Selection of Computer Codes for U.S. Department of Energy Safety Analysis Applications

Revision 1

Dae Y. Chung
National Nuclear Security Agency
Office of Environment, Safety and Health Support
19901 Germantown Road
Germantown, MD 20874-1290
Phone: 301.903.3968
Email: dae.chung@nnsa.doe.gov

Kevin R. O'Kula

Patrick R. McClure

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Executive Summary

Defense Nuclear Facilities Safety Board Technical Report 25 (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for safety analysis decisions and to control safety-related systems. The development and maintenance of a collection, or "Toolbox," of high-use safety analysis codes is one of the major corrective measures recommended in TECH-25. 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.

A Safety Analysis Software Group, organized to direct actions addressing TECH-25, has reviewed the results of the DOE Software Quality Assurance (SQA) Survey to identify computer codes widely used for support of safety basis documentation. Survey results are categorized in terms of type of analysis applications, and then evaluated with screening and quantification criteria to identify candidate codes for the Toolbox. This process identifies the following software for the Safety Analysis Toolbox.

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

Strengths and weakness of the proposed Toolbox codes are discussed, along with individual SQA status. The recommended quality assurance(QA) requirements to be applied in future gap analysis are those found in American Society of Mechanical Engineers (ASME) NQA-1-1997, Part II, Subpart 2.7, and ASME NQA-1a-1999 Addenda.

In addition, it is proposed that code-specific guidance reports be generated to provide DOE safety analysts with applicability information, appropriate regimes, recommended configurations, and other pertinent information. Guidance reports of this nature will allow contractor organizations to apply the Toolbox codes as part of "safe harbor" methodology, to support preparation of 10 CFR 830 Subpart B, *Safety Basis Requirements*.

Table of Contents

List of Figures and Tables

1.0 Introduction

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 the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer code 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.

One of the corrective measures recommended in TECH-25 software is the development and maintenance of a computer code Toolbox of accident and consequence codes. A Toolbox of this nature would, in principle, contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes that are managed and maintained for DOE-wide application.

This report summarizes key considerations for establishing a Toolbox of "safe harbor" accident analysis computer codes for DOE facility use. Specifically, survey results are summarized in terms of type or category for accident analysis applications, and integrated with screening criteria to identify constituent codes for Toolbox purposes. Strengths and weakness of the proposed Toolbox codes are discussed along with the current SQA status. Estimates of the specific levels of effort to comply with SQA standards are provided.

Submittal of this report completes Action 2.0 of the DOE response plan to TECH-25 (DOE 2000).

2.0 Context for Use of Safety Analysis Software

TECH-25 noted that computer codes play a prominent role in ensuring safe operation of DOE facilities. Furthermore, the DNFSB indicated that a thorough and effective approach to guaranteeing software quality and appropriate use is imperative. In particular, the DNFSB stated that SQA applied to accident analysis support and instrument and control (I&C) systems functions should ensure that:

- The numerical models are a valid representation of the physical phenomena of interest for the appropriate variables and within a defined applicable range (verification).
- The fundamental data used in the code are appropriate for the intended function.
- The results obtained when using the code within its established range of applicability are in reasonable agreement with available experimental benchmark data, other reference phenomenological data, alternative computer model predictions, or other independent data applicable (validation).
- Modifications of and improvements to software is tracked and documented in a central registry so that users will be aware of changes, physical and mathematical assumptions, and limitations of their analysis.

- Computer models are properly executed by safety analysts to support the authorization basis of the facility, and that the safety envelope is understood and appropriately interpreted. This understanding subsequently provides confidence that identified control sets are sufficient, and the safety basis is conservative.

- Principles comprising an acceptable set of applicable SQA standards flow down and are implemented in actual I&C systems.

The DNFSB suggested that problems with the implementation and use of software for safety analysis and I&C functions partially resulted from deficiencies in the software and limitations of encoded physical models. The DNFSB commented that a thorough and effective approach to maintaining sufficient software quality levels was needed. Improvements were recommended in the management of the codes that include computer model support and guidance; adherence to software standards; configuration management; and assessment of appropriate usage, audits, and training.

The DNFSB stated that it was not considered appropriate that all safety analysis and process control software undergo a program to upgrade the SQA level. Specifically, the role of the software, the nature of the facility, and the site-specific requirements should be considered to determine the appropriate SQA level. However, software upgrades should be explored particularly for software that is widely applied in support of authorization basis documentation of DOE nuclear facilities.

In this regard, the DNFSB suggested the concept of a developing and maintaining a set of computer codes, or "Toolbox." In a follow-on meeting, the DNFSB defined a Toolbox in terms of a small number of standard codes having widespread use and adequate pedigree, maintained, managed, and distributed for implementation by a central source. Toolbox software would receive a top priority for focusing limited resources for upgrade and maintenance purposes, as well as ensure DOE users are supported consistently in areas of error notification and code issue resolution.

With respect to the operation of DOE nuclear facilities, safety-related software is undoubtedly important aspect in building and maintaining a defensible, conservative authorization basis and operating facilities safely. Particularly with respect to maintaining the safety basis, application of software and interpretation of results constitute only part of what should be a larger, integrated picture. There are many other factors to be considered in ensuring safety at nuclear facilities and operations.

An adequate, technically defensible safety basis is in part described through Departmental Rules and Orders, and underlying standards and guides such as:

- 10 CFR 830, *Nuclear Safety Management*, Subpart B, *Safety Basis Requirements*
- DOE O 5480.21, *Unreviewed Safety Questions*
- DOE O 5480.22, *Technical Safety Requirements*
- DOE O 420.1, *Facility Safety*
- DOE-STD-1027-92, Change Notice No. 1, *Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports*
- DOE-STD-3009-94, Change Notice No. 1, *Preparation Guide for U.S. DOE Nonreactor Nuclear Facility Safety Analysis Reports*

- DOE G 420.1-1, *Nonreactor Nuclear Safety Design Criteria and Explosive Safety Criteria Guide for use with DOE O 420.1, Facility Safety,* and
- DOE G 421.1-2, *Implementation Guide for Use n Developing Documented Safety Analysis to Meet Subpart B of 10 CFR 830.*

However, the overarching philosophy is that of applying safety analysis and safety-related design software and using results obtained from them in the context of Integrated Safety Management (ISM) principles and guidelines. In the ISM context, the line management has the responsibility of assuring safety. The DOE line managers are responsible for ensuring the contractors prepare adequate and defensible safety analyses.

DOE nuclear facilities perform a safety analysis process in support of the development of a Safety Analysis Report (SAR) or Documented Safety Analysis (DSA). The safety analyses should systematically identify and analyze the hazards, quantify the source term and impacts of postulated accidents, and establish appropriate preventive and mitigative controls. This process is normally done with two sets of analyses, (1) the hazard analysis, and (2) the accident analysis. While a detailed overview is included in Appendix A on the characteristics of the phases of safety analysis, it is important to note that the hazard analysis phase is largely qualitative. In performing accident analysis, computer codes are often applied to quantify the source term from the accident sequence and/or to evaluate the potential consequences. While the accident analysis phase is quantitative, typically the process is based on sequential conservative inputs, assumptions, and computations. The result of this latter phase is that the overall outcome should result in sufficient margin to compensate for a non-conservative step, whether computer-based or not.

The results of the consequence phase of analysis are used primarily for the determination of Safety Class Structures, Systems, or Components (SSCs) (Appendix A to DOE-STD-3009-94). One of the major areas reviewed in examining the overall safety analysis is whether the subsequent safety classification of required systems is made correctly, and that the analysis has built in sufficient safety margin.

Data obtained from the field survey will be used to assess the degree of reliance on computer modeling for developing the safety bases for nuclear facilities. Category 2 facilities are expected to warrant the most frequent application of safety-related software. Conversely, Category 3 and lower facilities would merit relatively few applications of the same-level sophistication of software. An example of the latter might be addressing the near-field effects of a thermal plume emanating from a postulated fire in a Hazard Category 3 facility.

Consistent with the Department's ISM principles and guidelines, line management has the responsibility of assuring safety, including appropriate development, maintenance, and use of safety-related software that can potentially affect the safety at DOE's nuclear facilities. DOE personnel rarely develop or use the computer codes for performing safety analyses. DOE, however, is responsible for reviewing and approving safety basis documentation prepared by the management and operating contractors. Since DOE has not formally "licensed" the codes that are used in safety analysis, code usage and associated results are reviewed for their technical accuracy or appropriateness as part of the safety analysis review process. DOE-STD-3009-94 provides guidance in terms of what should be expected in terms of documentation when computer modeling is used as part of the accident analysis process.

2.1 Considerations and Protocol

As noted in the subject DNFSB report, SQA is a process for the systematic development, testing, documentation, maintenance, and execution of software. When applied to accident analysis codes, specifically those applied as estimation tools to quantify source terms (from fire, spill, and explosion events) and the subsequent atmospheric dispersion and consequences, robust SQA processes help ensure the adequacy of facility SSCs. Additionally, the associated safety documentation is a more defensible basis for safe operation of the facility in question, when under-girded by software at or above the level of the Toolbox codes.

A collection of software applied extensively for DOE facility safety, and configuration-controlled by an independent organization, is a key recommendation advised in TECH-25 to enhance SQA throughout the DOE safety analysis community. The Toolbox of accident analysis software ensures elimination of redundancies in error reporting & correction, release of new code versions and accompanying documentation, and provides a single authority for ensuring code improvements. The Toolbox maintainer is best conceptualized as a central software organization, composed of software quality experts and accident analyst code users, charged with keeping user groups aware of physical and mathematical assumptions and limitations stemming from use of a particular code. The maintainer would not necessarily be responsible for directly accomplishing software changes, but would work closely with the individual code owners such that user group issues are effectively resolved.

2.2 Defense Applications and Commercial Nuclear Sectors

The defense applications and commercial nuclear sectors apply SQA processes to safety-related design and analysis computer codes used for various purposes. Because of the related nature of these activities to use of software for DOE safety analysis, this section highlights several aspects of the SQA programs.

Defense Applications

The focus of the defense applications sector review will be on the Verification, Validation, & Accreditation (VV&A) phases of the SQA process. Although each branch has specific guidance, the overall framework and general format is discussed in two Department of Defense (DoD) documents (DoD 1996, DoD 1996a). These documents refer to running a computer model as a simulation. Hence, executing a software package is a modeling and simulation (M&S) of a process.

If a rigorous and formal implementation is followed based on the guidance documents, an independent VV&A (IVV&A) process is conducted. IVV&A refers to separation among software designer, user, and assessor groups. The intent of IVV&A is to provide the documented assurance that the selected M&S not only provides output that meets the expectations of the designer, but that the M&S is applicable to the specific task being performed. Furthermore, the guidance defines VV&A not merely as a step that is performed at the end of a project, but ideally as an ongoing process that starts during the design phase of the M&S.

The DoD guides also recommend a level of effort for a particular VV&A process that depends on which of the following categories the applicable M&S falls into:

1. Previously accredited based on verification and validation data that is available:
2. Previously accredited based on historical use;
3. Not previously accredited, but some verification and validation data available; and
4. Not previously accredited with no verification and validation available.

Commercial Nuclear

Depending on the specific nuclear technology and facility being licensed, the U.S. Nuclear Regulatory Commission (NRC) applies a graded approach to SQA requirements. Several areas are briefly discussed: power and fuel reprocessing plants, special nuclear material, and the Yucca Mountain project.

Under the requirements of Appendix B to 10 CFR Part 50, *Quality Assurance Criteria for Nuclear Power Plants and Fuel Reprocessing Plants*, every commercial plant and fuel processing plant applicant (for a construction permit) is required by the provisions of §50.34 to include in its preliminary SAR a description of the QA program to be applied to the design, fabrication, construction, and testing of the structures, systems, and components of the facility. Every applicant for an operating license is required to include, in its final SAR, information pertaining to the managerial and administrative controls to be used to ensure safe operation. Nuclear power plants and fuel reprocessing plants include structures, systems, and components that prevent or mitigate the consequences of postulated accidents that could cause undue risk to the health and safety of the public. QA requirements for the design, construction, and operation of those structures, systems, and components are established in Appendix B to 10 CFR 50. The requirements of Appendix B apply to all activities affecting the safety-related functions of those structures, systems, and components (including designing, purchasing, fabricating, handling, shipping, storing, cleaning, erecting, installing, inspecting, testing, operating, maintaining, repairing, refueling, and modifying).

As used in Appendix B, "quality assurance" comprises all those planned and systematic actions necessary to provide adequate confidence that a structure, system, or component will perform satisfactorily in service. In this case, QA includes quality control, which comprises those QA actions related to the physical characteristics of a material, structure, component, or system that provide a means to control the quality of the material, structure, component, or system to predetermined requirements.

Although these sections do not specifically address software quality, it does indicate that QA criteria apply to activities (e.g., design, test, operation, and modification) associated with safety-related functions of structures, systems, and components important to safety. By inference, software used to support such activities would be expected to be subject to applicable requirements of Subpart B.

Similar arguments for judicious application of SQA to software-supported safety-related design and analysis activities may be interpreted from Part 70 (*Domestic Licensing of Special Nuclear Material*) and Section 142 (*Quality Assurance Criteria*) to Part 63 (*Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada*). In the latter example, the DOE QA program for the Yucca Mountain site characterization includes a discussion of how the applicable requirements of Appendix B are met (DOE 1998). The QA program contains controls for software that appear in ASME NQA-1-1997, Part II, Subpart 2.7, such as: (1) software life cycles, baselines, and controls; (2) software verification and validation; (3) software configuration management; (4) defect reporting and resolution; (5) control of the use of the software; and (6) software documentation. It should be noted that the NRC has reviewed this plan and found it acceptable.

2.3 Candidate Software

DOE has outlined a process, directed by a Safety Analysis Software Group (SASG), for identifying initial codes for the Safety Analysis Toolbox in a response plan to the DNFSB (DOE, 2000). The SASG was formed in early 2001 and is composed of representatives from National Nuclear Security Agency – Defense Programs (NNSA-DP) national laboratories and sites, and several line organizations within DOE. The primary task of the SASG shall be to review responses from a survey of SQA practices, processes, and procedures from DOE contractors. A section of data from this survey will identify those codes broadly used for facility accident analysis at DOE laboratories and sites. Once this set is known and the individual codes screened for meeting minimum threshold criteria and compliance with minimum SQA standards, tailored programs will be proposed to bring tool-box constituent codes into an acceptable state of SQA readiness for accident analysis applications.

The major steps of this process have been completed, including

- Development, distribution, and receipt of a DOE Safety Contractor Survey of SQA practices, processes, and procedures[1];
- Analysis of survey results;
- Identification of computer codes that are widely applied in support of accident analysis;
- Screening the high-use codes with minimum requirements criteria as a down-select process; and
- Determination of candidate codes for the Toolbox.

2.4 Safe Harbor Computer Codes

Review of the DOE SQA Survey indicates that over two hundred computer codes are used in some manner for one or more safety analysis functions in DOE facility hazard, accident, criticality safety and emergency preparedness areas (Attachment 1). The Survey also suggests that safety analysis contractors have applied widely varying approaches to software development, testing, documentation, maintenance, and usage (Appendix B). Furthermore, few, if any programs, are fully compliant with governing DOE Orders and industry guidelines, such as DOE G 200.1-1, DOE G 414.1-1, DOE O 200.1, DOE O 414.1, DOE O 420.1, ASME NQA-1-1997 Part II Subpart 2.7, and American National Standards Institute (ANSI)/American Nuclear Society (ANS)-10.4-1987.

While SQA upgrade of several hundred computer codes is resource-prohibitive, it is feasible to attempt to upgrade a handful of codes recognized to be high-use to a minimum level and establishing an initial Toolbox. It is expected that at minimum, some remedial effort will be required with most of the Toolbox candidate codes. Assuming that the effort is achievable on a code-specific basis in a timely manner, the codes may then be ready for configuration control, and subsequent DOE safety applications through the Toolbox distribution organization (Figure 1).

[1] For the remainder of this report, the survey shall be referred to as the "DOE SQA Survey," or "Survey."

