality assurance
18. Training

Napier (2002b) is the System Design Document for GENII 2.0. It defines details of the overall structure of the software, the major software components, their data file interfaces, and specific mathematical models to be used. The design represents a translation of the requirements (Napier, 1995) into a description of the software structure, software components, interfaces, and necessary data. The design focuses on the major components and data communication links that are key to the implementation of the software within the operating framework.

Criterion 4.5 — The error reporting forms for GENII 1.485 (see Figure 4-1) provided a formal method of problem mitigation. A similar methodology does not exist for GENII 2.0.

Criterion 4.10 — The hardware requirements for GENII 1.485 are an IBM PC/AT or compatible computer, an 80287 math coprocessor, 640 KB of random access memory, a minimum of 5 MB on-line disk storage, and operating under DOS 3.1 or later (Napier, 1988b). Hardware requirements for GENII 2.0 are Windows® 95, 98, NT, or 2000[4], using Pentium processors, and disk storage in excess of 60 MB. FRAMES and GENII make use of the memory swapping capabilities of Windows, so the programs should run on any Windows-compatible computer. However, they will generally run fastest on machines with 256Mbytes of memory or more (Napier, 2002a). GENII 2.0 will not run in the DOS environment.

[4] The documentation from which this sentence was extracted (Napier, 2002a) was written before the advent of Windows XP. Experience shows that GENII 2.0 also runs under Windows XP.

Criterion 4.13 — GENII 1.485 has already been thoroughly reviewed and tested and there are no plans to pursue these issues again. GENII 2.0 has been reviewed at PNNL and several EPA clients, and it went through an advisory review with the EPA Science Advisory Board. This board suggested some additional capabilities that have not yet been implemented. The code author developed the code as general-purpose software and "importance to safety" was not an issue in its development. Standardization was an important consideration and was a direct response to the issue of testability and complexity of the older version. GENII 2.0 is very similar to 1.485 but it is not the same and is intended for a different set of users.

In summary, the GENII 1.485 User's Guide (Napier, 1988b), p 5.1, states: "The design process consisted of developing and internally testing software, developing test cases, and documenting software in accordance with the design input. The GENII package has been extensively tested and verified by hand, using the hand calculation worksheets of (the Code Maintenance Manual) and benchmarked against similar Hanford environmental dosimetry programs. A 10-volume set of test documentation is available for review from the authors upon request. The design process concluded with analysis of the final design by means of a Final Internal Development Review (FIDR). Two external peer reviews were held, as described in (the Conceptual Representation volume); these constitute the FIDR for the GENII package."

4.4.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Design," except for Item 12 (see Appendix B), and several e-mail communications with the code developer (Bruce Napier) have helped to clarify issues.

4.4.3 Software Quality-Related Issues or Concerns

There are no additional SQA related issues or concerns in "Design."

4.4.4 Other Areas for Improvement

No other areas of improvement have been identified.

4.4.5 Recommendations

Recommendations related to this topical area are provided in Table 4.4-2.

Table 4.4-2 — Recommendations for Design Phase Topic

Recommendation Number	Relates to Table 4.4-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
4.1	4.5	See recommendation 2.1 on criterion 2.6.		
4.2	4.11, 4.12, 4.13, 4.14	When GENII 2.0 is complete, a comprehensive independent review must be documented to cover all aspects of these items	Two FTE months	Four months

Additional Detail

No additional detail is needed on the above recommendations.

4.5 Topical Area 5 Assessment: Implementation Phase

This area corresponds to the requirement entitled *Implementation Phase* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.5.1 Criterion Specification and Result

This topical area is "graded" for GENII 1.485 and "required" for GENII 2.0. Table 4.5-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.5-1 — Subset of Criteria for Implementation Phase Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
5.1	The implementation process resulted in software products such as computer program listings and instructions for computer program use.	Yes for 1.485. Partial for 2.0	1.485: Napier (1988c) is the code maintenance manual, containing listings of all source code. Napier (1988b) is the user's manual. 2.0: Napier (2002a) is the user's guide. Program listings are not yet published.
5.2	Implemented software was analyzed to identify and correct errors.	Yes for 1.485. Partial for 2.0.	1.485: an error reporting and corrective action process was used during development. 2.0: used an informal error reporting process

Criterion Number	Criterion Specification	Met?	Summary Remarks
5.3	The source code finalized during verification (this phase) was placed under configuration control.	Yes for 1.485. No for 2.0.	1.485: Configuration control was in place during code development. Current configuration control is provided through RSICC, the distributor of the code, who will not release revised code unless tested and verified. 2.0: code is not yet finalized
5.4	Documentation during verification included a copy of the software, test case description, and associated criteria that are traceable to the software requirements and design documentation.	Yes for both	Although the documentation reviewed (Table 1-2) does not specifically address the items provided to the testers, the code author affirms that these items were given to them.

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

Criterion 5.1 — GENII 2.0 has not been finalized. Code listings should become available after completion and final testing of code.

Criterion 5.2 — See recommendation 2.1 (on Criterion 2.6) for a discussion of this.

Criterion 5.3 — The appendix to Napier (1988a), the system design document, states: "Configuration control shall be a feature of the software to protect the basic code from unauthorized changes. A control mechanism with sign-off procedures shall be implemented to protect the software from unauthorized modifications. Needed changes shall be validated before modification are permitted." Bruce Napier is the current custodian of GENII 1.485 although at times past others had been assigned this duty. The code is distributed through RSICC at Oak Ridge, TN. Together, they provide the current configuration control.

Criterion 5.4 — The code author (Bruce Napier) states (e-mail in Appendix A): "The test cases were generally designed to meet the needs of certain types of calculation, and were done first on the computer (using the code and documentation to run) and then again on the GENII-specific hand calculation worksheets. The criteria were that the numbers had to match to two significant figures (which is all that the GENII code transfers internally at certain steps)."

4.5.2 Sources and Method of Review

E-mails with the code author addressed some of these issues. In addition, all of the documentation listed in Table 1-2 was reviewed with attention to "Implementation," except for Item 12 (see Appendix B).

