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

Software Quality Assurance Improvement Plan: ALOHA Gap Analysis

Final Report

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

May 2004

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FOREWORD

This report documents the outcome of an evaluation of the Software Quality Assurance (SQA) attributes of the chemical source term and atmospheric dispersion computer code, ALOHA 5.2.3, 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 the Defense Nuclear Facilities Safety Board Recommendation 2002-1.

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

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REVISION STATUS

Page/Section	Revision	Change
1. Entire Document	1. Interim Report	1. Original Issue
1. Entire Document	1. Final Report, May 3, 2004	1. Updated all sections per review comments.

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CONTENTS

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TABLES

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FIGURES

Page

None

Software Quality Assurance Improvement Plan: ALOHA 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 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 ALOHA 5.2.3 software for chemical source term and atmospheric dispersion and consequence analysis, is one of the codes designated for the toolbox. To determine the actions needed to bring the ALOHA 5.2.3 code 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 ALOHA 5.2.3 against identified criteria.

The balance of this document provides the outcome of the ALOHA gap analysis compliant with NQA-1-based requirements as contained in U.S. Department of Energy, *Software Quality Assurance Plan and Criteria for Safety Analysis Toolbox Codes*, (DOE, 2003e). 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 *User Instructions* (7). A third requirement, *Configuration Control* (9), is partially met. Improvement actions are recommended for ALOHA to fully meet *Configuration Control* (9) criteria and the remaining seven requirements. This evaluation outcome is deemed acceptable because: (1) ALOHA is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of ALOHA is limited to those analytic applications for which the software is intended.

Suggested remedial actions for this software would warrant upgrading software documents. The complete list of revised 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 Manual.

As part of this effort, the draft National Oceanic and Atmospheric Administration (NOAA) theoretical description memorandum for ALOHA 5.0 (Reynolds, 1992), which is the main source of information for technical information, should be updated for recent upgrades, technically reviewed, and issued as final.

It is estimated that a concentrated program to upgrade the SQA pedigree of ALOHA to be compliant with the ten criteria discussed here would require fourteen to sixteen full-time equivalent (FTE)-months. Technical review of the chemical databases associated with this software is assumed to have been performed, and is not included in the level-of-effort estimate.

A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report. It is recommended that this version be evaluated relative to the software improvement and baseline document recommendations, as well as the full set of SQA criteria discussed in this report. If this version is found to be satisfactory, it should replace version 5.2.3 as the designated version of the software for the toolbox.

It was determined that the ALOHA 5.2.3 code does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of the software for supporting safety analysis. Informed use of the code can be assisted by appropriate use of current ALOHA documentation prepared by NOAA and the ALOHA code guidance report for DOE safety analysts, *ALOHA Computer Code Application Guidance for Documented Safety Analysis*, (DOE, 2004). Furthermore, while SQA improvement actions are recommended for ALOHA, no evidence has been found of programming, logic, or other types of software errors in ALOHA 5.2.3 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 on the results of a gap analysis for Version 5.2.3 of the ALOHA computer code. The intent of the gap analysis is to determine the actions needed to bring the designated 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. 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 (leak path factor 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, ALOHA Version 5.2.3, is likely to require some degree of quality assurance improvement before meeting current SQA standards. The analysis of this document evaluates ALOHA Version 5.2.3 relative to current software quality assurance criteria. It assesses the extent 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 basis, by which to evaluate each designated toolbox code. This evaluation process, a gap analysis, 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 complete 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 provides key information to DOE, code developers, and code users.

DOE obtains the following benefits:

- Estimate 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 is provided:

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

DOE safety analysts and code users 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 ALOHA 5.2.3 code, one of the six designated toolbox codes for safety analysis. While ALOHA 5.2.3 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 here 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 ALOHA 5.2.3 code as part of DOE's implementation plan on SQA improvements.

1.6 Methodology for Gap Analysis

The gap analysis for ALOHA 5.2.3 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 reported here utilizes ten of the fourteen topical areas listed in DOE (2003e) related to software quality assurance to assess the

quality of the ALOHA 5.2.3 code. The ten areas are those particularly applicable to the software development, specifically: (1) Software Classification, (2) SQA Procedures/Plans, (5) Requirements Phase, (6) Design Phase, (7) Implementation Phase, (8) Testing Phase, (9) User Instructions, (10) Acceptance Test, (12) Configuration Control, and (13) Error Impact. Each area, or requirement, is assessed individually in Section 4.

Requirements 3 (Dedication), 4 (Evaluation), and 14 (Access Control), are not applicable for the software development process, and thus are not evaluated in this review. Requirement 4 (Evaluation) is an outline of the minimum steps to be undertaken in a software review, and is complied with by evaluating the areas listed above. Requirement 11 (Operation and Maintenance) is only partially applicable to software development, and is interpreted to be applicable mostly to the software user organization.

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 (O'Kula, 2003). The core section of the template is attached as Appendix A to the present report. While the ALOHA software developers did not provide a written response using the template, they provided information intermittently through less formal means.

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.
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.

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

Phase	**Procedure**
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.

1.7 Summary Description of Software Being Reviewed

The gap analysis was performed on version 5.2.3 of the Areal Locations of Hazardous Atmospheres (ALOHA) code (NOAA, 1999a) as this was the current version during the course of the evaluation.[2] ALOHA 5.2.3 was released in 1999. ALOHA is a public domain code that is part of a system of software that is known as the Computer-Aided Management of Emergency Operations (CAMEO) that was developed to plan for and respond to chemical emergencies. It is also widely used throughout the DOE complex for safety analysis applications.