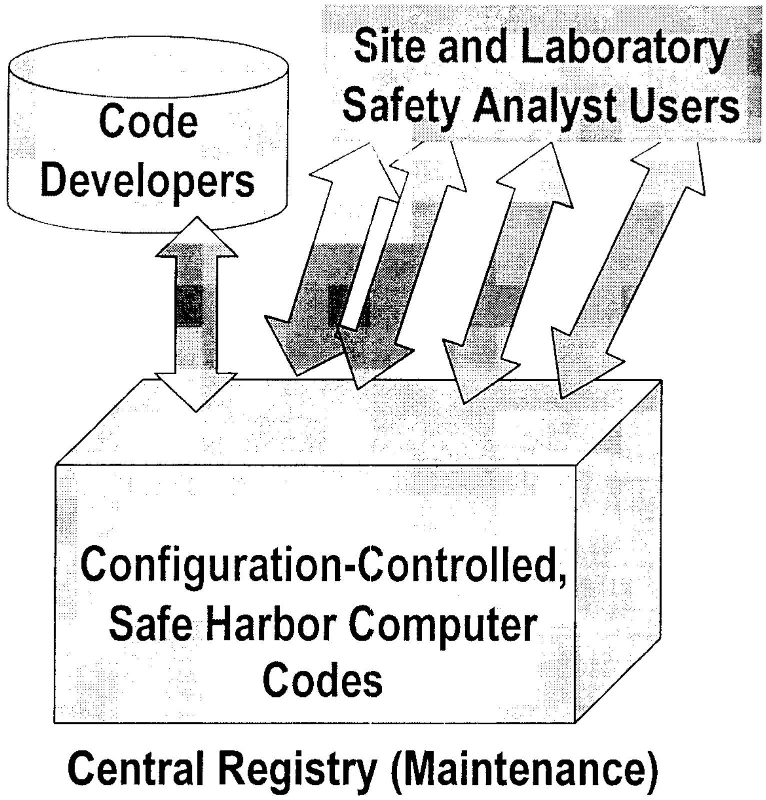

Figure 1. Toolbox distribution of codes & interface among code developers, users & registry.

The central registry organization would serve as the maintenance organization for the set of Toolbox codes. It would function for configuration control, distribution, and as a point of contact for dispositioning user issues. While a location has not been decided, an existing software center or one of the national laboratories is best able to support these functions with existing infrastructure.

In the context of 10 CFR 830, the Nuclear Safety Management rule, these codes may be thought of as "safe harbor" tools to be applied as appropriate for support of safety basis documentation. While the safety analyst would still need to justify the specific application, input parameters, and user assumptions, the burden would be limited. In most situations, the user would need to reference the Toolbox code and version, and demonstrate that the code is being applied in the proper context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as Toolbox-supported.

As an interim action, the SASG will issue a guidance document for each Toolbox code. The guidance will contain:

- Applicability guidance;
- Appropriate regimes, recommended configurations, and conditions to avoid;
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications;
- Default input values for site-independent parameters; and

- Citations of identified SQA documentation.

It is planned to guidance documents during calendar year (CY) 2002. The issuance of such documentation will allow qualified use of the Toolbox codes to support 10 CFR 830 safety analyses.

Maintaining Non-Toolbox Codes: Many sites apply software that has been tailored to their facilities and specific site (site-specific software). Similarly, an organization may have developed safety analysis software that is specific to a relatively unique process (process-specific software). Examples include, but are not limited to, a Lagrangian dispersion model that accounts for complex wind fields and terrain effects, or a damage model developed for high-explosive yield events, for site-specific and process-specific applications, respectively. As long as there is an ongoing and satisfactory SQA process associated with the single-site or unique-application software, the abandonment of computer codes and their safety basis applications is not desirable. Moreover, it is discouraged since there is a potential for "force-fitting" the standard Toolbox code to an application for which it is not suited, or spending an inordinate level of resources to explain the likely differences in outcome with the Toolbox code's predictions.

The preferred course of action in this case would be to continue to support the site- and process-specific code applications, *and* ensure that robust SQA processes are followed. If practicable, it would also be advised that an equivalency document be prepared, demonstrating that the chosen computer code is as appropriate as the standard tool for the application in question. Where significant deviations in results are found, justification for using the non-Toolbox code output is recommended. Additionally, periodic comparisons are recommended to the standard Toolbox code for applications that, on the basis of engineering judgment, are new application regimes or otherwise provide useful points of comparison. Good software application practice would be to document the basis for appreciable differences as identified.

An analogous situation occurred in the commercial nuclear industry in the 1970s and early 1980s with issuance of Regulatory Guide 1.145. A computer code, PAVAN[2], for quantification of dilution factors in compliance with the Regulatory Guide was made available to licensees. Most licensees, while applying PAVAN initially, later demonstrated equivalency with their own software. Commercial users have continued to develop their own codes, and PAVAN is not often applied today.

Rebaselining Analysis with Toolbox Codes: For some safety analysis organizations, switchover to a Toolbox code will be necessary. Inadequate QA documentation, instances of user misapplication, poor training, substandard support/maintenance/user assistance, and nonsystematic and inconsistent error notification are indications that a Toolbox code should be considered. However, each situation must be assessed given the status of the non-standard code QA and the specific demands upon it to support safety basis documentation.[3]

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[2] Bander, T.J., *PAVAN: An Atmospheric Dispersion Program for Evaluating Design Basis Accidental Releases of Radioactive Materials from Nuclear Power Stations*, NUREG/CR-2858 (PNL-4413). U.S. DOE Pacific Northwest Laboratory (November 1982).

[3] In situations where unique or questionable SQA status software pose application issues, the SASG can be contacted to assist the contractor.

2.5 Accident Phenomenology and Consequence Evaluation Program

Before results of the DOE Survey are discussed, it is helpful to outline the precursor study, the Accident Phenomenology and Consequence (APAC) Methodology Evaluation project (O'Kula, 1997). Much of the context for the current SASG can be better understood through a description of the earlier program and its process.

The APAC Methodology Evaluation Program was originated in 1995 at the request of the DOE DP Office. The purpose of the Program was to evaluate the accident analysis approaches (i.e., computer models and input assumptions) applied to support authorization basis documentation. This program was formed to address the increasing disparity in the application of codes and engineering methods among DOE Sites documented in SAR, Basis for Interim Operation (BIO), and hazard analysis documents. An Executive Committee directed the program and guided the evaluation process of software for source term development, in-facility transport, and dispersion/consequence analysis.

APAC Working Groups were formed through identification of the major areas required in accident analysis found in most DOE SARs written following guidance in DOE-STD-3009-94, and related documentation used in concert with the DOE Source Term Handbook, DOE-HDBK-3010-94 (DOE, 1994 and 1994 a). The Handbook provided a context for examining source term and dispersion/consequence analysis areas using six working groups:

Source Term Analysis
1. Fire Working Group (FWG)
2. Explosions and Energetic Events (EEE)
3. Spills Analysis (SWG)

In-Facility Transport Analysis

4. In-Facility Transport (IFT)

Atmospheric Dispersion/Consequence Analysis

5. Radiological Dispersion/Consequence (RDC)
6. Chemical Dispersion and Consequence Assessment (CDCA).

Each Working Group reviewed currently used computer models in its technical area. Computer models were identified by reviewing SARs and other Safety Basis documentation gleaned from the DOE facilities, as well as direct consultation with numerous accident and consequence analysts. Table 1 indicates the number of computer models evaluated by each group, staff participating, and the level of review depth. In total, on the order of fifty analysts supported the APAC in some capacity during the program. Nearly 200 were noted, reviewed, or evaluated in depth during the course of APAC evaluation.

As noted in Table 1, as many as ten safety analysts, model developers, and other technical support comprised each working group. Although approximately 50 individuals were involved in computer model evaluation, Working Group coordination, Executive Committee, or review capacity, the time-averaged support amounted to about three full-time equivalents per year. The program required approximately four years to complete.

Table 1. Computer Model Evaluation By Working Group

Working Group	Personnel	Decreasing Depth of Review →		
		Tier 1	Tier 2	Tier 3
1. Fire	6	5	-	-
2. Explosions and Energetic Events	9	-	-	10 (Models and Methods)
3. Spills	6	5	6	13
4. In-Facility Transport	6	5	-	-
5. Radiological Dispersion/Consequence	10	11	4	-
6. Chemical Dispersion & Consequence Assessment	7	14	11	110
Total Staff & Total Computer Models by Tier	44	40	21	133
Total Evaluated Models		194		

Generalized Evaluation Process and Code/Model Recommendations

The generalized evaluation process conducted by each Working Group followed these steps:

(I) Review of the regulatory documentation;
- (I.a) Identification of best practices - methods, assumptions, and parameter values to be followed as a norm;

(II) Development of Evaluation Criteria, including (1) General Software Quality and User Interface characteristics; (2) Technical Model Adequacy; (3) Application Environment (source term and range of applicability);
(III) Selection of candidate codes; and
(IV) Development of Test Problems. Several groups also conducted a limited ranking of computer models, i.e., quantitative "scoring" of computer models against detailed criteria.
(V) The Working Groups then executed the process on each code until all were evaluated.
(VI) Documentation and required rework of any of the process phases concluded the program.

A Tier 1 evaluation consisted of a thorough examination of code attributes and software documentation (approximately phases 1 through 3 above), and running one or more test problems. A Tier 2 evaluation was more limited, and did not include running the code against test problems. Several groups performed "Tier 3" reviews, and in these cases, the review was an acknowledgment of the availability of a computer model for the particular application, but was based on an abbreviated assessment of the code that omitted Tier I test case execution and a Tier II level of evaluation. A working group-specific summary of codes and recommendations is found in Appendix C.

Summary of APAC Evaluation Working Group Computer Code Recommendations

The SASG used the APAC Evaluation process to identify candidate computer codes for Toolbox consideration. These models, as noted in the discussion and tables above are restated in Table 2. A screening process will then be applied to rebaseline the APAC-recommended models in light of more recent regulatory requirements and new modifications made by several code organizations.

Table 2. Final APAC Methodology Evaluation Working Group Model Recommendations

APAC Phenomenology Area	Computer Models or Methodologies Appropriate for Accident and Consequence Analysis for Safety Basis Documentation
1. Fire	FIRAC/FIRIN, FPETool, CFAST
2. Explosion	TNT, Baker-Strehlow, or TNO model; as necessary, use the hydrodynamic codes.
3. Spill	ALOHA CASRAM HGSYSTEM HOTSPOT KBERT
4. In-Facility Transport	MELCOR, CONTAIN, GASFLOW
5. Radiological Dispersion and Consequence	MATHEW/ADPIC MACCS GENII UFOTRI (tritium)
6. Chemical Dispersion and Consequence Assessment	ALOHA DEGADIS HGSYSTEM SLAB EPIcode (Tier II model)

2.6 Rebaselining APAC Program Results: DOE SQA Survey Integration

Since the APAC Methodology Evaluation Program concluded in the late 1990s, computer models for accident analysis and usage patterns in the DOE Complex have changed. The SASG decided that although the earlier, comprehensive APAC program provides a useful starting point, it would be necessary to establish a new baseline, i.e., calibrate the older results against current day needs and application patterns on the part of users. The responses of the DOE Survey of Software Quality Processes, Practices, and Procedures ("DOE SQA Survey") were used in conjunction with "reasonable interpretation" of the APAC evaluations.

The DOE SQA Survey was transmitted in mid-2000 to site and laboratory safety contractors responsible for nuclear facility safety. The response was nearly 100%, and included 18 organizations at 11 DOE sites. The results identified clear trends in the use of computer models for facility safety basis purposes. However, to best apply the Survey results in light of the earlier APAC Program, it was deemed appropriate to develop a simple set of screening criteria.

The SASG defined screening criteria in terms of two categories. The first, a "go, no-go" set of criteria, are used to answer usage and appropriateness for meeting minimum requirements. If a computer model passed the threshold determinations, it was then evaluated relative to another set of criteria. These criteria are quantitative in terms of adequacy and quality of the software, and draw heavily from the APAC evaluations. The two sets of criteria are listed in Tables 3 and 4, respectively.

Results from the DOE SQA Survey were binned by general categories of accident phenomena, loosely equivalent to those used in the APAC Methodology Evaluation effort. The categories were as follows:

- Radiological Atmospheric Dispersion
- Chemical Atmospheric Dispersion
- Fire (zone fire modeling)
- Explosion
- In Facility Transport (Leak Path Factor)
- Criticality (and Shielding)
- Chemical Spill and Releases
- Other or Special Purpose (such as 3-D flow codes, heat conduction codes).

Upon review of the currently available software reported in the DOE SQA Survey, the mode of application of this software, and the analysis requirements imposed on accident analysts for DOE safety basis documentation, several categories were determined outside current scope, and will not be reviewed any further by the SASG. The Criticality software area is not central to the concerns articulated in the TECH-25 core issues of safety analysis. Furthermore, the SQA Survey results showed that this area is addressed mostly with engineering calculations, review of NUREG/CR-6410 (NRC, 1998), calculations using MCNP and/or SCALE systems of computer codes. Both of these code systems have appropriate SQA programs. It was also concluded that DNFSB Recommendation 97-02 and the DOE response and implementation plans covered the criticality area to a greater requisite depth than could the SASG.

Table 3. Computer Code Screening Criteria – "Threshold Requirements Met"

Criteria	Pass/Fail Level
Code Usage in the DOE Complex	Fail – 1 or no sites use this code Pass – 2 or more DOE sites use this code
Code meets minimum requirements*	Fail – Code does not meet the minimum model requirements for each code category Pass – Code meets the minimum model requirements as for each code category

Minimum requirements:

Radiological Dispersion and Consequence Analysis

- Ability to handle multiple weather data to meet requirements in DOE STD 3009-94, Appendix A for direction-independent 95th percentile χ/Q
- Ability to handle elevated releases
- Ability to modify dispersion coefficients

Fire Modeling

- DOE G-420.1/B-0, G-440.1/E-0, Implementation Guide for use with DOE Orders 420.1 and 440.1 Fire Safety Program
- ASTM E1355, Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models
- ASTM E1472, Standard Guide for Document Computer Software for Fire Models
- ASTM E1591, Standard Guide for Data for Fire Models
- ASTM E1895, Standard Guide for Determining Uses and Limitations of Deterministic Fire Models

Chemical Dispersion, Spills, Fire, In-Facility Transport/Leakpath Factor Analysis

- Follow & Supplement DOE STD-3009-94
- Follow & Supplement DOE-HDBK-3010-94

The second category to be omitted and not within the purview of the SASG is that of explosion (deflagration and detonation) computer codes. Several sites, notably Pantex and Lawrence Livermore National Laboratory (LLNL) use specific codes to determine blast effects, explosive yield, and overpressure among other consequences. However, there is not a specific workhorse code that is used at multiple locations that can justify consideration as part of the DOE Safety Analysis Toolbox. It should be noted that the APAC Working Group avoided recommendation of specific computer codes due to the complexity of this area. It is the expectation of the SASG that each site requiring use of an explosion code to support its Safety Basis demonstrate that the software has sufficient SQA measures in place.

Table 4. Quantitative Ranking Criteria

Criteria	Maximum Points	Scoring Mechanism
Capability and Versatility of Code	40	Assign a score based on APAC[4] detailed scoring scheme in APAC reports for each code category or have SASG qualitatively score each code based on input from the group Suggested scoring: Assign a score of 1 to 40 based on APAC data or qualitative data
Number of Code Users	20	Assign a score based upon SASG survey. Suggested scoring: Assign a score of 20 if five or more sites use code. Assign a score of 15 if three to four sites use code. Assign a score of 10 if at least two sites use code; 5 for one site.
APAC recommended code	10	Assign a score based on whether the code was recommended for usage by APAC. Suggested scoring: Assign a score of zero for non-recommended codes, assign a score of 10 for recommended codes
QA status	10	Assign a score based on code QA status Suggested scoring: Assign a score of zero for no or low documented QA. Assign a score of 5 for moderate QA. Assign a score of 10 for good to excellent QA.
User Interface	10	Assign a score based on a qualitative evaluation of code user interface. Suggested scoring: Assign a score of 0 for a poor interface. Assign a score of 5 for a good interface. Assign a score of 10 for a very good interface
Origin of Code	5	Assign a score based upon code origin. Suggested scoring: 5 if the code was developed, at least in part, by a DOE site, 0 if not. A score of 2 was applied for partial DOE site origin.
Code Sponsor	5	Assign a score based upon code sponsor. Suggested scoring: 5 if the code is sponsored, at least in part, by DOE, 0 if not.
Total Points	100	

[4] Accident Phenomenology and Consequence (APAC) Code Evaluation Project (1995 – 1998).