4.5.3 Software Quality-Related Issues or Concerns

There are no other SQA-related issues or concerns in "Implementation Phase."

4.5.4 Other Areas for Improvement

No other areas for improvement have been identified.

4.5.5 Recommendations

Recommendations related to this topical area are provide in Table 4.5-2.

Table 4.5-2 — Recommendations for Implementation Phase Topic

Recom-mendation Number	Relates to Table 4.5-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
5.1	5.1	Make GENII 2.0 code listings available upon completion and final testing of code.	One FTE week	One month

4.6 Topical Area 6 Assessment: Testing Phase

This area corresponds to the requirement entitled *Testing Phase* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.6.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.6-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.6-1 — Subset of Criteria for Testing Phase Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
6.1	The software was validated by executing test cases.	Yes for 1.485. No for 2.0.	1.485: code was validated by being thoroughly tested (Napier, 1988a, 1988b) 2.0: code not yet completed, so testing is not complete
6.2	Testing demonstrated the capability of the software to produce valid results for test cases encompassing the range of permitted usage defined by the program documentation. Such activities provide evidence to ensure that the software adequately and correctly performed all intended functions and does not perform adverse unintended functions.	Yes for 1.485. No for 2.0.	1.485: code was thoroughly tested (Napier, 1988a, 1988b) 2.0: code not yet completed, so testing is not complete
6.3	Testing demonstrated that the computer program properly handles abnormal conditions and events as well as credible failures appropriate warning or error messages are provided to the user when the code is used improperly (e.g., an input is specified outside acceptable range).	Yes for 1.485. No for 2.0.	1.485: code was thoroughly tested (Napier, 1988a, 1988b) 2.0: code not yet completed, so testing is not complete
6.4	Test Phase documentation includes test procedures or plans and the results of the execution of test cases. The test results documentation demonstrates successful completion of all test cases or the resolution of unsuccessful test cases and provides direct traceability between the test results and specified software requirements.	Yes for 1.485. No for 2.0.	1.485: code was thoroughly tested (Napier, 1988a, 1988b) 2.0: code not yet completed, so testing is not complete

Criterion Number	Criterion Specification	Met?	Summary Remarks
6.5	Test procedures or plans specify the following, as applicable:	Yes for 1.485.	1.485: code was thoroughly tested (Napier, 1988a, 1988b)

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

Criteria 6.1 – 6.5 — Napier (1988b) states that there is a ten-volume set of test documentation available for inspection by interested parties. These documents are not included in those reviewed here, as they are at the offices at PNNL. The GENII 2.0 User's Guide (Napier, 2002a), in reference to Version 1.485, states: "GENII Version 1 has been included in the International Atomic Energy Agency's VAMP project (VAlidation of Model Predictions - an acronym for the Coordinated Research Program on Validation of Models for the Transfer of Radionuclides in Terrestrial, Urban and Aquatic Environments), an international effort to compare environmental radionuclide transport models with measured environmental data. Results for test scenario CB (based on environmental measurements following the Chernobyl accident) indicated that dose estimates from GENII were comparable to, although slightly higher than, those of other participating models, which is consistent with its primary function as a prospective analysis tool. The models included in the code have been validated to various degrees by additional studies, however these have not been compared directly to output from the code."

4.6.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Testing Phase," except for Item 12 (see Appendix B).

4.6.3 Software Quality-Related Issues or Concerns

There are no other SQA-related issues or concerns in "Testing Phase."

4.6.4 Other Areas for Improvement

No other areas of improvement in the "Testing Phase" have been identified.

4.6.5 Recommendations

Recommendations related to this topical area are provide in Table 4.6-2.

Table 4.6-2 — Recommendations for Testing Phase Topic

Recom-mendation Number	Relates to Table 4.6-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
6.1	All	Document all testing of GENII 2.0.	Three FTE months	Six months

4.7 Topical Area 7 Assessment: User Instructions

This area corresponds to the requirement entitled *User Instructions* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.7.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.7-1 lists the subset of criteria reviewed for this topical area and summarizes the findings. Both versions of GENII are addressed (i.e., Versions 1.485 and 2.0).

Table 4.7-1 — Subset of Criteria for User Instructions Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
7.1	A description of the model is documented and made available to users.	Yes for both	1.485: Napier, 1988a 2.0: Napier, 2002b
7.2	User's manual or guide describes software and hardware limitations and identifies/includes approved operating	Yes for both	1.485: Napier, 1988b 2.0: Napier, 2002a Lahey Fortran-77 or F-99

Criterion Number	Criterion Specification	Met?	Summary Remarks
	systems (for cases where source code is provided, applicable compilers should be noted).		compiler used. Source code in: 1.485: Napier, 1988c 2.0: not provided
7.3	User's manual or guide includes description of the user's interaction with the software.	Yes for both	1.485: Napier, 1988b 2.0: Napier, 2002a and 2003
7.4	User's manual or guide includes a description of any required training necessary to use the software.	Yes for 1.485. No for 2.0.	1.485: A required training course is described in the system requirements document, not the user's manual. 2.0: Training is available (e.g., at EFCOG meetings) but it is not described in the User's Manual.
7.5	User's manual or guide includes input and output specifications.	Yes for both	1.485: Napier, 1988b 2.0: Napier, 2002a
7.6	User's manual or guide includes a description of user messages initiated because of improper input and how the user can respond.	Yes for both	1.485: Napier, 1988b 2.0: Napier, 2002a
7.7	User's manual or guide includes information for obtaining user and maintenance support.	Yes for 1.485. Partial for 2.0.	1.485: Readme.93 file on Distribution Disk 03 2.0: Napier, 2002a

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

Criterion 7.2 — Both versions of GENII were written and compiled using the Lahey Fortran (F-77 or F-99) software, except for the user interface of GENII 1.485 (Apprentice), which was written using Microsoft QuickBasic. Source code for GENII 1.485 is given in Volume 3 of PNL-6584, *Code Maintenance Manual* (Napier, 1988c). It is also can be found on Distribution Disk02 by double clicking on SOURCE.EXE, which will unpack all the routines, both those in Fortran and those in QuickBasic. Source code is not provided for GENII 2.0.