Specifically, ALOHA performs calculations for source terms and downwind concentrations. Source term calculations determine the rate at which the chemical material is released to the atmosphere, release duration, and the physical form of the chemical upon release. The analyst specifies the chemical and then characterizes the initial boundary conditions of the chemical with respect to the environment through the source configuration input. The ALOHA code allows for the source to be defined in one of four ways (i.e., direct source, puddle source, tank source, or pipe source) in order to model various accident scenarios. The source configuration input is used to either specify the chemical source term or to provide ALOHA with the necessary information and data to calculate transient chemical release rates and physical state of the chemical upon release.

The ALOHA code considers two classes of atmospheric transport and dispersion based upon the assumed interaction of the released cloud with the atmospheric wind flow.

[2] A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report.

- For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, ALOHA treats the released chemical as neutrally buoyant.
- Alternatively, if the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either neutrally buoyant or dense-gas type of atmospheric transport and dispersion.

In addition to the source term and downwind concentration calculations, ALOHA allows for the specification of concentration limits for the purpose of consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). ALOHA refers to these concentration limits as level-of-concern (LOC) concentrations. Safety analysis work uses the emergency response planning guidelines (ERPGs) and temporary emergency exposure limits (TEELs) for assessing human health effects for both facility workers and the general public (Craig, 2001). While ERPGs and TEELs are not explicitly a part of the ALOHA 5.2.3 chemical database[3], ALOHA 5.2.3 allows the user to input an ERPG or TEEL value as the LOC concentration.

A brief summary of ALOHA that was supplied code developer is summarized in Table 1-2.

Table 1-2 — Summary Description of ALOHA Software

Type	Specific Information
Code Name	ALOHA (Areal Locations of Hazardous Atmospheres)
Version of the Code	Version 5.2.3
Developing Organization and Sponsor Information	DOC/NOAA/NOS Office of Response and Restoration And EPA Office of Emergency Prevention, Preparedness, and Response
Auxiliary Codes	Codes ALOHA is a standalone program but can be used in conjunction with CAMEO and MARPLOT. For more information, see http://response.restoration.noaa.gov
Software Platform/Portability	Available for Macintosh computers running OS 8, OS 9, or OS X; Available for any personal computer that runs Windows 98, 2000, NT, XP, or ME operating systems.
Coding and Computer(s)	C Code
Technical Support Point of Contact	Robert Jones NOAA/ORR 7600 Sand Point Way, Seattle, WA 98115 206-526-4278 Robert.jones@noaa.gov
Code Procurement Point of Contact	A self-extracting installer can be downloaded from: http://www.epa.gov/ceppo/cameo/aloha.htm Mark W Miller DOC/NOAA/NOS/ORR 7600 Sand Point Way, Seattle, WA 98115 206-526-6272 mark.w.miller@noaa.gov

[3] The ALOHA 5.2.3 chemical database incorporates two sets of concentration limits that are used in the chemical industry to address worker safety issues: (1) immediately dangerous to life or health (IDLH) and (2) threshold limit value – time weighted average (TLV-TWA). ALOHA 5.3, which was released in March 2004 just prior to the issuance of this report, does include TEELs and ERPGs.

Type	Specific Information
Code Package Label/Title	aloha.exe – Windows alohains.sit.hqx - Macintosh
Contributing Organization(s)	DOC/NOAA/NOS Office of Response and Restoration and EPA Office of Emergency Prevention Preparedness and Response
Recommended Documentation - Supplied with Code Transmittal upon Distribution or Otherwise Available	1. The ALOHA manual is a 1.5 MB PDF file (aloha.pdf) that can be downloaded directly from http://www.epa.gov/ceppo/cameo/aloha.htm
Input Data/Parameter Requirements	The location and chemical must be selected from scrolling lists. In some cases, the user must specify the concentration level to be displayed. Wind speed, direction, ground roughness, cloud cover, humidity, air temperature, and inversion height must be selected. The inputs needed to specify the source strength depend upon the scenario chosen; the simplest is the direct source and requires the mass or volume release rate.
Summary of Output	Output is provided in text and graphical form, including - rate at which the pollutant is entering the atmosphere as a function of time - indoor and outdoor concentrations as a function of time at a user-defined location - spatial distribution corresponding to the condition that the maximum concentration exceeds a user-specified level of concern
Nature of Problem Addressed by Software	ALOHA provides conservative estimates of the spatial distribution of the peak concentration of a pollutant following an acute release. To accomplish this, ALOHA contains an extensive database of chemical properties, models for estimating the amount of material entering the atmosphere for a wide range of scenarios, and Gaussian and dense gas (based on DEGADIS) dispersion models.
Significant Strengths of Software	ALOHA contains an extensive database of chemical properties so no additional information beyond the chemical identity is required. ALOHA has submodels for estimating the amount of pollutant entering the atmosphere (source strength). ALOHA has a dispersion model capable of accounting for the gravity effects on dense gas dispersion. ALOHA displays uncertainty associated with wind direction. ALOHA's interface is designed to assist users by including intelligent default entries where appropriate, reasonableness checks for input and context sensitive helps which include data entry guidance.
Known Restrictions or Limitations	ALOHA is designed to estimate the airborne concentration of pollutants over a relatively short time, one hour, and short spatial extent, 10 kilometers. With this restriction, the use of steady-state meteorology is acceptable. ALOHA does not account for steering by local topography, particulates, or reactions (including fire).
Preprocessing (set-up) time for Typical Safety Analysis Calculation	5 - 15 minutes
Execution Time	1 – 10 seconds
Computer Hardware Requirements	Any computer capable of running the operating systems noted above can run ALOHA.