3.0 Software Candidates for DOE Safety Analysis Toolbox

The high-use computer models determined from the DOE SQA Survey, and those recommended from the APAC Methodology Evaluation program, are listed in Table 5. If a computer model was high-use (two or more sites) and met minimum performance requirements as interpreted from regulatory standards for that area, they are evaluated using the criteria discussed in Table 3 and 4. Examples of the regulatory standards for accident phenomenology include Appendix A of DOE Standard STD-3009-94 for radiological dispersion and consequence codes. Similarly, for fire zone modeling, DOE G-420.1/B-0, G-440.1/E-0, Implementation Guide for use with DOE Orders 420.1 and 440.1 Fire Safety Program, and associated American Society for Test Materials (ASTM) Standard Guides. The specific score by criterion is shown in Appendix D.

The quantitative criteria are used to identify strengths and weaknesses of the software potentially earmarked for the DOE Safety Analysis Toolbox. In this manner, any remedial actions identified by the SASG and recommended to the software owners can be prioritized. Secondly, the quantitative evaluation process facilitates impartial comparison of APAC Program recommended codes. Other than the Radiological Dispersion and Consequence Working Group, other working groups did not previously perform quantitative evaluations. Finally, use of quantitative criteria allows computer codes that were not reviewed by the APAC program to be considered in the SASG process.

By category of source term type and dispersion phenomenology, Table 5 highlights the codes that are candidates for the DOE Safety Analysis Toolbox including:

- Radiological Dispersion and Consequence Analysis – MACCS2, GENII
- Chemical Dispersion and Consequence Analysis – ALOHA, EPIcode
- Fire (Zone Models) – CFAST
- In-Facility Transport – MELCOR
- Chemical Release & Spills – ALOHA, EPIcode.

Note that the current list contains six models, since both ALOHA and EPIcode have source term and subsequent dispersion modules.

Despite having elements of a good, independent SQA program, two codes, HOTSPOT and RSAC-6, were not selected. Neither code can perform calculations in a mode compliant with the requirements of DOE STD-3009-94, Appendix A, without writing a "shell" set of instructions. While this is not a difficult task, a compensatory step such as this invites site-to-site nonstandardization. Also, the survey and informal checking by the found that RSAC-6 has not been applied outside of INEEL, and therefore does not meet the multiple-site use criterion outlined in Table 5.

Brief summaries are provided for each of the candidate codes. Strengths and weaknesses, and the respective SQA status are covered in later sections.

Table 5. Survey Code Screening

Computer Code	Threshold Criteria		Quantitative Criteria
	Usage	Meets Minimum Requirements	Total
	>=2 =1	Yes = 1	
Radiological Dispersion and Consequence Analysis			
MATHEW/ADPIC	0	1	80
MACCS MACCS2	**1**	**1**	**86**
GENII	**1**	**1**	**69**
HOTSPOT	1	0	64
UFOTRI	0	1	32
Chemical Dispersion and Consequence Analysis			
ALOHA	**1**	**1**	**75**
DEGADIS	0	1	50
HGSYSTEM	0	1	67
SLAB	0	1	59
EPIcode	**1**	**1**	**65**
Fire (Zone Models)			
CFAST	**1**	**1**	**65**
FIRAC/FIRIN	0	1	70
FPETool	0	1	40
In-Facility Transport			
CONTAIN	0	1	40
MELCOR	**1**	**1**	**80**
GASFLOW	0	1	65
Chemical Release & Spills			
ALOHA	**1**	**1**	**70**
CASRAM	0	1	50
EPIcode	**1**	**1**	**65**
HGSYSTEM	0	1	57
Other Special Purpose			
FLUENT	**1**	**N/A**	**See Text.**

ALOHA: The Areal Locations of Hazardous Atmospheres (ALOHA) code was jointly developed by the U.S. Environmental Protection Agency (EPA) and the hazardous materials division of National Oceanic and Atmospheric Administration (NOAA). It is part of the Computer-Aided Management of Emergency Operations (CAMEO) program and is used primarily for emergency response situations and for training. As such, it is user-friendly, allowing easy data input and convenient output of areal maps with contours of concentration of hazardous chemicals. Many of the internal features of the code are hidden from the user in order to make it more user-friendly. The code is intended for the evaluations of the consequences of chemical releases, but not intended for radiological, releases. If the chemical released is a heavy gas, a heavy-gas model (i.e., a stripped-down version of DEGADIS) is used; otherwise, a neutrally buoyant Gaussian model is used. To quote from the ALOHA User's Manual (EPA, 1995):

> ALOHA can predict the rates at which chemical vapors may escape into the atmosphere from broken gas pipes, leaking tanks, and evaporating puddles. It can then predict how a hazardous gas cloud might disperse in the atmosphere after an accidental chemical release. ... Its chemical library contains information about the physical properties of about 900 common hazardous chemicals. Its computations represent a compromise between accuracy and speed: it has been designed to produce good results quickly enough to be of use to responders. ALOHA is designed to minimize operator error.

The user identifies a unique release location, the released pure chemical, and weather data (i.e., constant weather conditions only), describes the chemical escape from containment (e.g., a broken pipe); and requests the type of output, such as the chemical concentration isopleth (e.g., downwind regions of equivalent air concentration). The user can also view graphs of predicted chemical concentrations at any location of special interest, such as a school or hospital, and the chemically induced doses to persons at that location. In order to derive a profile of concentration with distance, multiple runs with different input distances are required since ALOHA can only be executed for one downwind-crosswind distance conjugate pair. One of the ALOHA code's strengths is that it can a address a wide range of chemical accident sequences with its very mature 947 item chemical data base library and release types such as direct, puddle, pipe, and tank. ALOHA is very interactive and aids the analyst during its application. It prevents the analyst from evaluating inconsistent scenarios, such as a tank that is 168% full, with appropriate warning messages.

ALOHA, like all Gaussian models that are steady-state by definition, is not reliable for very low wind speeds, for very stable atmospheric conditions, for shifting winds and terrain-steering situations, or for concentration patchiness. ALOHA does permit changes in the wind direction parameter every 15-minutes when the Site Acquisition of Meteorology (SAM) component is applied.[5] Because ALOHA does not calculate plume rise for ground level releases, it does not realistically account for the enormous buoyancy effects of fires. ALOHA only addresses pure chemicals and consequently is not capable of analyzing the complexities of atmospheric chemistry associated with chemical reactions and mixtures of chemicals. Since ALOHA does not have any algorithms that account for dry deposition, wet deposition, plume depletion, and resuspension, it does not do particularly well for releases that contain particulates (i.e., non-gases). ALOHA is a

[5] The user has an option of "attaching" a small meteorological tower to provide real-time data. When used in this mode, changes in wind direction allow the plume to bend in the downwind direction. This is known as the segmented Gaussian plume.

straight-line, or at best, a segmented plume Gaussian model, which limits its ability to address complex flows associated with complex terrain.

ALOHA is maintained by the EPA. Version 5.2.3 can be obtained from the EPA web site (http://www.epa.gov/ceppo/cameo/aloha.htm).

CFAST: The computer software, Consolidated Model of Fire Growth and Smoke Transport (CFAST), was developed by the National Institute of Standards and Technology (NIST). This software operates under the shell program Fire Growth And Smoke Transport (FAST). CFAST is capable of predicting the environment in a multi-compartment structure subjected to a fire. It calculates the time evolving distribution of smoke and fire gases and the temperature throughout a building during a user-specified fire. CFAST is the result of a merger of ideas that came out of the FAST and the CCFM.VENTS development projects at NIST. The organization of the CFAST suite of programs is thus a combination of the two models. Although it may not be all-inclusive, CFAST has demonstrated the ability to make reasonably good predictions. Also, it has been subject to close scrutiny to insure its correctness. Thus it forms a prototype for what constitutes a reasonable approach to modeling fire growth and the spread of smoke and toxic gases.

CFAST is a member of a class of models referred to as zone or finite element models. This means that each room is divided into a small number of volumes (called layers), each of which is assumed to be internally uniform. That is, the temperature, smoke and gas concentrations within each layer are assumed to be exactly the same at every point. In CFAST, each room is divided into two layers. Since these layers represent the upper and lower parts of the room, conditions within a room can only vary from floor to ceiling, and not horizontally. This assumption is based on experimental observations that in a fire, room conditions do stratify into two distinct layers. While we can measure variations in conditions within a layer, these are generally small compared to differences between the layers.

CFAST consists of a collection of data and computer programs, which are used to simulate the important time-dependent phenomena involved in fires. The major functions provided include calculation of:

- the production of enthalpy and mass (smoke and gases) by one or more burning objects in one room, based on small- or large-scale measurements;
- the buoyancy-driven as well as forced transport of this energy and mass through a series of specified rooms and connections (e.g., doors, windows, cracks, ducts); and
- the resulting temperatures, smoke optical densities, and gas concentrations after accounting for heat transfer to surfaces and dilution by mixing with clean air.

CFAST is based on solving a set of equations that predict state variables (pressure, temperature and so on) based on the enthalpy and mass flux over small increments of time. These equations are derived from the conservation equations for energy mass, and momentum, and the ideal gas law. These conservation equations are always correct, everywhere. Thus, any errors that might be made in these areas likely arise from simplifying assumptions or from processes left out.
CFAST Version 3.1.6 is available from NIST. Information can be obtained from http://cfast.nist.gov/.

EPIcode: The Emergency Prediction Information code, or EPIcode, was originally developed at LLNL. EPIcode has many similarities to the ALOHA and ARCHIE codes in that it is a straight-line Gaussian model with an extensive chemical library. Unlike ALOHA, EPIcode can only address direct and puddle chemical release scenarios since it does not contain pipe and tank sub-models. However, EPIcode can assess area releases, fire releases, and explosion releases. The EPIcode chemical library is slightly smaller than that in ALOHA, but it still addresses more than 600 specific chemicals. EPIcode is available in a DOS version, but a new Windows version is presently under development. EPIcode also has the capability to assess the effects of fires and explosions.

To quote from the EPIcode manual (Homann, 1996):

> The EPIcode program was developed to provide emergency response personnel and emergency planners with a software tool to help evaluate the atmospheric release of toxic substances. EPIcode allows fast estimation and assessment of chemical release scenarios associated with accidents from industry and transportation. The software cab also be used for safety analysis planning purposes on facilities handling toxic materials. Additionally, this program can provide a rapid first-order check against complex and more data-intensive models running on larger computers.

EPIcode is menu-driven and user friendly, requiring minimal user training. It contains a good graphics package. The EPIcode User Manual also contains 11 case studies showing how the code can assess a wide range of chemical accident scenarios.

EPIcode Revision 6.0 is currently available from Homann Associates, Inc. (epicode@aol.com), which maintains and upgrades the code. The code author, Steve Homann, can also be contacted directly at shomann@llnl.gov.

GENII: Version 2.0 was released by the DOE Pacific Northwest National Laboratory (PNNL) in 1999, and is supported by the U.S. EPA. GENII Version 2 is the latest in a series of generalized software systems to provide a state-of-the-art, technically peer-reviewed, documented set of programs for calculating radiation dose and risk from radionuclides released into the environment. The GENII System includes capabilities for calculating radiation doses following postulated chronic and acute releases. Radionuclide transport via air, water, or biological activity may be considered in an integrated manner. Air transport options include both puff and plume modes, with each allowing use of an effective stack height or calculation of plume rise from buoyant or momentum effects (or both). Building wake effects can be included in acute atmospheric release scenarios.

Four independent atmospheric models, one surface water model, three independent environmental accumulation models, one exposure module, and one dose/risk module, is supplied with GENII. Computer programs are of several types: user interfaces (i.e., interactive, menu-driven programs to enable scenario generation and data input), internal and external dose factor libraries, environmental dosimetry programs, and Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES)-supplied file viewing routines.

GENII 2.0 data entry is accomplished by interactive, menu-driven user interfaces. Default exposure and consumption parameters are provided for the maximum exposed individual and the average (population), and may be modified by the user. Source term information may be entered as radionuclide release quantities for transport scenarios, or as basic radionuclide concentrations in environmental media. For input of basic or derived concentrations, decay of parent radionuclides and ingrowth of radioactive decay products prior to the start of the exposure scenario may be considered. A single code run can accommodate unlimited numbers of radionuclides including the source term and any radionuclides that accumulate from decay of the parent, because the system works sequentially on individual decay chains.

The current code package provides interfaces, through FRAMES, for external calculations of atmospheric dispersion, geohydrology, biotic transport, and surface water transport. Target populations are identified by direction and distance (radial or square grids for Version 2) for individual receptors, population groups, and for intruders into contained sources.

GENII Version 1 implemented dosimetry models recommended by the International Committee on Radiological Protection (ICRP) in Publications 26, 30, and 48, and approved for use by DOE O 5400.5. GENII Version 2 implements the same models but has capabilities to use ICRP Publications 56 through 72, and the related risk factors published in Federal Guidance Report 13. Risk factors in the form of EPA-developed slope factors are also included.

DOE users may contact PNNL (http://mepas.pnl.gov:2080/FRAMES/GENII/Download.html) and Bruce Napier (BRUCE.NAPIER@pnl.gov) for requests for, and technical questions on GENII.

MACCS/MACCS2: The MELCOR[6] Accident Consequence Code Systems (MACCS) code, and its successor code, MACCS2, is based on the straight-line Gaussian plume model. MACCS (Chanin, 1990, 1992a, 1992b) was developed originally for the NRC, whereas MACCS2 is an enhanced version that was developed with DOE applications in mind. These codes evaluate doses and health risks from the accidental releases of radionuclides. To quote from the *MACCS2 User's Guide* (Chanin 1998):

> The principal phenomena considered in MACCS/MACCS2 are atmospheric transport and deposition under time-variant meteorology, short-term and long-term mitigative actions and exposure pathways, deterministic and stochastic health effects, and economic costs. ... The MACCS2 package includes three primary enhancements: (1) a more flexible emergency response model, (2) an expanded library of radionuclides, and (3) a semi-dynamic food chain model. The new code features allow detailed evaluations of risks to workers at nearby facilities on large DOE reservations and allow the user to assess the potential impacts of over 500 radionuclides that cannot be considered with MACCS.

MACCS/MACCS2 cannot be considered user-friendly, but the user has control over nearly every input parameter. These include the following:

- Mesh intervals for the spatial grid,
- Receptor position and population distribution,
- Weather scenario [constant weather, various variable-weather scenarios (e.g., using one year of hourly averages of wind speed and direction, stability class, precipitation), and type of weather sampling],

[6] (MELCOR) Methods for Estimation of Leakages and Consequences of Releases) is an integrated code package for severe accident and source term modeling code (see next section).

- Dispersion parameter set and power law constants,
- Release height, number and duration of plumes,
- Radionuclides (i.e., over 800 radionuclides are available in the MACCS2 dose conversion factor database, an increase of over 500 from MACCS),
- Organ doses and health risks to evaluate,
- Dose conversion factor files,
- Evacuation timing and routes,
- Costs of decontamination and interdiction,
- Sensible heat[7],
- Radiation shielding parameters, and
- Deposition and resuspension.

The entire list includes other features, further demonstrating the versatility of the code. However, these are of lesser importance from a DOE safety basis perspective and are not included here.

MACCS2 can be obtained from the Radiation Safety Information Computational Center (http://www-rsicc.ornl.gov/rsic.html) at Oak Ridge National Laboratory. Information on MACCS2 can be downloaded from http://epicws.cped.ornl.gov/codes/ccc/ccc6/ccc-652.html. The technical point of contact is Nathan Bixler at Sandia National Laboratories (nbixler@sandia.gov).

MELCOR: MELCOR (Methods for Estimation of Leakages and Consequences of Releases) is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. Major uses of MELCOR for nonreactor facilities include estimation of confinement behavior due to radiological source terms (and their sensitivities and uncertainties in a variety of applications), evaluation of leakpath factors, and survivability of fans, filters, and other Engineering Safety Features (ESFs).

The MELCOR code is composed of an executive driver and a number of major modules, or packages, that together model the major systems of a reactor plant and their generally coupled interactions.