Criterion 7.4 — The appendix to Napier (1988a), the system requirements document, p A.15, states: "A short training program shall be developed at the completion of the code to instruct potential users on the execution of the code. A detailed stepwise instruction manual shall also be prepared. Training should consist of class sessions and hand-out instructions, with opportunity for hands-on testing of the code." This training was provided on GENII 1.485 after it was released but such training is no longer available. Training for GENII 2.0 has been available at annual EFCOG meetings but there is no guarantee this will continue. Training would be useful for GENII (either version). The

intuitive nature of the user interface and the documentation (e.g., Napier, 1988b, 2002a, 2003) is helpful but not enough for a first-time user.

Criterion 7.6 — In GENII 1.485, user input is primarily through the Apprentice program, which prompts the user for input and requires incorrect or incompatible entries to be corrected. Appendix B of the GENII 1.485 User's Manual (Napier, 1988b) gives an extensive discussion of error handling within GENII, not just that of Apprentice. For GENII 2.0, the FRAMES user interface provides error messages when input is incomplete, out of bounds, or conflicting. However, the current version has bugs. For example, it is possible to be trapped in an unending loop of error messages.

Criterion 7.7 — The GENII 1.485 User's Manual gives the names of the authors of GENII but not the contact information. The primary contact person is the lead author of the code, Bruce Napier (509-375-3916). In addition, RSICC has provided a "Readme" file with the name and telephone number of a very knowledgeable user of the code (Paul D. Rittman - 509-376-8715), who can also be contacted in case of problems. For GENII 2.0, the FRAMES Constituent Database user interface gives the contact information for the lead author of GENII (Bruce Napier).

4.7.2 Sources and Method of Review

The user's manual for GENII 1.485, *GENII – The Hanford Environmental Radiation Dosimetry Software System. Volume 2: User's Manual* (Napier, 1988b), was reviewed for this Gap Analysis. Section 2 of that document gives the code overview, including user interaction levels and data file descriptions. Section 3 gives specific user instructions for both user interaction levels 0 and 1. Section 4 discusses system requirements and Section 5 discusses quality assurance topics. Appendix A gives an input/output example and Appendix B gives an extensive discussion of error messages. A revision to some of the data files for GENII 1.485 was issued in 1993 and another in 1996, but these did not change the code or its usage.

The User's Guide for GENII 2.0, *GENII Version 2 User's Guide* (Napier, 2002a) and *Getting Started with GENII Version* 2 (Napier, 2003) were reviewed for this Gap Analysis. The User's Guide provides details on all the options available in GENII 2.0, whereas the Getting Started document provides an introduction useful for evaluating simple, but typical, scenarios.

Correspondence (e-mails and telephone conversations) with an expert user of GENII 2.0 and with Bruce Napier has also been reviewed. These are included as Appendix A of this document. The expert user of GENII 2.0 was identified by Bruce Napier as William Joyce[5], in whose opinion GENII 2.0 should not be used for DSAs. This was supported to some extent by the e-mails from Napier (see Appendix A).

[5] Mr. Joyce is a Senior Safety Engineer with ATL International, Corp., 20010 Century Blvd, Suite 500, Germantown, MD 20874.

4.7.3 Software Quality-Related Issues or Concerns

An item not discussed in the documentation is memory management. GENII 1.485 was developed in the DOS environment and was expected to be run in that environment. Experience shows that it can be run in a DOS window in the Windows environment[6]. However, this has potential problems in that memory management is different between DOS and Windows and there is a possibility of problems arising in the Windows environment. This needs to be verified by an extensive comparison of results using an older computer that is DOS based with a newer computer that is Windows based.

The bug in error handling of GENII 2.0 (see Criterion 9.6) needs to be fixed.

4.7.4 Other Areas for Improvement

The GENII 2.0 user guidance (Napier, 2002b, 2003) doesn't always match the operations the user needs to perform. For example, in a number of cases, the instructions say to right-click a button whereas the correct procedure is a left-click. In addition, some of the screens the user sees are not in the same order given in the guidance.

GENII 1.485 can determine 95th percentile consequences in only one direction (sector) at a time. It would be very helpful to the analyst for GENII 1.485 to automatically determine the 95th percentile consequences in every sector at the site boundary and other user-selected distance (such as 100 m). This can be done now only by setting up multiple runs of GENII 1.485. GENII 2.0 cannot determine 95th percentile consequences except perhaps in a manner involving a random sampling of the weather and compiling statistics that would yield 95th percentile values. However, this has not yet been tested.

4.7.5 Recommendations

Recommendations related to this topical area are provide in Table 4.7-2.

[6] The Radiation Safety Information Computational Center (RSICC) at Oak Ridge verified the performance of GENII 1.485 on a 486 PC under the MS DOS 6.2 and Windows 95 operating systems. Testing conducted during the preparation of this Gap Analysis shows that GENII 1.485 also can be executed in Windows 98SE and XP.

Table 4.7-2 — Recommendations for User Instructions Topic

Recommendation Number	Relates to Table 4.7-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
7.1	Criterion 7.2	Verify that GENII 1.485 runs correctly in a Windows environment (including XP)	One workday	One workday
7.2	Criterion 7.5	Correct the user guidance for GENII 2.0.	One FTE week	Two weeks
7.3	Criterion 7.6	The error message-handling problem needs to be fixed.	One FTE week	Two weeks

Additional Detail

Recommendation 7.1 – The estimate of one workday is for the comparison testing, which would consist of running the same scenarios side by side on DOS-based and Window-based computers. Should differences in results be found, use of GENII 1.485 would have to be restricted to only DOS-based computers.

4.8 Topical Area 8 Assessment: Acceptance Test

This area corresponds to the requirement entitled *Acceptance Test* Table 3-2 of the DOE SQA plan (DOE 2003e). During this phase of the software development, the software becomes part of a system incorporating applicable software components, hardware, and data, and is accepted for use. Much of this testing is the burden of the user organization, but the developing organization shoulders some responsibility.