Type	Specific Information
Computer Software Requirements	None
Other Versions Available	N/A
Individual(s) completing this information form: Name: Organization: Telephone: Email: Fax:	 Mark W Miller DOC/NOAA/NOS/ORR 206-526-6272 mark.w.miller@noaa.gov 206-526-6329

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

Table 1-3 — Software Documentation Reviewed for ALOHA

No.	Reference
1.	*ALOHA User's Manual (*NOAA, 1999a)
2.	*ALOHA 5.2.3 Online Help* (NOAA, 1999b)
3.	*ALOHA Theoretical Description* (Reynolds, 1992) – Draft document
4.	*ALOHA User's and ARCHIE: A Comparison*, Report No. HAZMAT 93-2 (M. Evans, 1993)
5.	*Quality Assurance of ALOHA* (M. Evans, 1994) – Draft document
6.	http://www.nwn.noaa.gov/sites/hazmat/cameo/alotech/quality.html
7.	http://www.nwn.noaa.gov/sites/hazmat/cameo/aloha.html
8.	http://www.epa.gov/ceppo/cameo/instruct.htm
9.	http://response.restoration.noaa.gov/cameo/aloha.html
10.	http://response.restoration.noaa.gov/cameo/alohafaq/history.html

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 ALOHA 5.2.3 SQA program, in general, met criteria for *Software Classification* and *User Instructions*, which refer to Requirements 1 and 7, respectively. A third topical area, *Configuration Control*, partially met criteria, but it and the remaining seven topical quality areas were judged either not wholly compliant with the SQA criteria, and/or lacked documentation to confirm compliance. The eight areas that should be addressed for improvement actions are listed in Section 2.2 (Exceptions to Requirements). Details on the evaluation process relative to the requirements and the criteria applied, are found in Section 4.

2.2 Exceptions to Requirements

Exceptions to criteria found for ALOHA 5.2.3 are listed below in Table 2-1. The requirement is given, the reason the requirement was not met is provided, and action(s) are listed to correct the exceptions. The ten criteria evaluated are those predominantly executed by the software developer. However, it is noted that criteria for SQA Procedures/Plan, Testing, Acceptance Test, Configuration Control, and Error Notification also have requirements for the organization implementing the software. These criteria were assessed in the present evaluation only from the code developer perspective.

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 Plans and Procedures were not available for the gap analysis.	SQA Plans and Procedures should be developed and made available for review.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document does not exist for review. Thus, it was necessary to infer requirements from draft model description and user guidance documents.	A Software Requirements Document should be prepared and made available for review.
3.	Design Phase (Section 4.4)	A Software Design Document does not exist for review. Thus, it was necessary to infer the intent of the design from draft model description and user guidance documents.	A Software Design Document should be prepared and made available for review. As part of this effort, the draft NOAA theoretical description memorandum for ALOHA 5.0 (Reynolds, 1992), which is the main source for technical information, should be updated for recent upgrades, technically reviewed, and issued as final.
4	Implementation Phase (Section 4.5)	Documentation to support the implementation is lacking.	A verifiable, written set of SQA plans and procedures including

No.	Criterion	Reason Not Met	Remedial action(s)
			implementation, test case descriptions, and associated criteria related to design should be made available.
5.	Testing Phase (Section 4.6)	A Software Testing Report Document does not exist for review. The documentation of results from validation and benchmark activities are incomplete and in the form of summaries that are found at ALOHA websites.	A Software Testing Report Document should be prepared and made available for review.
6	Acceptance Test (Section 4.8)	A verifiable, written set of SQA plans and procedures, which would include acceptance testing documentation, is lacking.	Documented acceptance testing should be developed.
7	Configuration Control (Section 4.9)	A Configuration Control process is in place at NOAA, but limited documentation was forwarded to allow a gap analysis to be performed.	While a Configuration Control process is apparently functional at NOAA, written documentation should be prepared and made available for review.
8.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report does not exist for review.	While a Software Problem Reporting system is apparently in place, written documentation should be provided to the Central Registry for verification of its effectiveness.

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. These recommendations are listed in Table 2-2.

Table 2-2 — Summary of Important Recommendations for ALOHA

No.	Recommendation
1.	Correct a reported IDLH bug (e-mail to Mark Miller at NOAA on 11/13/2003). The footprint information gives results for the distance that corresponds to the maximum threat zone for IDHL. When the centerline concentration output is requested at this distance, the concentration results are expected to be the IDLH concentration or very close to it. This is not always the case. (Note: The footprint information output seems to be the source of problem, and neither footprint output or IDLH data are typically not used in DSA applications.)