Nuclear facility response to off-normal or accident conditions include:

- thermal-hydraulic response of the primary reactor coolant system, the reactor cavity, the containment, and the confinement buildings:
- core uncovering (loss of coolant), fuel heatup, cladding oxidation, fuel degradation (loss of rod geometry), and core material melting and relocation;
- heatup of reactor vessel lower head from relocated fuel materials and the thermal and mechanical loading and failure of the vessel lower head, and transfer of core materials to the reactor vessel cavity;
- core-concrete attack and ensuing aerosol generation;

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[7] The sensible heat (enthalpy) of an air parcel is the sum of its internal (thermal) energy and the potential energy associated with its pressure and density. It is to be contrasted with latent heat and radiant heat.

- in-vessel and ex-vessel hydrogen production, transport, and combustion;
- fission product release (aerosol and vapor), transport, and deposition;
- behavior of radioactive aerosols in the reactor containment building, including scrubbing in water pools, and aerosol mechanics in the containment atmosphere such as particle agglomeration and gravitational settling; and
- impact of engineered safety features on thermal-hydraulic and radionuclide behavior.

The various code packages have been written using a carefully designed modular structure with well-defined interfaces between them. This allows the exchange of complete and consistent information among them so that all phenomena are explicitly coupled at every step. The structure also facilitates maintenance and upgrading of the code.

Initially, the MELCOR code was envisioned as being predominantly parametric with respect to modeling complicated physical processes (in the interest of quick code execution time and a general lack of understanding of reactor accident physics). However, over the years as phenomenological uncertainties have been reduced and user expectations and demands from MELCOR have increased, the models implemented into MELCOR have become increasingly best estimate in nature. The increased speed (and decreased cost) of modern computers (including PCs) has eased many of the perceived constraints on MELCOR code development. Today, most MELCOR models are mechanistic, with capabilities approaching those of the most detailed codes of a few years ago. The use of models that are strictly parametric is limited, in general, to areas of high phenomenological uncertainty where there is no consensus concerning an acceptable mechanistic approach.

Current uses of MELCOR often include uncertainty analyses and sensitivity studies. To facilitate these uses, many of the mechanistic models have been coded with optional adjustable parameters. This does not affect the mechanistic nature of the modeling, but it does allow the analyst to easily address questions of how particular modeling parameters affect the course of a calculated transient. Parameters of this type, as well as such numerical parameters as convergence criteria and iteration limits, are coded in MELCOR as sensitivity coefficients, which may be modified through optional code input.

MELCOR modeling is general and flexible, making use of a "control volume" approach in describing the nuclear facility. No specific nodalization of a system is forced on the user, which allows a choice of the degree of detail appropriate to the task at hand.

The most recent update of the MELCOR computer code manuals corresponds to MELCOR version 1.8.5, released to users in October 2000. The new version contains many new modeling features as well as improvements to existing models. New models include an iodine chemistry model, updates to several of the code default values, improvements to the hygroscopic aerosol model, and enhancements to both the user control function feature and plotting features.

Volume 1 contains a primer that describes MELCOR's phenomenological scope, organization (by package), and documentation. The remainder of Volume 1 contains the MELCOR User's Guides, which provide the input instructions and guidelines for each package. Volume 2 contains the MELCOR Reference Manuals, which describe the phenomenological models that have been implemented in each package. A new volume to this publication is added with the MELCOR 1.8.5 release that contains a portfolio of sample demonstration problems. These problems are a combination of experiment analyses, which illustrate code model performance against data, and full plant analyses showing MELCOR's performance on larger realistic problems.

The NRC endorsed Version 1.8.5 of MELCOR in May 2000. It is available from the NRC to eligible domestic and foreign requestors by submitting requests to www.nrc.gov/RES/MELCOR/obtain.html.

Process-Specific Software

In the Special Purpose category, the proprietary code FLUENT is used at several locations to examine mixing phenomena and multidimensional effects associated with deflagration events. However, there are insufficient common applications in the same topical area to warrant consideration of FLUENT as a candidate Toolbox code. It would be expected that each laboratory or site applying FLUENT have sufficient SQA procedures in effect before quantitative results are used as part of Safety Basis documentation.

Several sites with accident analysis issues concerning high-explosive detonation phenomena have developed their own suites of software. Again, there is inadequate justification for this software to be included in a common DOE software Toolbox since the user group is relatively isolated, and the site in question is expected to have the proper SQA program in place.

3.1 Strengths of Candidate Codes

Strengths of the six software packages have been discussed earlier in the code summaries provided in the previous section, as well as information gleaned from accident analysis sources. Table 6 reviews the major strengths in list form, associated with each code.

Table 6. Code Strengths

Computer Code	Major Strengths
ALOHA Version 5.2.3	• EPA-maintained • CAMEO-supported, large (> 900) chemical database • Easily understood user interface • Dense gas behavior model • Area release capability
CFAST Version 3.1.6	• FAST/CFAST is a widely available software package that is maintained by NIST. • Versions are being developed which are compatible with newer Windows operating systems. (Unlike other fire modeling software, which is not compatible with Windows 98 and higher.) • Training is provided by SFPE and others. • User interface is simple and easy to understand. • It is a workhorse for not only DOE contractors, but recognized throughout the fire protection industry.
EPIcode Revision 6.0	• Useful chemical library (~600 chemical species) • Elevated plumes may be modeled • Area release capability • Fire and explosion release models
GENII Version 2	• User-friendly, environmental transport system • State-of-the-art software engineering • Acute and chronic time frames • Large radionuclide grouping capable of being handled per execution • ICRP 26/30 and 60 doses; FGR 13 Risks • Excellent tabular and graphics reports of output data • Near-complete SQA Program
MACCS2 Version 1.12	• Large radionuclide grouping capable of being handled per execution • Large Dose conversion factor database (~800 radionuclides) • ICRP 26/30 and 60 dose models • Successor to CRAC, CRAC2, and MACCS computer codes • User-driven input options for meteorology, source term description, dispersion parameter sets, receptor location
MELCOR 1.8.5	• Modular architecture – User specified • Fast-running, implementation of many mechanistic features • NRC-based pedigree • Primary and Confinement/Containment; ESF modules

3.2 Limitations/Weaknesses of Candidate Codes

ALOHA

A limitation of ALOHA for most DOE safety basis applications is that it is a tool designed primarily for emergency preparedness support. As such, the user may infer the proper meteorological conditions characteristic of the site and facility in question and apply persistent meteorology assumptions. For large DOE sites, the spatial extent of the model may demand application of extrapolation methods since output concentration results are limited to 10 kilometers.

While dense gas behavior may be modeled in some source geometries (e.g., pipe break), other sources demand the user input this information. This is not an insurmountable problem but may demand more time and resources than available. Additionally, sensible heat and elevated sources are not treatable in ALOHA.

Chemical species in concentrations less than maximum cannot be modeled with the current code. User-supplied interpolation schemes must be applied. A major limitation of this code is the lack of a full set of SQA documentation. Each site must determine compliance activities appropriate for safety analysis support.

CFAST

An important limitation of CFAST is the absence of a fire growth model. At the present time, the CFAST owner indicates it is not practical to adapt currently available fire growth models for direct inclusion in CFAST. Therefore, the system utilizes a user specified fire, expressed in terms of time specified rates of energy and mass released by the burning item(s). The user must obtain these data from measurements taken in large- and small-scale calorimeters, or from room burns.

The provided data and procedures only relate directly to burning of items initiated by relatively large flaming sources. Little data are currently available for release rates under smoldering combustion, or for the high external flux and low oxygen conditions characteristic of post-flashover burning. While the model allows multiple items burning simultaneously, it does not account for the synergy of such multiple fires. Thus, for other ignition scenarios, multiple items burning simultaneously (which exchange energy by radiation and convection), combustible interior finish, and post-flashover conditions, the model can give estimates that are often nonconservative (the actual release rates would be greater than estimated). At present, the only sure way to account for all of these complex phenomena is to conduct a full-scale room burn and use the pyrolysis rates directly. The CFAST developers indicate that subsequent versions of the model will include detailed combustion models that can be used as the source fire.

The basic assumption of CFAST and all zone fire models is that each room can be divided into a small number of control volumes, each of which is internally uniform in temperature and composition. In CFAST, all rooms have two zones except the fire room, which has an additional zone for the fire plume. The boundary between the two layers in a room is called the interface.
It has generally been observed that in the spaces close to the fire, buoyantly stratified layers form. While in an experiment the temperature can be seen to vary within a given layer, these variations are small compared to the temperature difference between the layers.

Beyond the basic zone assumptions, the model typically involves a mixture of established theory (e.g., conservation equations), empirical correlations where there are data but no theory (e.g., flow and entrainment coefficients), and approximations where there are neither (e.g., post-flashover combustion chemistry) or where their effect is considered secondary compared to the "cost" of inclusion. An example of a widely used assumption is that the estimated error from ignoring the variation of the thermal properties of structural materials with temperature is small. While this information would be fairly simple to add to the computer code, data are scarce over a broad range of temperatures even for the most common materials.

With a highly complex model such as CFAST, the only reasonable method of assessing impacts of assumptions and limitations is through the verification process, which is ongoing at the Building and Fire Research Laboratory. Until the results of this process are available, the user should be aware of the general limits of zone modeling and some specific manifestations in CFAST. These include the following:[8]

1. Burning can be constrained by the available oxygen. However, this "constrained fire" (a "type 2" fire, see page 17) is not subject to the influences of radiation to enhance its burning rate, but is influenced by the oxygen available in the room. If a large mass loss rate is entered, the model will follow this input until there is insufficient oxygen available for that quantity of fuel to burn in the room. The unburned fuel (sometimes called excess pyrolyzate) is tracked as it flows out in the door jet, where it can entrain more oxygen. If this mixture is within the user-specified flammable range, it burns in the door plume. If not, it will be tracked throughout the building until it eventually collects as unburned fuel or burns in a vent. The enthalpy released in the fire room and in each vent, as well as the total enthalpy released, is detailed in the output of the model. Since mass and enthalpy are conserved, the total will be correct. However, since combustion did not take place adjacent to the burning object, the actual mass burned could be lower than that specified by the user. The difference will be the unburned fuel.

2. An oxygen combustion chemistry scheme is employed only in constrained (type 2) fires. Here user-specified hydrocarbon ratios and species yields are used by the model to predict concentrations. A balance among hydrogen, carbon, and oxygen molecules is maintained. Under some conditions, low oxygen can change the combustion chemistry, with an attendant increase in the yields of products of incomplete combustion such as CO. Guidance is provided on how to adjust the CO/CO2 ratio. However, not enough is known about these chemical processes to build this relationship into the model at the present time. Some data exist in reports of full-scale experiments (e.g., reference), which can assist in making such determinations.

3. The entrainment coefficients are empirically determined values. Small errors in these values will have a small effect on the fire plume or the flow in the plume of gases exiting the door of that room. In a multi-compartment model such as CFAST, however, small errors in each door plume are multiplicative as the flow proceeds through many compartments, possibly resulting in a significant error in the furthest rooms. The data available from validation experiments indicate that the values for entrainment coefficients currently used in most zone models produce good agreement for a three-compartment configuration. More data are needed for larger numbers of rooms to study this further.

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[8] This discussion was provided by the NIST organization.

4. In real fires, smoke and gases are introduced into the lower layer of each room primarily due to mixing at connections between rooms and from the downward flows along walls (where contact with the wall cools the gas and reduces its buoyancy). Doorway mixing has been included in CFAST, using an empirically derived mixing coefficient. However, for smoke flow along a wall, the associated theory is only now being developed and is not included in the model. This may produce an underestimate of the lower layer concentrations. The most important manifestation of this underestimate will be the temperature distribution between the upper and lower layers caused by radiation.

5. The only mechanisms provided in zone models to move enthalpy and mass into the upper layer of a room are two types of plumes: those formed by the burning item(s) in the fire room, and those formed by the jet of upper layer gases flowing through an opening. Thus, when the model calculates the flow of warm, lower layer gases through a low opening (e.g., the undercut of a "closed" door) by expansion of the smoke layer, they are assigned to the lower layer of the room into which they flowed where they remain until the upper layer in the source room drops to the level of the undercut and the door jet forms. Thus, for a time the receiving room can show a lower layer temperature that exceeds that in the upper layer (a physically impossible condition). A better understanding of the flow within compartments in the context of a zone fire model would allow us to remove this anomaly. However, no hazard will exist during this time as the temperatures are low, and no gas species produced by the fire are carried through the opening until the upper layer drops to the height of the undercut.

EPIcode

The primary limitation of EPIcode for DOE safety basis applications is that it does not have a dense gas option. While conservative in most far-field applications, this limitation may yield nonconservative results for close-in receptor calculations.

Similar to ALOHA, EPIcode does not statistically sample site or facility meteorology. The user is required to entire meteorological conditions appropriate for receptor of interest.

Finally, user sites must also recognize that as a proprietary code, EPIcode applications will inherently place greater SQA demands on the user than a code from the public domain.

GENII

Most limitations and undesirable features present in earlier versions of GENII that precluded unqualified endorsement as a safety basis code in the APAC Evaluation Program appear to have been removed (O'Kula 1997). The user must be able to work within the FRAMES operating system, and as such, experience in this environment is recommended.

During this limited review activity, no appreciable weaknesses were identified with respect to GENII and potential safety basis applications.

MACCS2

The major weakness in MACCS2 is programmatic, that of loss of robust SQA processes "undergirding" the current program. While the root causes and effects are documented in TECH-25 and earlier documentation, compensatory actions are still not in place.

A key objective of the SASG will be to document remedial actions and recommendations (see Section 2.3). Since the DOE Software Survey indicates that MACCS2 is a high-use code, it is essential that actions are implemented in a timely manner to ensure that calculations for support of 10 CFR 830 compliant DSAs are defensible.

The software upgrade in terms of DOE DSAs that should be addressed as soon as possible is that impacting calculations containing multiple plume segments (Gregory 1998). Other identified errors in the MACCS2 software, while deserving corrective action as part of good SQA processes and practices, are insignificant relative to most DOE applications.

Other improvements are recommended, as resources are available. Included are improvements to the user interface. MACCS2 still uses a DOS-based operating system, and requires experienced user insights to correctly build an input file. An NRC-sponsored program is planned to improve this feature by developing a WINDOWS-based system. However, it is unclear whether this modification will be carried over to the mainstream MACCS2 version.

The treatment of several source term types important to DOE applications could be improved in MACCS2. Sensible heat algorithms for modeling fire source terms have been implemented for some customers, but systematic treatment of this phenomenology should be standardized in the version of the code available to all DOE users. Additionally, the code does not presently treat deflagration/detonation events accurately. While MACCS2 may not be suitable for mechanistically modeling highly energetic source terms, User's Manual documentation could be expanded to include methods of modeling these events (Steele 1998).

Other user options for treating various aspects of dispersion phenomenology can be explored in future versions of MACCS2. These include plume duration, building wake effects, plume trajectory, puff/plume rise behavior, mixing layer penetration, resuspension, and wet and dry deposition features. While expanded user options would be useful to the DOE consequence analyst, they are not critical to completing current analyses.

MELCOR

As indicated earlier, most current DOE applications require MELCOR modules that model containment/confinement systems, without need of the reactor-based portions of the code. Storage requirements can be considerable, and may present problems for some users. In the context of most DOE needs, the benefits of the MELCOR-aided analysis, especially when only a portion of the code is applied, must be evaluated against engineering calculation-based approaches.

As in all applications, the DOE analyst must observe that MELCOR is designed as a fast-running, lumped-parameter computer code. Multidimensional effects should be explored with other codes.

Experience and skill of the user are especially important in benefiting from use of MELCOR. Although many MELCOR models will reduce the timestep to lower values when needed, very rapid phenomena, certain phenomenological events, or numerical problems encountered by the code may necessitate use of a smaller maximum timestep supplied by the user for portions of the transient. As a result, the current code is somewhat dependent on the user to select proper timesteps. It is expected that later versions may offer automatic timestep controls.

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While recommendations were made as part of the APAC Evaluation Program (as noted in Appendix E), many of these have been implemented. Table 7 lists known limitations of currently available code versions, as discussed above.