4.8.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.8-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.8-1 — Subset of Criteria for Acceptance Test Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
8.1	To the extent applicable to the developer, acceptance testing includes a comprehensive test in the operating environment(s).	Yes for 1.485. No for 2.0.	1.485: Napier (1988b) states that the code was tested on PCs from many manufacturers. 2.0: acceptance testing is not yet complete but Napier (2002a) states but the test plan has been developed and testing underway
8.2	To the extent applicable to the developer, acceptance testing was performed prior to approval of the computer program for use.	Yes for 1.485. No for 2.0.	1.485: the code delivered to RSICC for distribution had been tested prior to release. 2.0: acceptance testing is not yet complete
8.3	The acceptance testing comprehensively evaluates software performance against specified software requirements. To the extent applicable to the developer, software validation was performed to ensure that the installed software product satisfies the specified software requirements.	Yes for 1.485. No for 2.0.	Both codes were developed under NQA-1 guidelines. This includes testing against software requirements. 1.485: acceptance testing complete and code in use. 2.0: acceptance testing is not yet complete
8.4	Acceptance testing documentation includes results of the execution of test cases for system installation and integration, user instructions (Refer to Requirement 7 above), and documentation of the acceptance of the software for operational use.	Yes for 1.485. No for 2.0.	1.485: extensive test documentation is available on all aspects of code development 2.0: acceptance testing is not yet complete

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

> Criterion 8.1 — The GENII 1.485 User's Manual (Napier, 1988b), p 4.1, states: "Portions of the GENII Software Package have been tested on a number of IBM-PC/AT compatible machines. Versions of GENII have been established on microcomputers manufactured by GRID, NEC, Hewlett-Packard, and IBM. The IBM machines have included the new PS/2 System 50 and System 80. No machine-based incompatibilities have been found." The GENII 2.0 User Guide (Napier, 2002a), p 6, states: "A comprehensive test plan has been developed and testing is underway."

Criterion 8.2 — The preface to the RSICC distribution package of GENII 1.485 states that the authors of the code affirm that the code was tested prior to submission to RSICC for distribution to users.

Criterion 8.3 — The GENII 2.0 User Guide (Napier, 2002a), pp 5-6 states: "Both GENII versions were developed under QA plans based on the American National Standards Institute (ANSI) standard NQA-1 as implemented in the PNNL Quality Assurance Manual. All steps of the code development have been documented and tested, and hand calculations have verified the code's implementation of major transport and exposure pathways for a subset of the radionuclide library. A collection of hand calculations and other verification activities is available. A comprehensive test plan has been developed and testing is underway." The latter sentence refers to GENII 2.0, not 1.485.

Criterion 8.4 — Napier (1988b) states that there is a ten-volume set of test documentation available for inspection by interested parties.

4.8.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Acceptance Test," except for Item 12 (see Appendix B). The list in Appendix B includes a summary of developer/user testing and peer review of GENII for which documentation is available.

4.8.3 Software Quality-Related Issues or Concerns

There are no other SQA-related issues or concerns in "Acceptance Test."

4.8.4 Other Areas for Improvement

No other areas of improvement have been identified.

4.8.5 Recommendations

Recommendations related to this topical area are provide in Table 4.8-2.

Table 4.8-2 — Recommendations for Acceptance Test Topic

Recom-mendation Number	Relates to Table 4.8-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
8.1	All	Complete the documentation of acceptance testing for GENII 2.0	Two FTE months	Four months

4.9 Topical Area 9 Assessment: Configuration Control

This area corresponds to the requirement entitled *Configuration Control* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.9.1 Criterion Specification and Result

This topical area is "required" for both GENII 1.485 and 2.0. Table 4.9-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.9-1 — Subset of Criteria for Configuration Control Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
9.1	For the developers, the methods used to control, uniquely identify, describe, and document the configuration of each version or update of a computer program (for example, source, object, and back-up files) and its related documentation (for example, software design requirements, instructions for computer program use, test plans, and results) are described in implementing procedures.	Yes for both	1.485: Configuration control followed PNO-MA-70, the PNL version of the NQA-1 Quality Assurance Manual that existed during development. In addition, a series of "software change packets" have been maintained. 2.0: Formal procedures for configuration control follow the current PNNL "Software Based Management System" (SBMS). Notebooks and backups are also used for this purpose. (See Appendix A.)
9.2	Implementing procedures meet applicable criteria for configuration identification, change control, and configuration status accounting.	Yes for both	See the comments above, for Criterion 9.1.

Additional Detail

The following provides additional detailed explanation on selected criteria in the above table:

> Criteria 9.1 and 9.2 — Configuration control followed/follows procedures formalized in SQA methods used at PNL/PNNL during the development of each version of GENII. These procedures have evolved over the years, and thus, the procedures used for Version 2.0 are not identical to those used for Version 1.485. The author of the code(s) has kept informal notebooks and copies of earlier versions.

4.9.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Configuration Control," except for Item 12 (see Appendix B), as well as e-mails with the code developer.

4.9.3 Software Quality-Related Issues or Concerns

There are no SQA-related issues or concerns in "Configuration Control."

4.9.4 Other Areas for Improvement

No additional areas of improvement in "Configuration Control" have been identified.

4.9.5 Recommendations

There are no recommendations related to this topical area.

4.10 Topical Area 10 Assessment: Error Impact

This area corresponds to the requirement entitled *Error Impact* in Table 3-2 of the DOE SQA plan (DOE 2003e).

4.10.1 Criterion Specification and Result

This topical area is "graded" for both GENII 1.485 and 2.0. Table 4.10-1 lists the subset of criteria reviewed for this topical area and summarizes the findings.