No.	Recommendation
2.	Provide method to write-protect the Chemical Library. In previous versions of ALOHA, the Chemical Library was protected from inadvertent changes by requiring the use of another program, ChemManager. In the current version, this is not the case; permanent changes may be made within ALOHA code itself. This allows any user to permanently change the chemical library. This is especially problematic, in that users have previously been allowed to make changes knowing that they could not alter the chemical library itself. Allowing some method of protecting the chemical library would be beneficial. Although this can be done within the operating system itself by write protecting the ChemLib file, not all users will be knowledgeable enough to know this, and not all installations will write protect the file.
3.	Add capability to model release durations that are greater than one hour and downwind distances that are greater than 10 km. Although we recognize the purpose of this limitation, for safety analysis purposes, it is standard procedure to model releases using persistent meteorology and a straight-line Gaussian plume to a receptor at the site boundary. As many DOE sites are quite large (hundreds of square miles), this forces an analyst to use another tool to perform the same task. Rather than increasing the limit, we would rather it be removed altogether. While this may allow for unrealistic real-time use, it is typically required for bounding consequence calculations.
4.	Add capability to output consequences for multiple receptors in a single ALOHA run. DSA analyses may need a set of several receptors (e.g., 30m, 100m, 500m, 1km etc.) for which consequences must be determined for every postulated accident scenario. Having the ability to get this output without having to perform a run for each receptor would save time and money on performance and review, and decrease the size of documents. In tandem with the above request, the ability to output a graph of concentration versus centerline distance would be helpful, especially for elevated releases in which the maximum downwind concentration is desired and the distance where this occurs cannot be known apriori.
5. a.) b.)	Add capabilities to facilitate evaporation calculations for chemicals that are not part of ALOHA's library: Add capability to directly input vapor pressure rather than the only option being for ALOHA to calculate it from chemical properties. Occasionally, releases must be modeled for chemicals that are not in ALOHA's library. For some chemicals, though not all physical property data needed by ALOHA to calculate the vapor pressure is available, the vapor pressures themselves are available. It would be helpful if a vapor pressure could be directly entered and used by ALOHA to calculate an evaporative source term. Add capability so a simpler evaporation model as an option to use (one that did not require quite so much physical property data) when insufficient physical property data is known to use the ALOHA evaporation model. The uncertainty in the release quantity is usually far greater than that in the calculation of evaporative source term so the loss of accuracy would not normally be a problem.
6.	Add capability to read from a file of hourly meteorological data over a one-year period, calculate consequences for each hourly entry, and output the 50th and 95th percentile results.

No.	Recommendation
7.	Add capability for ALOHA either to use other sets of dispersion coefficients in addition to the two that are currently available (rural or urban) or to make user-specified adjustments to the dispersion coefficients as noted below:
a.)	Add capability to use the surface roughness input to adjust the rural vertical dispersion coefficient when the input value is greater than 3 cm and less than 100 cm. This will allow more accurate modeling for the majority sites that have surface roughness characteristics that fall in between the two extremes of flat grassland and an urban environment.
b.)	Add capability to adjust the horizontal dispersion coefficients for averaging time to account for specific exposure times that associated with toxic exposure guidelines of interest.
8.	Add capability to model dry deposition. A simple point depletion model could serve this purpose.
9.	For puddle modeling, allow model to calculate surface area from input of volume (or mass) and puddle depth. When using the code for planning rather than for response, this would be more useful than the current options of inputting the area or diameter, then the volume, depth, or mass.
10.	Add explosion modeling capability. A number of DOE sites have begun to look at explosive dispersal of toxicological material. It would be useful to be able to use the Gaussian plume model of ALOHA to estimate downwind concentrations.
11.	Reword or remove from the initial screen, the limitation on modeling particulates. As dispersion of small (respirable) particles is similar to that of gases, ALOHA is often used in the DOE complex to model respirable aerosols, including powders. The wording of this limitation, for some customers, unnecessarily calls into question this practice.
12	Update, technically review, and issue as final the draft NOAA theoretical description memorandum for ALOHA 5.0 that is the main source of information for technical information (Reynolds, 1992).
13.	Add capability to use long filenames for ALOHA save files.

2.4 Conclusion Regarding Codes Ability to Meet Intended Function

The ALOHA 5.2.3 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, *ALOHA Computer Code Application Guidance for Documented Safety Analysis*, (DOE 2004), it is judged that it will meet its intended function.

3.0 Lessons Learned

Additional opportunities and venues should be sought for training and user qualification on safety analysis software. This is a long-term recommendation for ALOHA 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 sections follow the ten topical areas. Included in the software improvements section is an estimate of the resources required to upgrade ALOHA.

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

Subsection (This Report)	Corresponding Entry Table 3-3 from DOE (2003e) No.	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

4.1 Topical Area 1 Assessment: Software Classification

This area corresponds to the requirement entitled Software Classification in Table 3-2 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 software transmittal to make an informed determination of the classification of the software. A user of the ALOHA 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.

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.	It is concluded that sufficient information is provided with the documentation that is transmitted with the software for the user to make an informed determination of the classification of the software. For most DSA applications, the safety class or safety significant classification, or Level B in the classification hierarchy discussed in DOE (2003e), would be selected, which by definition relate 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.

4.1.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the bases for response to 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 and Plans in Table 3-3 of (DOE 2003e).

From the limited information received from the software developers, formal, published SQA procedures and plans were not developed. While it is possible that most elements of a compliant SQA program were followed in the development of ALOHA 5.2.3, the lack of written documentation prevents an independent evaluator from making a definitive confirmation. Based on discussions with the code developer, organizational management of the ALOHA 5.2.3 development probably ensured that some, maybe many, elements of a compliant SQA program were fulfilled in an informal manner.

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.

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

Criterion Number	Criterion Specification	Compliant	Summary Remarks
2.1	Procedures/plans for SQA (**SQA Plan**) have identified organizations responsible for performing work; independent reviews, etc.	Uncertain.	A verifiable, complete written set of SQA plans and procedures is lacking for ALOHA. Based on discussions with the code developer, organizational management of the ALOHA development probably ensured that some elements of a compliant SQA program were fulfilled in an informal manner.
2.2	Procedures/plans for SQA (**SQA Plan**) have identified software engineering methods.	Uncertain.	See Criterion 2.1 summary remarks.
2.3	Procedures/plans for SQA (**SQA Plan**) have identified documentation to be required as part of program.	Uncertain.	See Criterion 2.1 summary remarks.
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.	Uncertain.	See Criterion 2.1 summary remarks.
2.5	Procedures/plans for SQA (**SQA Plan**) have identified software reviews and schedule.	Uncertain.	See Criterion 2.1 summary remarks.
2.6	Procedures/plans for SQA (**SQA Plan**) have identified methods for error reporting and corrective actions.	Uncertain.	See Criterion 2.1 summary remarks.