3.3 Protocols for Upgrading Software Quality Assurance

Several sites require a level of SQA commensurate with the importance of the software application in a safety context. Determining the importance for a given computer code and its associated applications can be referred to as classifying the software level. While several hierarchies may be cited, an approach used at the Savannah River Site (SRS) is summarized here as a useful prototype. Table 8 delineates the SRS safety analysis software levels by application basis [Westinghouse Savannah River Company (WSRC) 2001]. It is suggested that Level B would contain most safety analysis software.

Implementation of Part II of ASME NQA-1-1997, Subpart 2.7, *Quality Assurance Requirements for Computer Software for Nuclear Facility Applications* (ASME 1997) and ASME NQA-1a-1999 *Addenda* (ASME 1999), are recommended by the SASG as appropriate protocols for existing or purchased software used for safety analysis. While many sites have developed protocols for achieving compliance with Subpart 2.7, two are outlined below as reasonable and compliant.

Table 7. Code Limitations

Computer Code	Weaknesses/Limitations
ALOHA Version 5.2.3	• Persistent meteorology • Establish algorithm for quantifying downwind concentrations beyond 10 km. • Allow non-pure chemicals to be modeled (e.g., 50% HNO_3) • Dense gas properties are limited by source geometry • Incomplete SQA Program/Processes • No sensible heat, nor elevated release options
CFAST Version 3.1.6	• Occasional non-convergence error w/o guidance diagnostic • Fire growth model • Inherent flaws in zone model representation of a fire
EPIcode Revision 6.0	• Persistent meteorology • No dense gas option • User assistance and inquiry services are limited • Incomplete SQA Program/Processes
GENII (Version 2)	• FRAMES Operating System dependent
MACCS2 1.12	• Upgrade verification and validation program, especially for new features added in MACCS2. • Update user interface (planned as part of NRC program) • Review sensible heat model to account for areal releases as well as stack releases. • Consider multiple year option to better sample site data sets that are greater than one year in length. • Improve close-in model for impacts of building aerodynamic effects, low windspeed conditions. • Detonation/deflagration (explosive release) approach to code documentation
MELCOR Version 1.8.5	• Skill level required is relatively high • Computer storage requirements may be in excess of typical user

Table 8. Software Level Hierarchy by Safety Analysis Application

Level	Classification Basis
A	Software applications that have a direct effect on nuclear safety protection systems such that the consequences of failure to perform as expected may have an adverse impact on the health and safety of the general public.
B	Those software applications important to compliance with regulatory requirements/commitments or required by law, except as defined in Level "C" below. Also includes software applications whose failure to properly function as expected may have an indirect effect on nuclear safety. Such software applications may cause individuals to take actions or make decisions that may have a non-immediate impact on nuclear safety or individual safety. Such software may also generate output that verifies compliance with regulations unrelated to nuclear safety or that is independently verified through alternate means prior to use for plant operations.
C	Those software applications important to continued operations of the business. This may involve non-nuclear facilities, trending or analysis of operational data, or provide operation or maintenance information to management in support of decisions regarding operating activities. Includes software applications whose failure to perform as expected could not affect nuclear safety but would have an unacceptable impact by: • Causing a monetary loss in excess of $1,000,000 (1981 dollars) including cleanup, equipment damage and production value, • Causing a loss of primary program capabilities in excess of six months. Also includes: • Software applications for any on-line monitor required by an environmental permit or regulation which directly measures discharges to the atmosphere, to ground water or to the surface water. • Software applications required by the SRS Emergency Plan for environmental monitoring or fore communications with local, state and Federal Government agencies.
D	Those software applications important to the day to day operation of the business, but whose failure to perform as intended will not affect the safety or reliability of nuclear facilities. Such software may be used to administratively control the business of operating the nuclear facilities, and their output may support decisions and activities not related to nuclear facility operations.
E	Software that is within scope of this procedure that is not included in the above classification levels.

Sandia National Laboratories Safety Support to the Waste Isolation Pilot Plant (WIPP): NP-19 is a Sandia National Laboratories (SNL) SQA plan for implementing an earlier version of the relevant ASME standard (NQA-2a-1990 Part 2.7). It was used for support of safety analysis services for WIPP, and has the following requirements:

- Create a **Primitive Baseline (PB)** document to establish the QA status of the existing computer code
- Write a **Requirements Document (RD)**
- Establish a **Verification and Validation Plan (VVP)** based on the RD
- Create an **Implementation Document (ID)** to describe the process of generating the executable software

- Create/Evaluate a **User's Manual (UM)**
- Generate a **Validation Document (VD)** (Measures performance of software against criteria specified in the VVP)
- Perform **I&C** to Verify Correct Installation on all Supported Platforms
- Implement a software **Configuration Control (CC)** System
- Implement a **Software Problem Reporting (SPR)** System.

Savannah River Site Procedure QAP 20-1, Software Quality Assurance: The SRS procedure QAP 20-1 defines the requirements and responsibilities for the control of quality of computer software, and is responsive to NQA-1-1997, Part II, Subpart 2.7, and ASME NQA-1a-1999 Addenda. Included under the procedure are scientific/modeling/engineering codes where the output is used for regulatory reporting, environmental modeling, or as an input to SAR-level documentation. The following QAP 20-1 requirements, in part analogous to those of NP-19, must be met for *existing and purchased* software[9], and may be summarized as requiring the following steps:

- Classify software.
- Prepare SQA Procedures/Plans, identifying responsible organization(s), required documentation, compliance methods, reviews, and methods for error reporting and corrective action.
- If off-the-shelf software is used, determine critical functions that provide evidence of software's suitability, establish methods to verify adequacy, and provide verifiable acceptance criteria (Dedication documentation).
- Perform evaluation (for existing software, i.e., not developed in accordance with established software development procedures) of software, determining software capabilities and limitations, specifying test plans and test cases, identifying instructions for use within capabilities, among key objectives.
- Define Software Requirements – define requirements for functionality, performance, design constraints, attributes, acceptance criteria, and external interfaces.
- Design and Implementation phases – defined for developed software only.
- Execute and document test cases – a Test Report shall include test procedures or plans and the results of the execution of test cases. The test results documentation shall demonstrate successful completion of all test cases or the resolution of unsuccessful test cases and provide direct traceability between the test results and specified software requirements.
- Installation and acceptance phase documentation shall be developed, and shall include results of the execution of test cases for system installation and integration, user instructions, and documentation of the acceptance of the software for operational use.
- Corrective, perfective, adaptive maintenance steps shall be approved, documented, verified and validated and controlled in accordance with related life cycle phases of the software.
- Implement a configuration control protocol for controlling, uniquely identifying, describing, and documenting the configuration of each version or update of a computer code and its related documentation. Describe in implementing procedures.
- Implement procedures for reporting software problems and taking appropriate actions.
- Specify methods for controlling access.

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[9] See full WSRC Procedure QAP 20-1 for full text. A summary is listed here.

A software documentation matrix is shown in Table 9 listing the various WSRC QAP 20-1 requirements (Column 1) for Level A, B, and C software (Columns 3 – 6). The matrix requirements for Level A/B are in excellent agreement with the NP-19 requirements suggested by SNL.

Considerations in the remainder of this report shall consider candidate Toolbox codes as Level B Classification in view of its use in the overall context of safety analysis. It is recommended that the overarching standard for compliance for Toolbox codes be NQA-1-1997, Part II, Subpart 2.7, and the NQA-1a-1999 Addenda.

Table 9. Software Documentation Requirements Matrix Based on Source and Application

SRS WSRC 1Q, QAP 20-1	WIPP SNL NP 19-1	Level A and B Existing Software	Level A and B Purchased Software	Level C Existing Software	Level C Purchased Software
Software Classification		X	X	X	X
SQA Procedures/Plans		X	X	X	X
Dedication			X		
Evaluation	PB	X		X	
Requirements	RD	X	X		
Design					
Implementation					
Testing	VVP, VD	X	X		
User Instructions	ID, UM	X	X		
Acceptance Test	I&C		X		X
Operation and Maintenance		X	X		
Configuration Control	CC	X	X	X	X
Error Impact	SPR	X	X		
Access Control		X	X		

Additional guidance for the computer code developing and maintenance organizations may be found in the IEEE standards. A detailed list is found in Appendix F.

3.4 Gap Analysis for Toolbox Code Candidates

Six computer codes are candidates for the Safety Analysis Toolbox. Of these six, only one, EPIcode, is proprietary, while the other five have been developed and/or maintained by government agencies, including:

ALOHA and GENII	-	U.S. EPA
CFAST	-	NIST
MACCS2 and MELCOR	-	NRC and DOE.

Preliminary review of the current status of the QA programs for these codes indicates a disparate level of compliance with current SQA norms. This is due largely to regulatory drivers in the area of the code domain, resource limitations, and code sponsor prioritization. Additionally, these software packages have different purposes and are relied on to varying degrees in the analysis of hazards, source term and accident phenomenology, and in the control selection process for DOE facilities.

An initial step to be taken with each of the Toolbox code candidates will be a "gap analysis." This analysis is an evaluation of the code against applicable SQA standards for use in safety analysis. Specifically, the SQA deficiencies of each code are identified, and the actions needed to bring each code into compliance with the standards are quantified.

A listing of known SQA issues is provided for Toolbox candidate in the following sections. Additional, detailed information would be expected through performance of a rigorous gap analysis.

ALOHA

Limited documentation is furnished with the code (e.g., User's Manual), but additional legacy information is still available. The EPA now maintains the code. While several sites have prepared elements of a SQA package, additional effort would have to be expended to bring ALOHA into reasonable agreement with Level B software criteria shown in Table 9.

CFAST

Because CFAST software has not been formally validated, some sites have used the method of "alternate calculations" to argue partial compliance with ASME NQA-1 requirements. It is recognized that alternate calculations are an interim measure, and some effort has been initiated to conduct a thorough software verification and validation effort. This effort is directed at validating the room temperature and the target heat flux prediction capabilities.

The fire protection community has begun to address weaknesses in fire modeling SQA. The recognized weaknesses include limited empirical data to allow benchmarking, software with no published sample problems to facilitate software verification, published evaluations with little or no discussion of uncertainties, and limited agreement on what constitutes reasonable design assumptions.

There are two major, non-proprietary, fire modeling validation efforts in progress. The first, which is being organized by the NRC and NIST, is the *International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications*. This multi-national project is intended to share the knowledge and resources of various participating organizations to evaluate and improve the state of the art of fire models for use in nuclear power plant fire safety and fire hazard analysis. The group has completed one benchmark exercise. At least one DOE site is adopting this benchmark as a verification sample problem to be used on each installation of CFAST. Documentation is presently being prepared to implement this sample problem.

The second effort, which is being organized by the Society of Fire Protection Engineers, is validating different sub-routines of CFAST and other fire software. Their first project was validation of DETACT, which is a program that predicts sprinkler and fire detector response. This effort is essentially complete and the final report is in final preparation. The next scheduled project is to evaluate ASET, which was developed to estimate room temperatures and smoke layer heights. This effort is in the very early stages.

EPIcode

EPIcode is a proprietary model currently maintained by Homann Associates. A User's Guide is supplied with the code, but no other supporting documentation. The code author maintains that EPIcode strictly applies the well-established Gaussian Plume Model, and that the same algorithms and methodologies are applied as outlined in the multiagency document *Technical Guidance for Hazards Analysis – Emergency Planning for Extremely Hazardous Substances*.[10]

An SQA effort may be problematic in view of the proprietary nature of the software and limited documentation available from the code author/maintainer. While Toolbox designation can be maintained, it is recommended that the SASG not undertake or oversee any SQA activities. The code, in a sense, would have a qualified designation, requiring each user organization demonstrate minimum SQA processes have been implemented.

GENII

The GENII package of codes was developed under a QA plan based on the ANSI standard NQA-1 as implemented in the PNNL Quality Assurance Manual, PNL-MA-70. All steps of the code development have been documented and tested, and hand calculations have verified the code's implementation of major transport and exposure pathways for a subset of the radionuclide library. External peer reviews were performed for the internal dosimetry portions of the code, and for the entire code package, during the development phase. Recommendations of the review committees were then incorporated into the final product.

GENII has been included in the Validation of Model Predictions (VAMP) project (an acronym for the Coordinated Research Program on Validation of Models for the Transfer of Radionuclides in Terrestrial, Urban, and Aquatic Environments), which is an international effort to compare environmental radionuclide transport models with measured environmental data. Results for test scenario CB (based on environmental measurements following the Chernobyl accident) indicated that dose estimates from GENII were comparable to, although slightly higher than, those of other participating models, which is consistent with its primary function as a prospective analysis tool. The models included in the code have been validated to various degrees by additional studies, however these have not been compared directly to output from the code.

The overall system design is documented in *GENII Version 2 Software Design Document* (Napier 1999). A series of example case is available electronically (Napier 1999).

[10] U.S. EPA, Federal Emergency Management Agency, and U.S. Department of Transportation, (December 1987).

MACCS/MACCS2

The Gaussian dispersion and consequence code, MACCS2, has been recently evaluated by the developer and maintenance organization, SNL. To meet minimum Subpart 2.7 requirements outlined in Table 9, minimum requirements to be satisfied include:

- Development of a Primitive Baseline report;
- Production of a Requirements Document;
- Generation of a Verification and Validation Plan;
- Development of an Implementation document;
- Update of a MACCS2 User's Manual (use parallel effort from NRC-supported program);
- Upgrade and review of a Validation document; and
- Installation and Checkout, Configuration Control, and Software Problem Reporting System documentation.

MELCOR

MELCOR support and development has been through the NRC and many, if not all, SQA processes appear to have been followed. It is anticipated that remedial SQA processes and program elements would be minimal since only some of the modular features would be on interest to non-reactor, DOE facility safety analysts. A limited SQA backfit process could, in principle, be applied to confinement/containment, ESF, and leakpath factor modules.

Summary of Estimated Effort to Achieve Minimum SQA Levels Appropriate for Nuclear Facilities

Once SQA criteria for the Toolbox codes have been established, in-depth gap analysis can be performed on each of six Toolbox codes, and a tailored verification and validation schedule developed. As a projected estimate, three resource levels are anticipated for conducting the required remedial process for meeting minimum requirements for "B Classification Level" software, consistent with NP-19 and QAP 20-1 implementing procedures for meeting NQA-1-1997, Part II, Subpart 2.7. These are:

1. Low (< 12 person-months)
2. Medium (1 – 2 person-years)
3. High (> 2 person-years)

Most code candidates would be expected to fall in the medium category. More accurate estimates, however, can only be obtained through a code-specific, gap analysis process.

4.0 Path Forward for Development of Safety Analysis Toolbox

The issues cited in TECH-25 are Complex-wide, and thus any response, including organization of a SASG and the steps toward formulating a Toolbox, must also have widespread support among DOE, its laboratories, and nuclear facility contractors. With this in mind, the SASG was formed with representation from key NNSA-DP sites, laboratories, and DOE field and line organizations.

Activity to date has reviewed the results of DOE SQA Survey, and rebaselined the earlier findings of the DOE APAC Program relative to updated, screening criteria. Six computer codes, including MACCS/MACCS2[11], GENII, ALOHA, EPIcode, CFAST, and MELCOR, have been recognized through this process as high-use software. They are identified as the initial candidates for DOE Safety Analysis Toolbox, and as such potentially can satisfy minimum SQA requirements for accident analysis.

4.1 Additional Actions

Additional steps still must be taken. Included are:

1. Provide code-specific guidance reports on use of the Toolbox codes to support 10 CFR 830 Subpart B Safety Basis documentation. These documents will provide guidance on use of the software for supporting safety basis accident analysis, specifically applicable regimes in accident and consequence analysis, default inputs, recommendations and caveats on certain modes of use.

2. Perform a gap analysis on each of the proposed Toolbox codes and determine the minimum actions to needed to bring each code into compliance with SQA verification and validation requirements.

3. Establish and implement a Central Registry as the organization "owning" the DOE Safety Analysis Toolbox. Define protocols for accessing codes, maintaining configuration control, addressing user issues, and updating and correcting software.

4. Revise or add SQA sections to the appropriate safety analysis standards and implementation guides.

More details are forthcoming on these and other SQA improvement actions. A master plan is in preparation under the direction of the DOE Office of Environment, Safety, and Health.