Table 4.10-1 — Subset of Criteria for Error Impact Topic and Results

Criterion Number	Criterion Specification	Met?	Summary Remarks
10.1	The developing organization's problem reporting and corrective action process addresses the appropriate requirements of its corrective action system and is documented in implementing procedures.	Yes for 1.485. No for 2.0	Napier (1988b) discusses how to report errors and request upgrades. An informal method is used for GENII 2.0. See criterion 2.6.
10.2	The process for evaluating, and documenting whether a reported problem is an error is documented and implemented.	No for both	Not specifically discussed in the documentation reviewed. However, the SQA procedures followed during development

Criterion Number	Criterion Specification	Met?	Summary Remarks
			(see criterion 9.1) do require problem reporting and documenting.
10.3	The process for disposition of the problem reports, including notification to the originator of the results of the evaluation, is documented and implemented.	No for both	Not specifically discussed in the documentation reviewed. However, the SQA procedures followed during development (see Criterion 12.1) do require proper disposition of problem reports.
10.4	A documented process provides guidance on determining how identified errors relate to appropriate software engineering elements and is implemented.	No for both	Not discussed in the documentation reviewed.
10.5	The process is documented and implemented for determining how an error impacts past and present use of the computer program.	No for both	Not discussed in the documentation reviewed.
10.6	The process is documented and implemented for determining how an error and resulting corrective action impacts previous development activities.	No for both	Not discussed in the documentation reviewed.
10.7	The process is documented and implemented describing how the users are notified of an identified error, its impact; and how to avoid the error, pending implementation of corrective actions.	No for both	Not discussed in the documentation reviewed.

4.10.2 Sources and Method of Review

All of the documentation listed in Table 1-2 has been reviewed with attention to "Error Impact," except for Item 12 (see Appendix B).

4.10.3 Software Quality-Related Issues or Concerns

For users of GENII 2.0 within PNNL, the existing Standards Based Management System (SBMS) process can be followed. There would be no software quality-related issues or concerns for these users. However, for users outside of PNNL, the process of error notification and corrective action needs to be formalized and documented so that users know how to report errors,

how PNNL will respond, how PNNL will notify other users of the problem, and how too avoid the problem.

4.10.4 Other Areas for Improvement

No other areas of improvement are noted.

4.10.5 Recommendations

Recommendations related to this topical area are provide in Table 4.10-2.

Table 4.10-2 — Recommendations for Error Impact Topic

Recom-mendation Number	Relates to Table 4.13-1 Criterion Number(s)	Recommendation	Est. FTE to Complete	Est. Calendar Duration
10.1	All	A formal error reporting and corrective action process needs to be implemented for GENII 1.485 and GENII 2.0 for users outside of PNNL.	One FTE month	Two months

4.11 Training Program Assessment

No regularly scheduled GENII training program is conducted. Training materials for Version 1.485 of GENII are still available, but there have been no requests made to the author (Bruce Napier) to use these for several years.

There have been discussions with the EPA about training on Version 2, and the author has given some Version 2.0 training at recent EPA NESHAPS meetings (held annually). Future training may be provided to the NRC headquarters staff. However, the latter is still in the planning stage.

The last known training to DOE safety analysis community occurred during the 2000 Energy Facility Contractors Group (EFCOG) Safety Analysis Working Group Workshop (April 2000). It is recommended that this forum be explored to provide DOE users with a regular opportunity for GENII training.

5.0 Conclusion

The GENII code gap analysis has been completed. For GENII 1.485, of the ten applicable topical quality areas for software developers, nine met the criteria fully, and one failed to meet the criteria. GENII 1.485 should create and follow a formal error reporting and corrective action process. For GENII 2.0, of the same ten general topical quality areas, two met the criteria fully, five met the criteria partially, and three failed to meet the criteria.

Recommendations are given for each of the topical areas in Section 4.0. It is estimated that approximately ten full-time equivalent (FTE) months would be required to perform all SQA upgrade tasks covered in Section 4.0. Because GENII 1.485 has been in use for many years and the code developer does not intend to make any further modifications, no similar estimates need be made. The error-reporting estimate for GENII 2.0 may be applied to GENII 1.485. It would be useful for personnel at RSICC to respond to Recommendation 7.1 regarding running the code in the DOS and Windows environments. This is estimated to require only about one day. The GENII 1.485 documentation would not need to be changed but documentation of the results could be included with the RSICC distribution package for GENII 1.485.

Training opportunities exist for both versions of GENII, but these are not routinely offered. It is recommended that training at the annual EFCOG Safety Analysis Working Group Workshop be offered to familiarize DOE and DOE contractor personnel on the GENII software and applications.

The GENII code was evaluated to determine if the code, as it currently stands, meets the intended function for the code in the context as described in the scope of this gap analysis. When the code is run for the intended applications, as detailed in the code guidance document, *Computer Code Application Guidance for Documented Safety Analysis*, (DOE 2003f), it is judged that GENII 1.485 will meet its intended function, but GENII 2.0 will not. Therefore, only GENII 1.485 can be recommended for DSA use at this time.

While completion of the GENII 2.0 development is encouraged, current DOE DSA support should be through the earlier code version, GENII 1.485. No evidence was found of software-induced errors in GENII 1.485 that have led to non-conservatisms in nuclear facility operations or in the identification of facility controls.

6.0 Acronyms and Definitions

ACRONYMS

ANS	American Nuclear Society
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
CD	Compliance Decision
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CSARP	Cooperative Severe Accident Research Program
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
IEEE	Institute of Electrical and Electronics Engineers
INEL	Idaho National Engineering Laboratory
IP	Implementation Plan
ISO	International Organization for Standardization
LPF	Leak Path Factor
MCAP	MELCOR Code Applications Program
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (code)
NRC	Nuclear Regulatory Commission
QAP	Quality Assurance Program (alternatively, Plan)
RSICC	Radiation Safety Information Computational Center
SNL	Sandia National Laboratories
SQA	Software Quality Assurance
SRS	Savannah River Site
V&V	Verification and Validation
WSRC	Westinghouse Savannah River Company

DEFINITIONS

The following definitions are taken from the Implementation Plan. References in brackets following definitions indicate the original source, not the Implementation Plan.