4.2.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement.

4.2.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures for ALOHA should be addressed.

4.2.4 Recommendations

Recommendations related to this topical area are provided as follows:

- It is recommended that a SQA plan be developed to provide a framework for configuration control, code maintenance, and support of future upgrades.

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 Result

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.	Yes.	Implicitly fulfilled. The ALOHA program was developed to provide emergency response personnel and emergency planners with a software tool to evaluate downwind concentrations from the atmospheric release of toxic substances. It is a widely used computer code, which demonstrates that it serves the needs of many analysts. The code is regularly upgraded to improve capabilities. Specific requirements can be inferred from various ALOHA documents.
3.2	Software requirements are specified, documented, reviewed and approved.	No.	Software requirements have not been formally established. A verifiable, written set of SQA plans and procedures, which would include software requirements, is lacking for ALOHA.
3.3	Requirements define the functions to be performed by the software and provide detail and information necessary to design the software.	Partial.	Information sources for the technical details of the ALOHA algorithms are given in the ALOHA User's manual (NOAA, 1999a), the online help with

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			ALOHA 5.2.3 (NOAA, 1999b), a NOAA report (Evans, 1993) and a draft NOAA theoretical description memorandum (for ALOHA 5.0) (Reynolds, 1992). Information from ALOHA websites is also available. The ALOHA code uses the well-established models, such as the Gaussian puff and plume models. The draft NOAA theoretical description memorandum (for ALOHA 5.0) comprehensively documents these models (Reynolds, 1992). The document, however, is in draft form and should be updated to reflect upgrades that have been made over the past ten years.
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.	The online user's documentation implicitly states requirements. The user's documentation also addresses, at least partially, installation, operating systems, external interfaces (e.g., MARPLOT) and design inputs.
3.5	Acceptance criteria are established in the software requirements documentation for each of the identified requirements.	No.	See Criterion 3.2 summary remarks.

4.3.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement. The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information (Reynolds, 1992).

4.3.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which would include written software requirements, for ALOHA should be addressed.

4.3.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Formal documentation of the software requirements as in intended in ALOHA 5.2.3 will be needed for ALOHA to meet all prerequisites for the DOE toolbox.
- The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information (Reynolds, 1992). It should be updated for recent upgrades, technically reviewed, and issued as final.

4.4 Topical Area 4 Assessment: Design Phase

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

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 documentation.
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.	Partial.	Design may be inferred from final software product, but design document was not made available for review.
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).	Partial.	Elements of this criterion may be inferred from documentation.
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.	Partial.	Elements of this criterion may be inferred from 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.	Not applicable to non-process, instrumentation and control software.	None.
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.	Partial.	Elements of this criterion may be inferred from documentation. A verifiable, written set of SQA plans and procedures, which would include software design documentation, is lacking for ALOHA.
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.	See Criterion 4.6 summary remarks.

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.		
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.	The ALOHA user documentation contains this 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.	Partial.	See Criterion 4.6 summary remarks.
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.	See Criterion 4.6 summary remarks.
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.	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.	Partial.	See Criterion 4.6 summary remarks.
4.13	The Independent Review (IR) 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.	Partial.	Significant review (see Criterion 4.5) was performed. Documentation of reviewer qualifications and independence is lacking.
4.14	The results of the IR are documented with the identification of the verifier indicated.	Partial.	See Criterion 4.13 summary remarks.
4.15	If review alone was not adequate to determine if requirements are met,	Partial.	See Criterion 4.5 summary remarks.

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	alternate calculations were used, or tests were developed and integrated into the appropriate activities of the software development cycle.		
4.16	Software design documentation was completed prior to finalizing the Independent Review.	Partial.	It appears that some reviews were conducted in parallel with design documentation preparation or before preparation of its equivalent,
4.17	The extent of the IR 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.	Elements of this criterion may be inferred from documentation. Integrated documentation of the design requirements is lacking, as is documentation of the review details and bases.

4.4.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement. The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information (Reynolds, 1992).

4.4.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which would include software design documentation, for ALOHA should be addressed.

4.4.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Formal documentation of the software design as in intended in ALOHA 5.2.3 will be needed for ALOHA to meet all prerequisites for the DOE toolbox.
- The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information (Reynolds, 1992). It should be updated for recent upgrades, technically reviewed, and issued as final.

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	Yes.	User guide, draft technical

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	software products such as computer program listings and instructions for computer program use.		description report as well as web-posted information, and executable file demonstrate that the essential features of this criterion are met.
5.2	Implemented software was analyzed to identify and correct errors.	Partial.	Practical steps were taken by the code developers to identify problems through the use of fractional factorial designs, which ALOHA draft documentation describes as "a method of experimental design commonly used in industrial research." Using this method, ALOHA output was systematically compared against that of reference models to "identify and eliminate code errors, to find flaws in model algorithms, to identify aspects of the model requiring additional evaluation, to ensure that all substantial deviations of ALOHA's estimates from predictions made by similar models are the result of intended differences in algorithms" (Evans, 1994). Thus, documentation, especially the quality assurance draft report (Evans, 1994), supports partial satisfaction of essential features of this criterion in general for ALOHA development, but does specifically address ALOHA 5.2.3, which was released post-1994. This document should be updated as necessary, reviewed, and issued in final form.
5.3	The source code finalized during verification (this phase) was placed under configuration control.	Partial.	Discussions with the code developers indicate that software is managed by the program manager (currently Mark Miller) and under the direct control of the project manager (currently Jerry Muhasky). The project manager implements all the changes to the source code and

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			maintains the code on his computer, using password protection to control access. The computer is backed up on a NOAA server as well as CD copies that are stored in secure off site locations. The code developers indicate that there are plans to formally document configuration control procedures.
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.	Partial.	The user's manual includes four sample problems that can serve as test cases. Guidance is given for each required input for each test case. Results are also given for each test case that can be compared to user-generated results. Not possible to trace to requirements and design descriptions since these are lacking documentation.