Augmenting Training on Use of Safety Analysis Software: The DOE Safety Analysis Working Group conducts an annual workshop each year, and has increased the attention given in the training area. The emphasis has been particularly strong in providing code-specific training in use and applications appropriate to many of the computer models reviewed earlier by the APAC Program, and more recently by the SASG. However, nearly all training modules lack the formalism of enabling objectives and graded testing. The SASG will evaluate the need and requirements for formal training later in the near future.

Resources and Organizational Interaction Relative to Toolbox Maintenance: Once institutionalized, the Toolbox codes will require one to two full-time equivalents per year for the maintenance function, as well as oversee timely dispositioning of user questions and issues. The manner of interaction between the tool-box maintainer and code owners and allocations of resources

[11] In the case of the MACCS code, the SASG concludes that either MACCS Version 1.5.11.1 or MACCS2 Version 1.12 can be applied as an interim computational tool until SQA upgrades are completed to MACCS2.

will deserve particular attention since the codes of interest span the full public domain to proprietary spectrum.

4.2 Opportunities

The Safety Analysis Toolbox concept and the oversight of the SASG will provide significant cost and resource savings when viewed in the context of safety analysis and associated safety basis documentation at numerous DOE laboratories and sites. While startup and initial activities may prove difficult, the payoff is appreciable. It must be remembered that the concept represents a fundamental paradigm shift relative to the current general pattern of site-by-site code control.

Chief among the benefits will be:

- Centralized configuration control of high-impact accident analysis software, thereby minimizing multiple, non-uniform, and substandard programs
- Unambiguous computer code versions and software documentation
- Single-point receipt of user inquiries, error notification, as well as user-specific and general user group responses
- Sources of test data for Toolbox codes and possibly, site-specific data sets (e.g., meteorology, site facility to boundary distances, and listing of Hazard 2 facilities).

Initial toll-box code identification and preliminary plans for code maintenance should be in place by the end of CY 2001.

4.3 Acknowledgement

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5.0 Acronyms and Definitions

ALOHA	Areal Locations of Hazardous Atmospheres
APAC	Accident Phenomenology and Consequence
ANS	American Nuclear Society
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
ASTM	American Society for Test Materials
BIO	Basis for Interim Operation
CAMEO	Computer-Aided Management of Emergency Operations
CC	Configuration Control
CDCA	Chemical Dispersion and Consequence Assessment
CFR	Code of Federal Regulations
Central Registry	An organization that will be responsible for the storage, control and long-term maintenance of the DOE Safety Analysis Toolbox codes
CFAST	Consolidated Model of Fire Growth and Smoke Transport
CY	calendar year
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DP	Defense Programs
DSA	Documented Safety Analysis
EEE	Explosions and Energetic Events
EPA	U.S. Environmental Protection Agency
EPIcode	Emergency Prediction Information code
ESF	Engineering Safety Feature
FAST	Fire Growth And Smoke Transport
FWG	Fire Working Group
Gap Analysis	Evaluation of the SQA attributes of a computer code against established requirements
I&C	instrument and control
ID	Implementation Document
IFT	In-Facility Transport
IVV&A	Independent VV&A
ISM	Integrated Safety Management
M&S	modeling and simulation
MACCS	MELCOR Accident Consequence Code Systems
MELCOR	Methods for Estimation of Leakages and Consequences of Releases
NNSA	National Nuclear Security Agency

NIST	National Institute of Standards and Technology
NOAA	National Oceanic and Atmospheric Administration
NRC	U.S. Nuclear Regulatory Commission
PB	Primitive Baseline
PNNL	Pacific Northwest National Laboratory
QA	Quality Assurance
RD	Requirements Document
RDC	Radiological Dispersion/Consequence
SAM	Site Acquisition of Meteorology
SASG	Safety Analysis Software Group – A group of technical experts formed by the Deputy Secretary in October 2000 in response to TECH-25 issued by the DNFSB. This group is responsible for determining what safety analysis and 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 NRC on code assessment as appropriate.
SAR	Safety Analysis Report
SPR	Software Problem Reporting
SQA	software quality assurance
SRS	Savannah River Site
SSC	Safety Class Structures, Systems, or Components
SWG	Spills Analysis
TECH-25	Defense Nuclear Facilities Safety Board Technical Report 25
Toolbox Codes	A small number of standard computer models (codes) supporting DOE safety analysis having widespread use and of sufficient pedigree that are maintained, managed and distributed by a central source. These codes are verified and validated and constitute a "safe harbor" methodology. That is to say, the analyst using these codes do not need to present additional defense as to their pedigree, provided that they are sufficiently qualified to use the codes and the input parameters are valid.
UM	User's Manual
VD	Validation Document
VVP	Verification and Validation Plan
WSRC	Westinghouse Savannah River Company

6.0 References

10 CFR 50	10 CFR 50, Appendix B, *Quality Assurance Criteria for Nuclear Power Plants and Fuel Reprocessing Plants.*
10 CFR 63	10 CFR 63, *Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada*, Section 63.142, *Quality Assurance Criteria.*
10 CFR 70	10 CFR 70. *Domestic Licensing of Special Nuclear Material.*
10 CFR 830	10 CFR 830, *Nuclear Safety Management*, Subpart B, *Safety Basis Requirements.*
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Appendix A. Overview of Use of Computer Software for Support of DOE Safety Analysis

The Department of Energy (DOE) evaluates and approves the operation of its nuclear facilities via a safety analysis process outlined in DOE Rule, 10CFR830 – Subpart B, DOE Order 5480.23 and DOE-STD-3009-94. This safety analysis process requires the development of a Safety Analysis Report (SAR) or Documented Safety Analysis (DSA) per the Rule language and includes two key analyses: (1) hazard analysis (HA) and (2) accident analysis.

The hazard analysis is the cornerstone of the DOE safety analysis process and is largely a qualitative process by which:

- the hazards in the facility are identified,
- a spectrum of accidents are postulated for each hazard,
- a qualitative evaluation of accident likelihood and consequence is made, and
- all preventive and mitigative systems or controls are identified along with a qualitative measure of their importance.

The final product of the hazard analysis gives rise to a list of which systems or controls are important to safety and therefore are designated as safety-significant. This designation will lead to a formal commitment on the part of the facility contractor to maintain the safety function of these systems through technical safety requirements (TSRs).

The other product derived from the hazard analysis is a list of so called "derivative design-basis accidents" (DBAs). These accidents will be examined in more detail in the accident analysis portion of the DOE safety process.

Accident analysis is a follow-on activity to the hazard analysis. The focus of the DBAs is public exposure, and therefore, a quantitative calculation of dose to the maximally exposed offsite individual (MOI) is made for each DBA. The purpose of the dose calculations is to determine if some of the safety-significant systems identified in the hazard analysis should have their safety designation raised to safety-class. Safety-class requires a higher degree of commitment to maintain its safety function via increased reliability, maintenance, etc.

In addition, because accident analysis involves quantitative calculations, the calculated values may be used to establish criteria used to measure the safety function of the system on some occasions. These criteria are referred to as safety functional requirements and include factors such as flow rates, temperature, etc.

Understanding the DOE safety process and the products derived from it is vital when evaluating the effect that tools, such as computer codes, have on the process.

Standardized Methodology for DOE Accident Analysis

The DOE has developed a standardized methodology for performing accident analysis. The method centers on an equation referred to as the "five-factor formula." The five-factor formula is as follows.

$$\text{Source Term} = \text{MAR} * \text{ARF} * \text{RF} * \text{DR} * \text{LPF} \;,$$

where

MAR = Material at Risk,
ARF = Airborne Release Fraction,
RF = Respirable Fraction,
DR = Damage Ratio, and
LPF = Leak Path Factor.

When the source term is known, it can be converted to a dose to the MOI as follows.

$$\text{Dose} = \text{Source Term} * \text{Breathing Rate} * \text{Dose Conversion Factor} * \chi/Q,$$

where χ/Q = the dilution factor.

The MAR is derived from the hazard analysis and represents the identified hazardous material present in the facility available for an accident to act upon. Therefore, it is not derived in the accident analysis but is brought forward from the HA.

The ARF and RF are based on experimental data for various impacts to the MAR. No computer codes are used to derive these values. Instead, the safety analysts use their expertise and DOE guidance via the Handbook (DOE-HDBK-3010-94) to derive the appropriate ARF and RF.

Breathing rate is normally set at a conservative value, and the dose conversion factors are based on Federal Guidance Report standards. This leaves only the DR, LPF, and χ/Q to be calculated as part of the accident analysis.

The safety analyst may use hand calculations or computer codes to calculate these parameters. The computer codes chosen by the safety analyst fall into several categories. The categories of codes are:

- radiological atmospheric dispersion codes,
- chemical atmospheric dispersion codes,
- fire modeling codes, and
- leak-path analysis codes.

The analyst will use one of these types of codes to calculate parameters such as DR, LPF, and χ/Q. The effect of the quality of these codes on the overall safety analysis process can be evaluated qualitatively by examining the role that these parameters play in the overall safety process. This is done in the next section.

Qualitative Effect of the Codes on Safety Analysis

The gross effect of the use of computer codes can be evaluated by examining their effect on the final MOI dose values calculated as part of the accident analysis. The values chosen or calculated for each parameter in the dose equation are near the conservative tail of any distribution that would be assigned to the individual parameter. Therefore, when each parameter is multiplied using the five-factor formula to obtain the dose, the conservatism in the calculation grows. This large conservatism in the calculation has always provided the DOE with a comfort zone when the doses are used to make decisions regarding safety. Even if a single value in the dose calculation were off by an order of magnitude, the resulting value would still not approach the mean value of dose if a cumulative distribution of dose also were calculated.

Each code and five-factor-formula parameter is discussed individually below. The types of code calculations include:

- atmospheric dispersion and radiological consequence,
- atmospheric dispersion and chemical consequence,
- in-facility transport used to calculate LPF, and
- fire modeling used to calculate DR and other information.

Atmospheric Dispersion and Radiological Consequence

The atmospheric dispersion and radiological consequence codes are used only to calculate the appropriate dilution factor and ultimately quantify the radiological dose. Their effect on safety then is related only to their input in selecting safety-class systems, structures, and components (SSCs).

The selection of safety-class SSCs is an important decision, but the decision to make an SSC safety-significant is made initially in the hazard analysis. The quality of the dose value will not affect the SSC being made a safety-significant SSC and having TSR coverage, only the designation of safety-class and therefore possibly the pedigree of the SSC.

Atmospheric dispersion is one area where a simple bounding hand calculation can be done easily to ensure that the code calculation is not off by many orders of magnitude. If the issue of safety-class determination is in question, a simple hand calculation may aid in the decision.

Atmospheric Dispersion and Chemical Consequence

A code of this class is used primarily to calculate an instantaneous or time-averaged concentration of a chemical downwind from an accident. Because the DOE does not have an Evaluation Guideline for chemicals, the chemical concentration calculated is not used to distinguish safety-class designation for SSCs. Therefore, the quality of the numbers does not affect this portion of the safety process.

Occasionally, chemical concentrations are used to help set limits on chemical inventory, and this may present more of a safety implication. When these code calculations are used to help set inventory limits, they have a direct effect on values used in TSRs and the quality of the calculation may be very important. Again, it is important to note that a hand calculation can be used to verify this value, and in most cases, surrogate values for inventory limits (such as EPA or OSHA limits) also can be used.

In-Facility Transport

Typically, control-volume-type codes are used to calculate an LPF for radionuclide releases from the point of origin to the outside of the facility. They are used to calculate a mitigated dose for a given accident. However, because the DOE safety process requires that an unmitigated dose (i.e., an LPF of 1.0) be used in the selection of safety-class SSCs, the dose values have no effect on safety SSC designation.

LPF values typically are not used to set functional requirements for SSCs. Therefore, the LPF values are not used to set limits or operational requirements in TSRs. This information indicates that although LPF calculations provide useful information to the safety analysis process, the quality of those values does not have a major effect on safety.

Fire Modeling Codes

Fire modeling codes are used primarily to calculate bulk room temperatures during a fire. Fire progression is estimated from this information. Information derived from these calculations includes such items as

- failure of fire barriers (e.g., walls, cans),
- extent of fire spread, and
- response of fire suppression (e.g., sprinklers).

The safety analyst uses fire calculations primarily to determine the damage ratio (DR). This is done by estimating a DR from the extent of fire spread and the failure of fire barriers. The DR then is used in calculating dose. As before, this has a direct effect on the selection of safety-class SSCs.

The other information that may be derived from the fire modeling is input to the functional requirements of some safety SSCs or administrative controls. Fire modeling has been used to determine combustible load limits for facilities and to set functional requirements such as sprinkler head temperatures.

The quality of the codes used to perform fire modeling could affect many decisions in the DOE safety analysis process, primarily because results could be used to determine operational limits. The concern for fire modeling accuracy is offset by the fact that safety analysts in the DOE community typically use extremely conservative boundary conditions, such as uniform combustible loadings, skipping fire ramping, and using peak burn rates, etc. These conservative assumptions provide for very conservative room temperatures and may offset quality in the room fire temperatures.

Conclusions

Uncertainty in the quality assurance of software applied for safety analysis in the DOE Complex is offset in part in the manner in which they are applied to support safety analysis. This is because of the following.

1. The hazard analysis is the cornerstone of the DOE safety process and the primary means of designating safety-significant SSCs for which TSRs will be derived.

2. Computer codes are primarily used to determine consequence dose from postulated accident sequences, and this value will be used only to determine the need to elevate a safety-significant SSC to a safety-class SSC. There is a great deal of conservatism in the dose calculations because all of the parameters are chosen conservatively.