Acceptance Testing	The process of exercising or evaluating a system or system component by manual or automated means to ensure that it satisfies the specified requirements and to identify differences between expected and actual results in the operating environment. [NQA-1]
Central Registry	An organization designated to be responsible for the storage, control, and long-term maintenance of the Department's safety analysis "toolbox codes." The central registry may also perform this function for other codes if the Department determines that this is appropriate.
Classification (Level of Software)	Determination of the level of SQA associated with a computer code commensurate with the importance of the software application. For the toolbox codes, classification level is determined as described in Appendix A of: "Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes."
Commercial Grade Item	An item satisfying a), b), and c) below: (a) Not subject to design or specification requirements that are unique to nuclear facilities. (b) Used in applications other than nuclear facilities. (c) Ordered from the manufacturer/supplier on the basis of specifications set forth in the manufacturer's published product description (for example, catalog). [IEEE Std. 7-4.3.2-1993]
Computer Code	A set of instructions that can be interpreted and acted upon by a programmable digital computer (also referred to as a module or a computer program).
Configuration Item	A collection of hardware or software elements treated as a unit for the purpose of configuration control. [NQA-1]
Configuration Management	The process that controls the activities, and interfaces, among design, construction, procurement, training, licensing, operations, and maintenance to ensure that the configuration of the facility is established, approved and maintained. (Software specific): The process of identifying and defining the configuration items in a system (i.e., software and hardware), controlling the release and change of these items throughout the system's life cycle, and recording and reporting the status of configuration items and change requests. [NQA-1]
Control Point	A point in the software life cycle at which specified agreements or control (typically a test or review) are applied to the software configuration items being developed, e.g., an approved baseline or release of a specified document or computer program. [NQA-1]
Commercial Grade Dedication	A process of evaluating (which includes testing) and accepting commercial grade items to obtain adequate confidence of their

	suitability for safety application. [IEEE Std. 7-4.3.2-1993]
Data Library	A data file for use with an executable code that is created and maintained by the controlling organization and is not intended for modification by the user.
Dedication (of Software)	The evaluation of software not developed under utilizing organization existing quality assurance plans and procedures (or not developed under NQA-1 standards). The evaluation determines and asserts the software's compliance with NQA-1 quality standards and its readiness for use in specific applications. (Typically applies to commercially available software.) The utilizing organization reviews the intended software application sufficiently to determine the critical functions that provide evidence of the software's suitability for use. Once the critical functions have been established, methods are defined to verify critical function adequacy and provide verifiable acceptance criteria. Acceptable dedication methods are implemented and required documentation is prepared.
Design Requirements	Description of the methodology, assumptions, functional requirements, and technical requirements for a software system.
Discrepancy	The failure of software to perform according to its documentation.
Error	A condition deviating from an established base line, including deviations from the current approved computer program and its baseline requirements. [NQA-1]
Executable Code	The user form of a computer code. For programs written in a compilable programming language, the compiled and loaded program. For programs written in an interpretable programming language, the source code.
Firmware	The combination of a hardware device and computer instructions and data that reside as read-only software on that device. [IEEE Standard 610.12-1990]
Gap Analysis	Evaluation of the SQA attributes of specific computer software against identified criteria.
Independent Verification and Validation (IV&V)	Verification and validation performed by an organization that is technically, managerially, and financially independent of the development organization.
Nuclear Facility	A reactor or a nonreactor nuclear facility where an activity is conducted for, or on behalf of, DOE and includes any related area, structure, facility, or activity to the extent necessary to ensure proper implementation of the requirements established by 10 CFR 830. [10 CFR 830]
Object Code	A computer code in its compiled form. This applies only to programs written in a compilable programming language.
Operating Environment	A collection of software, firmware, and hardware elements that provide for the execution of computer programs. [NQA-1]

Safety Analysis and Design Software	Computer software that is not part of a Structure, System, or Component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure proper accident analysis of nuclear facilities; proper analysis and design of safety SSCs; and proper identification, maintenance, and operation of safety SSCs.
Safety Analysis Software Group (SASG)	A group of technical experts formed by the Deputy Secretary in October 2000 in response to Technical Report 25 issued by the DNFSB. This group was responsible for determining if the safety analysis and Instrument and Control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment, as appropriate.
Safety-Class Structures, Systems, and Components (SC SSCs)	SSCs, including portions of process systems, whose preventive and mitigative function is necessary to limit radioactive hazardous material exposure to the public, as determined from the safety analyses. [10 CFR 830]
Safety-Significant Structures, Systems, and Components (SS SSCs)	SSCs, which are not designated as Safety-Class (SC) SSCs, but whose preventive or mitigative function is a major contributor to defense in depth and/or worker safety as determined from safety analyses. [10 CFR 830] As a general rule of thumb, Safety Significant (SS) SSC designations based on worker safety are limited to those SSCs whose failure is estimated to result in prompt worker fatalities, serious injuries, or significant radiological or chemical exposure to workers. The term, serious injuries, as used in this definition, refers to medical treatment for immediately life-threatening or permanently disabling injuries (e.g., loss of eye or loss of limb). The general rule of thumb cited above is neither an evaluation guideline nor a quantitative criterion. It represents a lower threshold of concern for which an SS SSC designation may be warranted. Estimates of worker consequences for the purpose of SS SSC designation are not intended to require detailed analytical modeling. Consideration should be based on engineering judgment of possible effects and the potential added value of SS SSC designation. [DOE G 420.1-1]
Safety Software	Includes both safety system software and safety analysis and design software.
Safety Structures, Systems, and Components (SSCs)	The set of SC SSCs and SS SSCs for a given facility. [10 CFR 830]
Safety System Software	Computer software and firmware that performs a safety system function as part of a SSC that has been functionally classified as SC or SS. This also includes computer software such as human-machine interface software, network interface software, programmable logic controller (PLC) programming language software, and safety management databases that are not part of an SSC but whose operation or malfunction can directly affect SS and SC SSC function.