4.5.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA website) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement.

4.5.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which would include test case descriptions as well as software requirements and design documentation, for ALOHA should be addressed.

4.5.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Formal documentation of the implication process as it relates to ALOHA 5.2.3 will be needed for ALOHA to meet all prerequisites for the DOE toolbox.

4.6 Topical Area 6 Assessment: Testing Phase

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

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.	Partial.	Documentation, especially the quality assurance draft

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			report (Evans, 1994), supports partial satisfaction of this criterion. Only partial credit is given since the document is draft form and only addresses early development of ALOHA. This document should be updated as necessary, reviewed, and issued in final form.
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.	Partial.	Draft ALOHA documentation suggests that essential features of this criterion have been partially met informally (Evans, 1994). Only partial credit is given since the document is draft form and only addresses early development of ALOHA. Practical steps were taken by the code developers to identify problems through the use of fractional factorial designs. Using this method, ALOHA output was systematically compared against that of reference models for various combinations of input values and the results analyzed to ensure that all substantial deviations of ALOHA's estimates from predictions made by similar models were the result of intended differences in algorithms (Evans, 1994). Thus, documentation, especially the quality assurance draft report (Evans, 1994), supports partial satisfaction of essential features of this criterion. This document should be updated as necessary, reviewed, and issued in final form.
6.3	Testing demonstrated that the computer program properly handles abnormal conditions and events as well as credible	Partial.	While there is no formal documentation that addresses this issue completely, the

Criterion Number	Criterion Specification	Compliant	Summary Remarks
	failures.		user's manual does address warning messages that ALOHA provides when the user enters an input outside the allowable range or when the user-specified inputs define conditions that may result in phenomena that is outside of the capabilities of ALOHA. An example of the latter case occurs when the user selects an air- or water-reactive chemical for analysis. ALOHA informs the user of the type of reaction and expected reaction products. For example, sulfur trioxide reacts with water to form sulfuric acid and heat. ALOHA does not account for resulting phenomena such as buoyancy from the heat.
6.4	Testing demonstrated that the computer program does not perform adverse unintended functions.	Partial.	See Criterion 6.2 summary remarks.
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.	Documentation, especially the quality assurance draft report (Evans, 1994), supports the satisfaction of essential features of this criterion. The results of comparisons of ALOHA predictions against field results as well as other computer codes are presented. This document should be updated as necessary, reviewed, and issued in final form. 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.	Significant testing on ALOHA has been performed as discussed in the summary remarks of Criterion 6.2 and Criterion 6.5. However, successful resolution of unsuccessful cases is not possible to verify, nor is traceability between test

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			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.	Significant testing on ALOHA has been performed as discussed in the summary remarks of Criterion 6.2 and Criterion 6.5. No comprehensive detailed record of test procedures and plans was available. It can be inferred that this criterion was partially met.

Additional Detail

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

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Criterion 6.1 — Details on the comparisons with field data are summarized below (Evans, 1994).

- Source term prediction for non-boiling pool evaporation – All ALOHA predictions were within 42% of measured evaporation rates.
- Source term prediction for liquefied propane – About 83% of ALOHA predictions were within a factor of two of measured vaporization rates.
- Atmospheric transport and dispersion predictions with Gaussian model – ALOHA predictions of mean downwind concentrations were on average 142% of the measured field data. ALOHA tended to underestimate concentrations at distances of 200 meters or more and overestimate concentrations closer in.
- Atmospheric transport and dispersion predictions with dense-gas model – ALOHA predictions were not compared directly with field measurements, but compared with results from the DEGADIS model that was calibrated to 12 trials from field experiments (Spicer, 1989). ALOHA predictions of mean downwind concentrations were on average 107% of DEGADIS predictions, and about 70% of DEGADIS predictions were within a factor of two of measured field concentrations.
- Atmospheric transport and dispersion predictions with dense-gas model for hydrogen fluoride (HF) releases – ALOHA predictions were not compared directly with field measurements, but compared with results from the DEGADIS model that was calibrated to 12 trials from field experiments (Spicer, 1989). ALOHA predictions of mean downwind concentrations were on average 48% of the measured field data.

4.6.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement.

4.6.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which includes test reports, for ALOHA should be addressed.

4.6.4 Recommendations

Recommendations related to this topical area are provided as follows:

- It is recommended that benchmark comparisons and validation cases be updated and formally documented (current documentation is in the form of draft summary document that is dated 1994).
- It is recommended that formal test report documentation be established for future upgrades to the code.