Appendix B. Summary from SQA Survey on Program and Order Compliance

Survey Targets: LLNL, LANL, SNL, SRS, Pantex, Rocky Flats, Y-12, INEEL, Nevada Test Site, Hanford (including ORP), WIPP, and ORNL. Only response from ORNL is the Y-12 survey. The Nevada Test Site stated they had no nuclear facilities. Although not a major target, YMP submitted a survey.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Development	LLNL	HCD/ABS--One code, HOTSPOT, was developed within HCD. No formal QA procedures.
	LANL	Varies by customer (note the majority of safety codes used for safety analysis of LANL nuclear facilities are not LANL developed codes). For specific customers, "Manufacturing Manual: Software Quality Assurance"; MFG-AP-0014 Rev. 0; and "TRU Waste Characterization Program: TWCP Quality Procedure", TWCP-QP-1.1-006 Rev. 7 are used.
	SNL	TA-V RREP QA Procedure, RREP 3-2, Computer Software Control; developed in-house, is mandatory for all software associated with the TA-V Nuclear Facilities; QA processes are peer review and testing.
	SRS	WSMS follows WSRC requirements on developing, testing, documenting, maintaining, and using computer codes used for safety analysis. Requirements are specified in standalone WSMS QA documentation, or are cited and referenced in WSRC documentation. This includes but is not limited to, the WSRC 1Q Manual, 11Q, Section 20-1, the E7 Manual, and WSMS Quality Assurance Procedures. Procedures are in-house developed and mandatory; QA processes are peer review.
	Pantex	In-house developed Software Quality Life Cycle (SQLC) Plant Standard STD-1875. Mandatory for all site-developed software, purchased software, contractor developed software, or design agency furnished software. The SQA process consists of peer reviews and approvals, and auditing.
	Rocky Flats	The Computer Software Management Manual (1-MAN-004-CSMM) contains the procedures followed for software development, testing, documentation, and maintenance. This manual was developed in-house using best industry practices and is mandatory; QA processes are peer review and independent verification and validation. The processes invoked by the CSMM have been reviewed and audited by the Software Engineering Institute at Carnegie-Mellon University and given a SEI Level certification. They have also been reviewed and audited for Software Quality Assurance by the Carlsbad Area Office for WIPP certification. Since virtually all of the codes used in the nuclear safety areas are provided by outside sources (Oak Ridge, Los Alamos, RSICC, etc.) we cannot vouch for the SQA processes used by those developers. However, the implementation of the codes on site is guided by the CSMM and V&V testing is performed as part of the installation and configuration management process mandated by the CSMM.
	Y-12	Y80-100, *Project Initiation*, Y80-200, *Feasibility Study/Requirements Definition*, Y80-400, *Functional System Design*, Y80-500, *Computer System Design*, Y80-515, *Manufacturing Applications User Interface Standard*, and Y80-600, *Programming and Implementation*. The current software control program is defined by the, *Software Development and Control*, Y80 Series procedures; the upcoming revision will be based on DOE's Software Engineering Methodology (SEM). The Nuclear Criticality Safety organization uses the following safety-related software: (1) SCALE/KENO: Standard Computer Analyses for Licensing Evaluation and (2) MCNP: Monte Carlo N-particle Transport Code System. This software is controlled by the Y80 Series procedures including the Nuclear Criticality Safety organization procedures. The procedures were developed in-house at Y-12, based on software industry practices at the time. The procedures determine a software classification for each system based on various criteria. This classification is then used to drive the mandatory portions of the actual development process. It is mandatory that all Y-12 software use the Y80 procedures for guiding development. A combination of walkthroughs, reviews, and testing regimens are used as the basis for ensuring quality, per the Y80 procedures.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Development cont'd	INEEL	INEEL Program Requirements Document (PRD)-115, "Configuration Management;" INEEL Standard (STD)-107, "Configuration Management Program;" INEEL Management Control Procedure (MCP) 550, "Software Management"; INEEL MCP-3630, "Computer System Change Control;" INEEL Guide (GDE)-59, "Guide for Computer System Change Control;" DOE-STD-1073-93, "Guide for Operational Configuration Management Program;" ANSI/IEEE STD-828-1998;" IEEE Standard for Software Configuration Plans;" ANSI/ANS-10.4-1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry." Compliance with the INEEL documents is mandatory. Software packages developed and maintained at INEEL that are used for nuclear facility safety analysis or for control of active Safety SSCs are subject to the INEEL CM Program, have received verification and validation (V&V), and have CM Plans in place. See survey for description of INEEL documents.
	YMP/TESS	•NQA-2, Subpart 2.7 •OCRWM Quality Assurance Requirements & Description •OCRWM AP-SI.1Q Software Management •NQA-2, Subpart 2.7 is the NRC Standard for software development, testing, documentation, maintenance and usage. OCRWM Quality Assurance Requirements & Description (QARD) reflects in total the requirements of NQA-2, Subpart 2.7. AP-SI.1Q Software Management is the implementing procedure for Supplement I of the QARD. Compliance with AP-SI.1Q is mandatory. SQA processes include independent peer review, inspection, audit, and verification and validation of software.
	Hanford/RL	•Fluor Hanford--Primarily HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements.* Procedures are in-house developed based on DOE Orders and other government agencies' requirements and mandatory. All the SQA processes listed in the survey are accepted in the procedures - they are based on defined scope and risk. The procedure requires that some form of change control and review process be established. Each project is allowed to define in their implementing procedures the specific configuration management processes they will apply. •Bechtel Hanford--In-house BHI-AT-01 Procedure 1.7 *Software Development & Maintenance*, and Bechtel Corp. Software Development Methodology Framework (SDMF). Procedures are based on industry standards and are mandatory. •PNNL Hanford–Any software developed or used at the Laboratory is required to be controlled in accordance with the Computer Software and Database Control subject area, which is aligned with the Software Systems Engineering Process (SSEP). The subject area was derived largely from the SSEP. The SSEP addresses each of the issues identified above. The subject area is mandatory for all PNNL staff. The SSEP is mandatory for all projects in the Information Science and Engineering Division and for all projects done for the Information Systems Engineering product line. The SSEP is more rigorous and more flexible than the subject area. However, each is based on the fundamental premise of defining a plan based on specific project or activity needs and executing the plan to develop, acquire, or use the software in involved. Both the subject area and the SSEP were developed at PNNL. The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/). It's also based to lesser extent on elements of IEEE standards, Department of Defense MIL-STD-498 (since replaced), and Iterative Process Models like the "Spiral Model" by Boehm and "Managed Evolutionary Development" by U.S. Patent Office.
	Hanford/ORP	•Tank Farm–HNF-PRO-309, *Computer Software Quality Assurance Requirements* and HNF-PRO-2778, *IRM Application System Life Cycle Standards.* Procedures developed in-house based on DOE Orders and other government agency requirements and are mandatory. Varying degrees of SQA processes are used based on the defined scope and risk of the specific project application. •Tank Waste–Procedure K70C515, *Code of Practice for Computer Program Use,* addresses all the elements of ASME NQA-1-1994, Part II, Subpart 2.7, including software life cycle, development and maintenance, software testing, software verification and validation, documentation, error identification and notification. Procedure was developed in-house based on the requirements of NQA-1-1994, Part II, Subpart 2.7 and DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplement I. It is mandatory. SQA activities are installation testing and validation.
	WIPP	WP 16-IT3117, WIPP internal, mandatory, use-dependent; WP 16-2, WIPP internal, optional, use-dependent.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Testing	LLNL	HCD/ABS--HOTSPOT, EPI runs compared against ARAC runs by developer. Other codes (MACCS, MACCS II, ALOHA, GEN II) are widely used and accepted, but have no formal QA.
	LANL	Varies by customer. For specific customers, "Manufacturing Manual: Software Quality Assurance"; MFG-AP-0014 Rev. 0; and "TRU Waste Characterization Program: TWCP Quality Procedure", TWCP-QP-1.1-006 Rev. 7 are used.
	SNL	TA-V RREP QA Procedure, RREP 3-2, Computer Software Control; developed in-house, is mandatory for all software associated with the TA-V Nuclear Facilities; QA processes are peer review and testing.
	SRS	WSMS follows WSRC requirements on developing, testing, documenting, maintaining, and using computer codes used for safety analysis. Requirements are specified in standalone WSMS QA documentation, or are cited and referenced in WSRC documentation. This includes but is not limited to, the WSRC 1Q Manual, 11Q, Section 20-1, the E7 Manual, and WSMS Quality Assurance Procedures. Procedures are in-house developed and mandatory; QA processes are peer review.
	Pantex	In-house developed Software Quality Life Cycle (SQLC) Plant Standard STD-1875. Mandatory for all site-developed software, purchased software, contractor developed software, or design agency furnished software. The SQA process consists of peer reviews and approvals, and auditing.
	Rocky Flats	The Computer Software Management Manual (1-MAN-004-CSSM) contains the procedures followed for software development, testing, documentation, and maintenance. This manual was developed in-house using best industry practices and is mandatory; QA processes are peer review and independent verification and validation.. The processes invoked by the CSMM have been reviewed and audited by the Software Engineering Institute at Carnegie-Mellon University and given a SEI Level certification. They have also been reviewed and audited for Software Quality Assurance by the Carlsbad Area Office for WIPP certification. Since virtually all of the codes used in the nuclear safety areas are provided by outside sources (Oak Ridge, Los Alamos, RSICC, etc.) we cannot vouch for the SQA processes used by those developers. However, the implementation of the codes on site is guided by the CSMM and V&V testing is performed as part of the installation and configuration management process mandated by the CSMM.
	Y-12	Y80-700, *Validation and Acceptance*. The current software control program is defined by the, *Software Development and Control*, Y80 Series procedures; the upcoming revision will be based on DOE's Software Engineering Methodology (SEM). The Nuclear Criticality Safety organization uses the following safety-related software: (1) SCALE/KENO: Standard Computer Analyses for Licensing Evaluation and (2) MCNP: Monte Carlo N-particle Transport Code System. This software is controlled by the Y80 Series procedures including the Nuclear Criticality Safety organization procedures. The procedures were developed in-house at Y-12, based on software industry practices at the time. The procedures determine a software classification for each system based on various criteria. This classification is then used to drive the mandatory portions of the actual development process. It is mandatory that all Y-12 software use the Y80 procedures for guiding development. A combination of walkthroughs, reviews, and testing regimens are used as the basis for ensuring quality, per the Y80 procedures.
	INEEL	INEEL Program Requirements Document (PRD)-115, "Configuration Management;" INEEL Standard (STD)-107, "Configuration Management Program;" INEEL Management Control Procedure (MCP) 550, "Software Management"; INEEL MCP-3630, "Computer System Change Control;" INEEL Guide (GDE)-59, "Guide for Computer System Change Control;" DOE-STD-1073-93, "Guide for Operational Configuration Management Program;" ANSI/IEEE STD-828-1998;" IEEE Standard for Software Configuration Plans;" ANSI/ANS-10.4-1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry." Compliance with the INEEL documents is mandatory. Software packages developed and maintained at INEEL that are used for nuclear facility safety analysis or for control of active Safety SSCs are subject to the INEEL CM Program, have received verification and validation (V&V), and have CM Plans in place. See survey for description of INEEL documents.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Testing cont'd	YMP/TESS	•NQA-2, Subpart 2.7 •OCRWM Quality Assurance Requirements & Description •OCRWM AP-SI.1Q Software Management •OCRWM AP-SV.1Q Control of Electronic Management of Data •NQA-2, Subpart 2.7 is the NRC Standard for software development, testing, documentation, maintenance and usage. OCRWM Quality Assurance Requirements & Description (QARD) reflects in total the requirements of NQA-2, Subpart 2.7. AP-SI.1Q Software Management is the implementing procedure for Supplement I of the QARD. Compliance with AP-SI.1Q is mandatory. SQA processes include independent peer review, inspection, audit, and verification and validation of software.
	Hanford/RL	•Fluor Hanford--Primarily HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements*. Procedures are in-house developed based on DOE Orders and other government agencies' requirements and mandatory. All the SQA processes listed in the survey are accepted in the procedures - they are based on defined scope and risk. The procedure requires that some form of change control and review process be established. Each project is allowed to define in their implementing procedures the specific configuration management processes they will apply. •Bechtel Hanford--In-house BHI-AT-01 Procedure 1.7, BHI-AT-01 Procedure 1.8 *Software Acquisition and Maintenance*, and BHI-DE-01-EDPI-4.36-01, *Project Calculations*. Procedures are based on industry standards and are mandatory. •PNNL Hanford–Any software developed or used at the Laboratory is required to be controlled in accordance with the Computer Software and Database Control subject area, which is aligned with the Software Systems Engineering Process (SSEP). The subject area was derived largely from the SSEP. The SSEP addresses each of the issues identified above. The subject area is mandatory for all PNNL staff. The SSEP is mandatory for all projects in the Information Science and Engineering Division and for all projects done for the Information Systems Engineering product line. The SSEP is more rigorous and more flexible than the subject area. However, each is based on the fundamental premise of defining a plan based on specific project or activity needs and executing the plan to develop, acquire, or use the software in involved. Both the subject area and the SSEP were developed at PNNL. The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/). It's also based to lesser extent on elements of IEEE standards, Department of Defense MIL-STD-498 (since replaced), and Iterative Process Models like the "Spiral Model" by Boehm and "Managed Evolutionary Development" by U.S. Patent Office.
	Hanford/ORP	•Tank Farm–HNF-PRO-309, *Computer Software Quality Assurance Requirements* and HNF-PRO-2778, *IRM Application System Life Cycle Standards*. Procedures developed in-house based on DOE Orders and other government agency requirements and are mandatory. Varying degrees of SQA processes are used based on the defined scope and risk of the specific project application. •Tank Waste–Procedure K70C515, *Code of Practice for Computer Program Use,* addresses all the elements of ASME NQA-1-1994, Part II, Subpart 2.7, including software life cycle, development and maintenance, software testing, software verification and validation, documentation, error identification and notification. Procedure was developed in-house based on the requirements of NQA-1-1994, Part II, Subpart 2.7 and DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplement I. It is mandatory. SQA activities are installation testing and validation.
	WIPP	WP 16-IT3117, WIPP internal, mandatory, use-dependent; WP 16-2, WIPP internal, optional, use-dependent.
Documentation	LLNL	HCD/ABS--Manuals are available for codes. No formal QA was done for manual content.
	LANL	Varies by customer. For specific customers, "Manufacturing Manual: Software Quality Assurance"; MFG-AP-0014 Rev. 0; and "TRU Waste Characterization Program: TWCP Quality Procedure", TWCP-QP-1.1-006 Rev. 7 are used.
	SNL	TA-V RREP QA Procedure, RREP 3-2, Computer Software Control; developed in-house, is mandatory for all software associated with the TA-V Nuclear Facilities; QA processes are peer review and testing.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Documentation cont'd	SRS	WSMS follows WSRC requirements on developing, testing, documenting, maintaining, and using computer codes used for safety analysis. Requirements are specified in standalone WSMS QA documentation, or are cited and referenced in WSRC documentation. This includes but is not limited to, the WSRC 1Q Manual, 11Q, Section 20-1, the E7 Manual, and WSMS Quality Assurance Procedures. Procedures are in-house developed and mandatory; QA processes are peer review.
	Pantex	In-house developed Software Quality Life Cycle (SQLC) Plant Standard STD-1875. Mandatory for all site-developed software, purchased software, contractor developed software, or design agency furnished software. The SQA process consists of peer reviews and approvals, and auditing.
	Rocky Flats	The Computer Software Management Manual (1-MAN-004-CSSM) contains the procedures followed for software development, testing, documentation, and maintenance. This manual was developed in-house using best industry practices and is mandatory; QA processes are peer review and independent verification and validation.. The processes invoked by the CSMM have been reviewed and audited by the Software Engineering Institute at Carnegie-Mellon University and given a SEI Level certification. They have also been reviewed and audited for Software Quality Assurance by the Carlsbad Area Office for WIPP certification. Since virtually all of the codes used in the nuclear safety areas are provided by outside sources (Oak Ridge, Los Alamos, RSICC, etc.) we cannot vouch for the SQA processes used by those developers. However, the implementation of the codes on site is guided by the CSMM and V&V testing is performed as part of the installation and configuration management process mandated by the CSMM.
	Y-12	Required deliverables provided at the end of each procedure. The current software control program is defined by the, *Software Development and Control*, Y80 Series procedures; the upcoming revision will be based on DOE's Software Engineering Methodology (SEM). The Nuclear Criticality Safety organization uses the following safety-related software: (1) SCALE/KENO: Standard Computer Analyses for Licensing Evaluation and (2) MCNP: Monte Carlo N-particle Transport Code System. This software is controlled by the Y80 Series procedures including the Nuclear Criticality Safety organization procedures and Y/DD-834 "LMES Y-12 Nuclear Criticality Safety Software application Software Document for the HP C-180 Workstation." The procedures were developed in-house at Y-12, based on software industry practices at the time. The procedures determine a software classification for each system based on various criteria. This classification is then used to drive the mandatory portions of the actual development process. It is mandatory that all Y-12 software use the Y80 procedures for guiding development. A combination of walkthroughs, reviews, and testing regimens are used as the basis for ensuring quality, per the Y80 procedures.
	INEEL	INEEL Program Requirements Document (PRD)-115, "Configuration Management;" INEEL Standard (STD)-107, "Configuration Management Program;" INEEL Management Control Procedure (MCP) 550, "Software Management"; INEEL MCP-3630, "Computer System Change Control;" INEEL Guide (GDE)-59, "Guide for Computer System Change Control;" DOE-STD-1073-93, "Guide for Operational Configuration Management Program;" ANSI/IEEE STD-828-1998;" IEEE Standard for Software Configuration Plans;" ANSI/ANS-10.4-1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry." Compliance with the INEEL documents is mandatory. Software packages developed and maintained at INEEL that are used for nuclear facility safety analysis or for control of active Safety SSCs are subject to the INEEL CM Program, have received verification and validation (V&V), and have CM Plans in place. See survey for description of INEEL documents.
	YMP/TESS	•NQA-2, Subpart 2.7 •OCRWM Quality Assurance Requirements & Description •OCRWM AP-SI.1Q Software Management •NQA-2, Subpart 2.7 is the NRC Standard for software development, testing, documentation, maintenance and usage. OCRWM Quality Assurance Requirements & Description (QARD) reflects in total the requirements of NQA-2, Subpart 2.7. AP-SI.1Q Software Management is the implementing procedure for Supplement I of the QARD. Compliance with AP-SI.1Q is mandatory. SQA processes include independent peer review, inspection, audit, and verification and validation of software.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Documentation cont'd	Hanford/RL	•Fluor Hanford--Primarily HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements.* Procedures are in-house developed based on DOE Orders and other government agencies' requirements and mandatory. All the SQA processes listed in the survey are accepted in the procedures - they are based on defined scope and risk. The procedure requires that some form of change control and review process be established. Each project is allowed to define in their implementing procedures the specific configuration management processes they will apply. •Bechtel Hanford--In-house BHI-AT-01 Procedure 1.7, BHI-AT-01 Procedure 1.8 *Software Acquisition and Maintenance*, and BHI-DE-01-EDPI-4.36-01, *Project Calculations*. Procedures are based on industry standards and are mandatory. •PNNL Hanford--Any software developed or used at the Laboratory is required to be controlled in accordance with the Computer Software and Database Control subject area, which is aligned with the Software Systems Engineering Process (SSEP). The subject area was derived largely from the SSEP. The SSEP addresses each of the issues identified above. The subject area is mandatory for all PNNL staff. The SSEP is mandatory for all projects in the Information Science and Engineering Division and for all projects done for the Information Systems Engineering product line. The SSEP is more rigorous and more flexible than the subject area. However, each is based on the fundamental premise of defining a plan based on specific project or activity needs and executing the plan to develop, acquire, or use the software in involved. Both the subject area and the SSEP were developed at PNNL. The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/). It's also based to lesser extent on elements of IEEE standards, Department of Defense MIL-STD-498 (since replaced), and Iterative Process Models like the "Spiral Model" by Boehm and "Managed Evolutionary Development" by U.S. Patent Office.
	Hanford/ORP	•Tank Farm–HNF-PRO-309, *Computer Software Quality Assurance Requirements* and HNF-PRO-2778, *IRM Application System Life Cycle Standards.* Procedures developed in-house based on DOE Orders and other government agency requirements and are mandatory. Varying degrees of SQA processes are used based on the defined scope and risk of the specific project application. •Tank Waste--Procedure K70C515, *Code of Practice for Computer Program Use,* addresses all the elements of ASME NQA-1-1994, Part II, Subpart 2.7, including software life cycle, development and maintenance, software testing, software verification and validation, documentation, error identification and notification. Procedure was developed in-house based on the requirements of NQA-1-1994, Part II, Subpart 2.7 and DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplement I. It is mandatory. SQA activities are installation testing and validation.
	WIPP	WP 16-IT3117, WIPP internal, mandatory, use-dependent; WP 16-2, WIPP internal, optional, use-dependent.
Maintenance	LLNL	HCD/ABS--HOTSPOT and EPI are tested by the developer with standard runs after modification. No formal QA documentation. Other codes are purchased or adopted when they become available. They are informally QA'd by comparison with older versions and other applicable codes.
	LANL	Varies by customer. For specific customers, "Manufacturing Manual: Software Quality Assurance"; MFG-AP-0014 Rev. 0; and "TRU Waste Characterization Program: TWCP Quality Procedure", TWCP-QP-1.1-006 Rev. 7 are used.
	SNL	TA-V RREP QA Procedure, RREP 3-2, Computer Software Control; developed in-house, is mandatory for all software associated with the TA-V Nuclear Facilities; QA processes are peer review and testing.
	SRS	WSMS follows WSRC requirements on developing, testing, documenting, maintaining, and using computer codes used for safety analysis. Requirements are specified in standalone WSMS QA documentation, or are cited and referenced in WSRC documentation. This includes but is not limited to, the WSRC 1Q Manual, 11Q, Section 20-1, the E7 Manual, and WSMS Quality Assurance Procedures.
	Pantex	In-house developed Software Quality Life Cycle (SQLC) Plant Standard STD-1875. Mandatory for all site-developed software, purchased software, contractor developed software, or design agency furnished software. The SQA process consists of peer reviews and approvals, and auditing.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Maintenance cont'd	Rocky Flats	The Computer Software Management Manual (1-MAN-004-CSSM) contains the procedures followed for software development, testing, documentation, and maintenance. This manual was developed in-house using best industry practices and is mandatory; QA processes are peer review and independent verification and validation.. The processes invoked by the CSMM have been reviewed and audited by the Software Engineering Institute at Carnegie-Mellon University and given a SEI Level certification. They have also been reviewed and audited for Software Quality Assurance by the Carlsbad Area Office for WIPP certification. Since virtually all of the codes used in the nuclear safety areas are provided by outside sources (Oak Ridge, Los Alamos, RSICC, etc.) we cannot vouch for the SQA processes used by those developers. However, the implementation of the codes on site is guided by the CSMM and V&V testing is performed as part of the installation and configuration management process mandated by the CSMM.
	Y-12	Y80-800, *Configuration Control*. The current software control program is defined by the, *Software Development and Control*, Y80 Series procedures; the upcoming revision will be based on DOE's Software Engineering Methodology (SEM). The Nuclear Criticality Safety organization uses the following safety-related software: (1) SCALE/KENO: Standard Computer Analyses for Licensing Evaluation and (2) MCNP: Monte Carlo N-particle Transport Code System. This software is controlled by the Y80 Series procedures including the Nuclear Criticality Safety organization procedures. The procedures were developed in-house at Y-12, based on software industry practices at the time. The procedures determine a software classification for each system based on various criteria. This classification is then used to drive the mandatory portions of the actual development process. It is mandatory that all Y-12 software use the Y80 procedures for guiding development. A combination of walkthroughs, reviews, and testing regimens are used as the basis for ensuring quality, per the Y80 procedures.
	INEEL	INEEL Program Requirements Document (PRD)-115, "Configuration Management;" INEEL Standard (STD)-107, "Configuration Management Program;" INEEL Management Control Procedure (MCP) 550, Software Management"; INEEL MCP-3630, "Computer System Change Control;" INEEL Guide (GDE)-59, "Guide for Computer System Change Control;" DOE-STD-1073-93, "Guide for Operational Configuration Management Program;" ANSI/IEEE STD-828-1998;" IEEE Standard for Software Configuration Plans;" ANSI/ANS-10.4-1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry." Compliance with the INEEL documents is mandatory. Software packages developed and maintained at INEEL that are used for nuclear facility safety analysis or for control of active Safety SSCs are subject to the INEEL CM Program, have received verification and validation (V&V), and have CM Plans in place. See survey for description of INEEL documents.
	YMP/TESS	•NQA-2, Subpart 2.7 •OCRWM Quality Assurance Requirements & Description •OCRWM AP-SI.1Q Software Management •NQA-2, Subpart 2.7 is the NRC Standard for software development, testing, documentation, maintenance and usage. OCRWM Quality Assurance Requirements & Description (QARD) reflects in total the requirements of NQA-2, Subpart 2.7. AP-SI.1Q Software Management is the implementing procedure for Supplement I of the QARD. Compliance with AP-SI.1Q is mandatory. SQA processes include independent peer review, inspection, audit, and verification and validation of software.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Maintenance cont'd	Hanford/RL	•Fluor Hanford--Primarily HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements*. Procedures are in-house developed based on DOE Orders and other government agencies' requirements and mandatory. All the SQA processes listed in the survey are accepted in the procedures - they are based on defined scope and risk. The procedure requires that some form of change control and review process be established. Each project is allowed to define in their implementing procedures the specific configuration management processes they will apply. •Bechtel Hanford--In-house BHI-AT-01 Procedure 1.7, BHI-AT-01 Procedure 1.8 *Software Acquisition and Maintenance*, and BHI-DE-01-EDPI-4.36-01, *Project Calculations*. Procedures are based on industry standards and are mandatory. •PNNL Hanford–Any software developed or used at the Laboratory is required to be controlled in accordance with the Computer Software and Database Control subject area, which is aligned with the Software Systems Engineering Process (SSEP). The subject area was derived largely from the SSEP. The SSEP addresses each of the issues identified above. The subject area is mandatory for all PNNL staff. The SSEP is mandatory for all projects in the Information Science and Engineering Division and for all projects done for the Information Systems Engineering product line. The SSEP is more rigorous and more flexible than the subject area. However, each is based on the fundamental premise of defining a plan based on specific project or activity needs and executing the plan to develop, acquire, or use the software in involved. Both the subject area and the SSEP were developed at PNNL. The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/). It's also based to lesser extent on elements of IEEE standards, Department of Defense MIL-STD-498 (since replaced), and Iterative Process Models like the "Spiral Model" by Boehm and "Managed Evolutionary Development" by U.S. Patent Office.
	Hanford/ORP	•Tank Farm–HNF-PRO-309, *Computer Software Quality Assurance Requirements* and HNF-PRO-2778, *IRM Application System Life Cycle Standards*. Procedures developed in-house based on DOE Orders and other government agency requirements and are mandatory. Varying degrees of SQA processes are used based on the defined scope and risk of the specific project application. •Tank Waste--Procedure K70C515, *Code of Practice for Computer Program Use,* addresses all the elements of ASME NQA-1-1994, Part II, Subpart 2.7, including software life cycle, development and maintenance, software testing, software verification and validation, documentation, error identification and notification. Procedure was developed in-house based on the requirements of NQA-1-1994, Part II, Subpart 2.7 and DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplement I. It is mandatory. SQA activities are installation testing and validation.
	WIPP	WP 16-IT3117, WIPP internal, mandatory, use-dependent; WP 16-2, WIPP internal, optional, use-dependent.
Usage	LLNL	•HCD/ABS--Printouts of ALOHA, HOTSPOT, and EPI code runs are included with the safety basis documents and QA'd as part of the document. •HCD/ABS--HOTSPOT is an LLNL-developed code adopted by DOE for evaluation of potential doses (50-yr CEDE based on ICRP-30 dose conversion factors). HCD uses it when reviewing radioactive material releases. •HCD/ABS--EPI is a commercially available code (by the developer of HOTSPOT) that models toxic material releases, giving respirable airborne material concentration as a function of distance from release point. •HCD/ABS--ALOHA is a NOAA product that models toxic material releases, giving respirable airborne material concentration as a function of distance from release point. One of its uses at LLNL is to model liquid and condensed gas releases from tanks. •HCD/ABS--GEN II and MACCS are more complex codes that are not generally used by HCD analysts for safety basis documents.
	LANL	Varies by customer. For specific customers, "Manufacturing Manual: Software Quality Assurance"; MFG-AP-0014 Rev. 0; and "TRU Waste Characterization Program: TWCP Quality Procedure", TWCP-QP-1.1-006 Rev. 7 are used.
	SNL	TA-V RREP QA Procedure, RREP 3-2, Computer Software Control; developed in-house, is mandatory for all software associated with the TA-V Nuclear Facilities; QA processes are peer review and testing.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Usage cont'd	SRS	WSMS follows WSRC requirements on developing, testing, documenting, maintaining, and using computer codes used for safety analysis. Requirements are specified in standalone WSMS QA documentation, or are cited and referenced in WSRC documentation. This includes but is not limited to, the WSRC 1Q Manual, 11Q, Section 20-1, the E7 Manual, and WSMS Quality Assurance Procedures. Procedures are in-house developed and mandatory; QA processes are peer review.
	Pantex	In-house developed Software Quality Life Cycle (SQLC) Plant Standard STD-1875. Mandatory for all site-developed software, purchased software, contractor developed software, or design agency furnished software. The SQA process consists of peer reviews and approvals, and auditing.
	Rocky Flats	This is determined by the specific software used by the analysts.
	Y-12	Y80-900, *Post-Implementation Review.* The current software control program is defined by the, *Software Development and Control*, Y80 Series procedures; the upcoming revision will be based on DOE's Software Engineering Methodology (SEM). The Nuclear Criticality Safety organization uses the following safety-related software: (1) SCALE/KENO: Standard Computer Analyses for Licensing Evaluation and (2) MCNP: Monte Carlo N-particle Transport Code System. This software is controlled by the Y80 Series procedures including the Nuclear Criticality Safety organization procedures and Y70-68-005, *Quality Assurance for Nuclear Criticality Safety Computer Calculations*, Y/DD-833, Lockheed Martin Energy Systems Y-12 Nuclear Criticality Safety Organization Plan for Administration of the HP Workstation, Y/DD-573, *MMES Y-12 Nuclear Criticality Safety Software Validation of Keno V.a on the HP 9000/Series 700 Workstation*, Y/DD-790, *Validation of MCNP4A for Criticality Safety and Shielding Analyses on the HP-735*, and Y/DD-860, *Validation of MCNP4B2 for Criticality Safety and Shielding Analyses on the HP C-180*. The procedures were developed in-house at Y-12, based on software industry practices at the time. The procedures determine a software classification for each system based on various criteria. This classification is then used to drive the mandatory portions of the actual development process. It is mandatory that all Y-12 software use the Y80 procedures for guiding development. A combination of walkthroughs, reviews, and testing regimens are used as the basis for ensuring quality, per the Y80 procedures.
	INEEL	INEEL Program Requirements Document (PRD)-115, "Configuration Management;" INEEL Standard (STD)-107, "Configuration Management Program;" INEEL Management Control Procedure (MCP) 550, "Software Management"; INEEL MCP-3630, "Computer System Change Control;" INEEL Guide (GDE)-59, "Guide for Computer System Change Control;" DOE-STD-1073-93, "Guide for Operational Configuration Management Program;" ANSI/IEEE STD-828-1998;" IEEE Standard for Software Configuration Plans;" ANSI/ANS-10.4-1987, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry." Compliance with the INEEL documents is mandatory. Software packages developed and maintained at INEEL that are used for nuclear facility safety analysis or for control of active Safety SSCs are subject to the INEEL CM Program, have received verification and validation (V&V), and have CM Plans in place. See survey for description of INEEL documents.
	YMP/TESS	•NQA-2, Subpart 2.7 •OCRWM Quality Assurance Requirements & Description •OCRWM AP-SI.1Q Software Management •OCRWM AP-SV.1Q Control of Electronic Management of Data •NQA-2, Subpart 2.7 is the NRC Standard for software development, testing, documentation, maintenance and usage. OCRWM Quality Assurance Requirements & Description (QARD) reflects in total the requirements of NQA-2, Subpart 2.7. AP-SI.1Q Software Management is the implementing procedure for Supplement I of the QARD. Compliance with AP-SI.1Q is mandatory. SQA processes include independent peer review, inspection, audit, and verification and validation of software.