Sample Input	Input data for a designated sample problem that is maintained by the controlling organization for distribution to users.
Software	Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Std. 610.12-1990]
Software Design Verification	The process of determining if the product of the software design activity fulfills the software design requirements. [NQA-1]
Software Development Cycle	The activities that begin with the decision to develop a software product and end when the software is delivered. The software development cycle typically includes the following activities: (a) Software design requirements (b) Software design (c) Implementation (d) Test And sometimes: (e) Installation. [NQA-1]
Software Engineering	The application of a systematic, disciplined, quantifiable approach to the development, operation, and maintenance of software; that is, the application of engineering to software; also: the study of these applications. [NQA-1]
Software Life Cycle	The activities that comprise the evolution of software from conception to retirement. The software life cycle typically includes the software development cycle and the activities associated with operation, maintenance, and retirement. [NQA-1]
Source Code	A computer code in its originally coded form, typically in text file format. For programs written in a compilable programming language, the uncompiled program.
System Software	Software designed to enable the operation and maintenance of a computer system and its associated computer programs. [NQA-1]
Test Case	A set of test inputs, execution conditions, and expected results developed for a particular objective, such as to exercise a particular program path or to verify compliance with a specific requirement. [NQA-1]
Test Case Input	Input data for a test case used to verify a modification to a module or a data library.
Test Plan (Procedure)	A document that describes the approach to be followed for testing a system or component. Typical contents identify the items to be tested, tasks to be performed, and responsibilities for the testing activities. [NQA-1]
Testing	An element of verification for the determination of the capability of an item to meet specified requirements by subjecting the item to a set of physical, chemical, environmental, or operating conditions. [NQA-1]

Testing (Software) The process of
(a) Operating a system (i.e., software and hardware) or system component under specified conditions.
(b) Observing and recording the results.
(c) Making an evaluation of some aspect of the system (i.e., software and hardware) or system component, in order to verify that it satisfies specified requirements and to identify errors. [NQA-1]

Toolbox Codes A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and meeting minimum qualification standards. These codes are sufficiently verified and validated, and may be said to constitute a "safe harbor" methodology. That is to say, the analysts using these codes do not need to present additional defense as to their qualification, if they are sufficiently qualified to use the codes and the input parameters are valid.

User Manual A document that presents the information necessary to employ a system or component to obtain desired results. Typically described are system or component capabilities, limitations, options, permitted inputs, expected outputs, possible error messages, and special instructions. Note: A user manual is distinguished from an operator manual when a distinction is made between those who operate a computer system (mounting tapes, etc.) and those who use the system for its intended purpose. Syn: User Guide. [IEEE 610-12]

Validation
1) The process of testing a computer program and evaluating the results to ensure compliance with specified requirements. [ANSI/ANS-10.4-1987]
2) The process of determining the degree to which a model is an accurate representation of the real-world from the perspective of the intended uses of the model. [Department of Defense Directive 5000.59, DoD Modeling and Simulation (M&S) Management]

Verification
1) The process of evaluating the products of a software development phase to provide assurance that they meet the requirements defined for them by the previous phase. [ANSI/ANS-10.4-1987]
2) The process of determining that a model implementation accurately represents the developer's conceptual description and specifications. [Department of Defense Directive 5000.59, DoD Modeling and Simulation (M&S) Management]

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Appendices

Appendix	Subject
A	COMMUNICATIONS WITH OTHERS
B	GENII BENCHMARKING AND V&V

APPENDIX A.— COMMUNICATIONS WITH OTHERS

E-mails

From: O'Kula, Kevin [mailto:Kevin.OKula@WXSMS.com]
Sent: Friday, September 19, 2003 4:42 PM
To: Joyce, William
Subject: Urgent Need for GENII Version 2 Guidance Document

William E. Joyce
Senior Safety Engineer
ATL International, Corp
20010 Century Blvd, Suite 500
Germantown, MD 20874

Mr. Joyce:

I work for Westinghouse Safety Management Solutions in Aiken, SC, and am supporting DOE in the area of SQA.

(deleted material not relevant to the gap analysis)

Bruce Napier recommended you as the most expert GENII Version 2 user he was aware of. Would you be interested in providing a rough draft of a guidance document?
...
Let me know at your earliest convenience.

Kevin O'Kula
Westinghouse Safety Management Solutions LLC
P. O. Box 5388
Aiken, SC 29804-5388
Phone: 803.502.9620
Fax: 803.502.9773
FEDX: 2131 South Centennial Avenue, Bldg. #3
Aiken, South Carolina 29803

From: O'Kula, Kevin [mailto:Kevin.OKula@WXSMS.com]
Sent: Thursday, September 25, 2003 11:19 AM
To: Napier, Bruce A
Subject: FW: Urgent Need for GENII Version 2 Guidance Document

Bruce:

I spoke at length with William yesterday.

He discussed his current work with GENII Version 2.0 for Dose Reconstruction, where he stated that the annual average conditions were being used. He strongly recommended that we not endorse it for accident analysis applications. Among other reasons, he said that the new version does not allow a 95th percentile X/Q based dose to be determined for acute (~1 hour) releases. Is this accurate?

We have seen more use of the "older" version, 1.485. For example, the ANL people are using it for the MOX EIS for both routine and accident releases. We asked them why they weren't using the new version, and they indicated that the NRC wanted them to apply 1.485. Could they have done this work for accident releases and found the 95th percentile dose with GENII Version 2.0?

Thanks,

Kevin

From: Napier, Bruce A [mailto:Bruce.Napier@pnl.gov]
Sent: Friday, September 26, 2003 6:07 AM
To: O'Kula, Kevin
Subject: HA: Urgent Need for GENII Version 2 Guidance Document

Version 2 is much different than 1.485.
We use hourly meteorology, not joint frequency data.
I have it set up for the acute release met model to start at a defined date and time. HOWEVER, the FRAMES system has a stochastic processor that wraps around all the GENII modules and allows variation in all the input parameters - and I have the date/time set up to input as Julian[7] hour. This means that I can actually run the whole thing a few thousand times, varying the start time. This has the effect of building the entire output dose distribution, not just the 95th percentile meteorology. This is a much different way of doing it than we have done before. The problem comes with the lack of completed testing - I am still quite skeptical that this is all working correctly. So I don't recommend it yet, either.

ALSO - since I never saw anybody use it, I have taken out the Winter/Spring/Summer/Fall output, and only use the Fall model. I suppose that I could put it all back in - but would you use it?