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 4.7-1 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 and made available to users.	Partial.	The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information (Reynolds, 1992). It should be updated for recent upgrades, technically reviewed, and issued as final. Currently, this draft NOAA theoretical description memorandum is not readily available.
7.2	User's manual or guide describes software and hardware limitations and identifies includes approved operating systems (for cases where source code is provided, applicable compilers should be noted).	Yes.	(NOAA, 1999a; NOAA, 1999b)
7.3	User's manual or guide includes description of the user's interaction with the software.	Yes.	(NOAA, 1999a; NOAA, 1999b)
7.4	User's manual or guide includes a description of any required training necessary to use the software.	Yes.	The user's manual does not state the need for any required general training. The inference can be made that formal training, while recommended, may not be required for general use of the code. The user's manual and web-posted information provide amble guidance, address specific issues that an analyst is likely to encounter, and cover worked sample problems. In addition, a fair amount of training material is posted on the

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			EPA website (http://www.epa.gov/ceppo/cameo/instruct.htm) . The user's manual does advise that a very specific type of ALOHA calculation, namely the calculation of dose from a chemical exposure, only be performed by someone trained in toxicology.
7.5	User's manual or guide includes input and output specifications.	Yes.	(NOAA, 1999a; NOAA, 1999b)
7.6	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.	(NOAA, 1999a; NOAA, 1999b)
7.7	User's manual or guide includes information for obtaining user and maintenance support.	Yes.	(NOAA, 1999a; NOAA, 1999b)

4.7.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement.

4.7.3 Software Quality-Related Issues or Concerns

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

4.7.4 Recommendations

Recommendations related to this topical area are provided as follows:

- The draft NOAA theoretical description memorandum (for ALOHA 5.0) is the main source of information for technical information on the models (Reynolds, 1992). It should be updated for recent upgrades, technically reviewed, and issued as final.

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 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

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

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).	Uncertain.	A verifiable, written set of SQA plans and procedures, which would include acceptance-testing documentation, is lacking for ALOHA.
8.2	To the extent applicable to the developer acceptance testing was performed prior to approval of the computer program for use.	Uncertain.	See Criterion 8.1 summary remarks.
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.	Uncertain.	See Criterion 8.1 summary remarks.
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.	Partial.	The user's manual includes four sample problems that can serve as test cases. Guidance is given for each required input for each test case. Results are also given for each test case that can be compared to user-generated results. These cases can be viewed as providing users and user groups with a mechanism for deciding if the ALOHA software is correctly installed and functioning properly.

4.8.2 Sources and Method of Review

Documentation that was distributed with the software package (plus information on ALOHA websites) and additional documentation that was supplied by the code developers for this effort were used as the primary bases for response to this requirement.

4.8.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which include acceptance-testing documentation for ALOHA should be addressed.

4.8.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Formal documentation of the acceptance testing process as it relates to ALOHA 5.2.3 will be needed for ALOHA to meet all prerequisites for the DOE toolbox.

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
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.	Partial.	Discussions with the code developers indicate that software is managed by the program manager (currently Mark Miller) and under the direct control of the project manager (currently Jerry Muhasky). The project manager implements all the changes to the source code and maintains the code on his computer, using password protection to control access. The computer is backed up on a NOAA server as well as CD copies that are stored in secure off site locations. The code developers indicate that there are plans to formally document configuration control procedures.
9.2	Implementing procedures meet applicable criteria for configuration identification, change control and configuration status accounting.	Partial.	See Criterion 9.1 summary remarks.

4.9.2 Sources and Method of Review

The requirement was assessed largely through discussions with the code developers.

4.9.3 Software Quality-Related Issues or Concerns

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

4.9.4 Recommendations

Recommendations related to this topical area are provided as follows:

- It is recommended that the code developers follow through with plans to formally document configuration control procedures.

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.	Partial.	NOAA controls the error notification and corrective actions process. An error notification and corrective action document was not available, making a thorough evaluation not possible.
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.	Upgrades are made to code has errors are discovered, frequently by users. The program manager evaluates whether a reported error reflects an error in the code. An error notification and corrective action document was not available, making a thorough evaluation not possible.
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.	If the program manager determines that an error exists in the code, the project manager responsible for the portion of the code in question as well as the originator of the error report are notified. An error notification and corrective action document was not available, making a thorough evaluation not possible.
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.	Uncertain.	An error notification and corrective action document was not available, making a thorough evaluation not possible.
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	The lead programmer/project manager makes changes in the source code if required to address the error and incorporates the new source code into the next release. If the error represents a safety issue then a new release is made as soon as possible. Copies of the incrementally changed code are kept as historical documentation. An error notification and corrective action document was not

Criterion Number	Criterion Specification	Compliant	Summary Remarks
			available, making a thorough evaluation not possible.
10.6	When a problem is determined to be an error, then action to document, evaluate and correct, as appropriate, is provided for handling how the corrective action impacts previous development activities	Partial.	See Criterion 10.5 summary remarks.
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.	Uncertain.	An error notification and corrective action document was not available, making a thorough evaluation not possible.

4.10.2 Sources and Method of Review

The requirement was assessed largely through discussions with the code developers. If a user detects a problem with the ALOHA software they can report these problems to the development team through the following methods: a problem reporting form at http://www.epa.gov/ceppo/cameo/bugform.htm, or contacting the CAMEO Specialist (ORR.cameo@noaa.gov) from http://response.restoration.noaa.gov/cameo/intro.html

4.10.3 Software Quality-Related Issues or Concerns

Lack of a verifiable, written set of SQA plans and procedures, which includes error notification and corrective action report, for ALOHA should be addressed.

4.10.4 Recommendations

Recommendations related to this topical area are provided as follows:

- Formal documentation of the error notification and corrective action process as it relates to ALOHA 5.2.3 will be needed for ALOHA to meet all prerequisites for the DOE toolbox.

4.11 Training Program Assessment

The software developer's does not have a published training program available for review. However, discussions with the software developer indicate that there is an active and frequent training program presented nationally on ALOHA/CAMEO.

Discussions are ongoing for the software developer to provide training at the Energy Facility Contractors Group (EFCOG) conferences. The winter session is during the Safety Basis Subgroup meeting and the summer session is the larger Safety Analysis Working Group, and historically has included training workshops.

4.12 Software Improvements

A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report. The main changes to the program are as follows according to the code developer:

- Windows source code was updated to a 32-bit application
- footprint output (i.e., concentration contour plot) can now be displayed with up to three level-of-concern concentrations) simultaneously
- evaporation algorithm was updated

- capability to model the evaporation from puddles of five aqueous chemical solutions was added
- chemical library was updated

In general according to the code developers, upgrades to ALOHA occur when features are requested by an outside agency (i.e. EPA), or internal discussion sees the benefit of a feature, and then the following steps are implemented. Once funding has been allocated to accomplish the upgrade, the ALOHA program manager assigns the upgrade to the personnel best suited to handle it. Once the team member has completed the development of the upgrade, the project manager ensures the source code is updated. Testing of the new version is completed and documented before the software version is updated and ready for release over the Internet.

It is estimated that a concentrated program to upgrade the SQA pedigree of ALOHA to be compliant with the ten criteria discussed here would require fourteen to sixteen full-time equivalent (FTE)-months. Technical review of the chemical databases associated with this software is assumed to have been performed, and is not included in the level-of-effort estimate.

5.0 Conclusion

The gap analysis for Version 5.2.3 of the ALOHA software, based on a set of requirements and criteria compliant with NQA-1, has been completed. 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 *User Instructions* (7). A third requirement, *Configuration Control* (9), is partially met. Improvement actions are recommended for ALOHA to fully meet *Configuration Control* (9) criteria and the remaining seven requirements. This evaluation outcome is deemed acceptable because: (1) ALOHA is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of ALOHA is limited to those analytic applications for which the software is intended.

Suggested remedial actions for this software would warrant upgrading software documents. The complete list of revised 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 Manual.

As part of this effort, the draft NOAA theoretical description memorandum for ALOHA 5.0 (Reynolds, 1992), which is the main source of information for technical information, should be updated for recent upgrades, technically reviewed, and issued as final.

It is estimated that a concentrated program to upgrade the SQA pedigree of ALOHA to be compliant with the ten criteria discussed here would require fourteen to sixteen full-time equivalent (FTE)-months. Technical review of the chemical databases associated with this software is assumed to have been performed, and is not included in the level-of-effort estimate.

A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report. It is recommended that this version be evaluated relative to the software improvement and baseline document recommendations, as well as the full set of SQA criteria discussed in this report. If this version is found to be satisfactory, it should replace version 5.2.3 as the designated version of the software for the toolbox.

It was determined that the ALOHA 5.2.3 code does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of the software for supporting safety analysis. Informed use of the code can be assisted by appropriate use of current ALOHA documentation prepared by NOAA and the ALOHA code guidance report for DOE safety analysts, *ALOHA Computer Code Application Guidance for Documented Safety Analysis*, (DOE, 2004). Furthermore, while SQA improvement actions are recommended for ALOHA, no evidence has been found of programming, logic, or other types of software errors in ALOHA 5.2.3 that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

6.0 Acronyms and Definitions

ACRONYMS:

AEC	Atomic Energy Commission
ALOHA	Areal Locations of Hazardous Atmospheres (designated toolbox software)
ANS	American Nuclear Society
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
CCPS	Center for Chemical Process Safety
CD	Compliance Decision
CFAST	Consolidated Fire and Smoke Transport Model (designated toolbox software)
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CSARP	Cooperative Severe Accident Research Program
DCF	Dose Conversion Factor
DIR	Defect Investigation Report
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
EH	DOE Office of Environment, Safety and Health
EIA	Electronic Industries Alliance
EM	DOE Office of Environmental Management
EPIcode	Emergency Prediction Information code (designated toolbox software)
EPRI	Electric Power Research Institute
FTE	Full-time equivalent
GENII	Generalized Environmental Radiation Dosimetry Software System - Hanford Dosimetry System (Generation II) (designated toolbox software)
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
IP	Implementation Plan
ISO	International Organization for Standardization
MACCS2	MELCOR Accident Consequence Code System 2 (designated toolbox software)
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (designated toolbox software)
NNSA	National Nuclear Security Administration
NRC	Nuclear Regulatory Commission
OCRWM	Office of Civilian Radioactive Waste Management
PSA	Probabilistic Safety Analysis (or Assessment)
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, 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.

Classification (Level of Software) — Determination of the level of software quality assurance 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 QA 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 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]

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 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.

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.

Sample Input — Input data for a designated sample problem which 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; and

(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 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 — 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 — 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

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	1.

Table 2. Summary Description of Subject Software	
Type	**Specific Information**
Documentation - Supplied with Code Transmittal upon Distribution or Otherwise Available	2. 3. 4. 5.
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[4]]

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.

Guidance for SQA Plans:

Requirement 2 – SQA Procedures/Plans (Table 3-2 of SQA Plan/Criteria (DOE, 2003a)
ASME NQA-1 2000 Section 200

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

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		

Type	Description	Frequency of training
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 correc
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.

REFERENCES

CFR Code of Federal Regulations (CFR). 10 CFR 830, Nuclear Safety Management Rule.

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DOE, U.S. Department of Energy (2000a). *Appendix A, Evaluation Guideline,* DOE-STD-3009-94, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Reports* (January 2000).

DOE, U.S. Department of Energy (2002). *Selection of Computer Codes for DOE Safety Analysis Applications* (August 2002).

DOE, U.S. Department of Energy (2003). *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, Letter (March 13, 2003); Report (February 28, 2003).

DOE, U.S. Department of Energy (2003a). *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes,* Interim Report, (September 2003).

DOE/EH, U.S. Department of Energy Office of Environment, Safety and Health (2003), *Designation of Initial Safety Analysis Toolbox Codes*, Letter, (March 28, 2003).