Bruce

Following a request from Jim Rhone for review of the SQA Plan and Criteria for the Safety Analysis Toolbox Codes Report, Napier sent this reply:

[7] By Julian hour, he means the number of hours since the beginning of the year, although this is not the correct use of this term.

From: Napier, Bruce A [mailto:Bruce.Napier@pnl.gov]
Sent: Tuesday, October 21, 2003 6:18 PM
To: Jim Rhone
Cc: Kevin.okula@wxsms.com; Eng, Tony
Subject: RE: GENII Code Developer Review

Hi guys;

I'm back from a few weeks of relative isolation in Siberia (and I must say, it is more comfortable there, where the email doesn't work and the phone doesn't either).

I'm trying to catch up with your needs...

I'm not looking forward to this.

I think that I should respond "twice" to your paperwork. Once for GENII 1.485 and once for GENII Version 2.0. They are sufficiently dissimilar that I think that we would be misleading people if we tried to do them together. So that you know what I'm thinking:

GENII 1.485 was developed under the earliest NQA-1 standards (1986 version):

- SQA Plan
  got one, out of date. Refers to PNNL manual no longer available, but I have the key chapters.
- Software Requirements Document
  got one, but the one we developed was VERY SHORT, and not nearly as detailed as the system now wants.
- Software Design Document
  I would say that the GENII PNL-6854 Volume 1 report covers this
- Test Case Description and Report
  We have a series of regression tests that we know the answers to, and ran all modifications against. We also have an extensive series of documented hand calculation worksheets that give "the right answer." This isn't in the format of a "report" - but I have several file cabinets full of the tests
- Software Configuration and Control Document
  This is also not in the format of a "document." We have hard copies of all the versions from 1.350 (the point at which we thought things were stable) through 1.485, including the "Software change packets." I have let RSICC do my distribution for years.

- Error Notification and Corrective Action Report
  We no longer do this, except in extraordinary circumstances (like last year's H3 debacle at Savannah River), when we tell RSICC and they tell the world.
- User's Manual, and other relevant documentation (model description, weekly or monthly reports to code sponsor, etc.).
  I think that GENII PNL-6854 Volume 2 report covers this

So that you understand: DOE quit funding any GENII support or maintenance in the early 1990's. I have lost the capability to make changes to the compiled Basic APPRENTICE routines (and I'd be afraid to mess with the Fortran routines, too, because I don't think that my old compiler will run on a recent machine, and I certainly don't want to try to change to a new one, because the code was so specific to the Lahey F77 compiler.) THERFORE, there have been NO official changes to the code since 1990.

GENII Version 2 keeps the name, and a few of the basic algorithms. Pretty much everything else is new.
This has been held up in the "development" phase for years because of lack of money to get it completed. I inch it along when I have personal time to do so.
The formal QA is weaker than for 1.485, in part because we are using the lab's "Good Practices" standards instead of NQA-1:

- SQA Plan
  got one, it's pretty short. It also refers to lab manuals, but at least these exist!
- Software Requirements Document
  got one, reasonably detailed and complete
- Software Design Document
  GENII Version 2 Software Design Document available
- Test Case Description and Report
  Since it isn't done, we don't have one of these.
- Software Configuration and Control Document
  all I've got is my notebooks and backups.

- Error Notification and Corrective Action Report
  I only have a few beta users; they let me know when it's broke and I fix it for them.
- User's Manual, and other relevant documentation (model description, weekly or monthly reports to code sponsor, etc.).
  GENII Version 2 Users Guide available, plus the "Getting Started with GENII" instructions that keep getting longer and longer...

HOWEVER: the whole thing was reviewed by the EPA Science Advisory Board (who have a report), and EPA paid some people to go over it this year. I have NOT seen the results of this review; I have no idea what they said or who did it. I am a tad disappointed that they spent the money and then didn't even bother to tell me the results.

Bruce

P.S. I don't think that I have any comments on the SQA Plan and Requirements (other than a couple of really minor typos).

From: VERN PETERSON [mailto:vlrep@msn.com]
Sent: Monday, January 05, 2004 3:27 PM

To: Napier, Bruce A
Subject: more questions

Bruce,

...

Here is another requirement I must assess for the gap analysis: "Documentation during verification included a copy of the software, test case description, and associated criteria that are traceable to the software requirements and design documentation." I don't know how to answer this but you probably do. When the independent reviewers/testers did verification of the code, did they have all these things mentioned? I assume they did but I can't find a statement to this effect in the 1.485 or 2.0 documentation. (It may be there but if so, I missed it.)

...

Vern Peterson

From: Napier, Bruce A
To: Vern Peterson
Sent: Tuesday, January 06, 2004 12:59 PM
Subject: RE: more questions

The test cases were generally designed to meet the needs of certain types of calculation, and were done first on the computer (using the code and documentation to run) and then again on the GENII-specific hand calculation worksheets. The criteria were that the numbers had to match to 2 significant figures (which is all that the GENII code transfers internally at certain steps).

So: YES they had the software.
YES they had the documentation. The GENII documentation, PNL-6584 Volume 1 contains the Design Requirements as an appendix. So YES, it's traceable.
YES they had test case descriptions (or wrote their own).
YES they had criteria.

Telephone conversations

Conversation between William Joyce and Vern Peterson, October 14, 2003

These are highlights from the conversation:

- GENII 2.0 is not appropriate for DSAs because it can't give 95th percentile consequences and because the JDF files developed at Hanford are not appropriate for DSA work – they don't meet DOE requirements (but new ones could be constructed that do meet DOE requirements)

- The ten receptor locations in GENII 2.0 are each forced to be at the nearest grid points, which may not be where the user wants them
- GENII 2.0 is meant for EPA NESHAPS, not DOE DSAs
- GENII 1.485 was developed in a DOS environment and therefore had to address the memory limit of <640 KB. The Windows memory management system is different and there is a potential that this may lead to problems.
- Neither GENII 1.485 nor GENII 2.0 are appropriate for DSA work, in his opinion.

APPENDIX B. — GENII BENCHMARKING AND V&V

(List provided by Bruce Napier)

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