I. SOFTWARE QUALITY ASSURANCE (SQA) INFORMATION		
1. What documented SQA programs or procedures do you follow for computer codes used for safety analysis in the areas of software development, testing, documentation, maintenance, and usage?		
Usage cont'd	Hanford/RL	•Fluor Hanford--Primarily HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements*. Procedures are in-house developed based on DOE Orders and other government agencies' requirements and mandatory. All the SQA processes listed in the survey are accepted in the procedures - they are based on defined scope and risk. The procedure requires that some form of change control and review process be established. Each project is allowed to define in their implementing procedures the specific configuration management processes they will apply. •Bechtel Hanford--In-house BHI-AT-01 Procedure 1.7, BHI-AT-01 Procedure 1.8 *Software Acquisition and Maintenance*, and BHI-DE-01-EDPI-4.36-01, *Project Calculations*. Procedures are based on industry standards and are mandatory. •PNNL Hanford--Any software developed or used at the Laboratory is required to be controlled in accordance with the Computer Software and Database Control subject area, which is aligned with the Software Systems Engineering Process (SSEP). The subject area was derived largely from the SSEP. The SSEP addresses each of the issues identified above. The subject area is mandatory for all PNNL staff. The SSEP is mandatory for all projects in the Information Science and Engineering Division and for all projects done for the Information Systems Engineering product line. The SSEP is more rigorous and more flexible than the subject area. However, each is based on the fundamental premise of defining a plan based on specific project or activity needs and executing the plan to develop, acquire, or use the software in involved. Both the subject area and the SSEP were developed at PNNL. The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/). It's also based to lesser extent on elements of IEEE standards, Department of Defense MIL-STD-498 (since replaced), and Iterative Process Models like the "Spiral Model" by Boehm and "Managed Evolutionary Development" by U.S. Patent Office.
	Hanford/ORP	•Tank Farm–HNF-PRO-309, *Computer Software Quality Assurance Requirements* and HNF-PRO-2778, *IRM Application System Life Cycle Standards*. Procedures developed in-house based on DOE Orders and other government agency requirements and are mandatory. Varying degrees of SQA processes are used based on the defined scope and risk of the specific project application. •Tank Waste--Procedure K70C515, *Code of Practice for Computer Program Use,* addresses all the elements of ASME NQA-1-1994, Part II, Subpart 2.7, including software life cycle, development and maintenance, software testing, software verification and validation, documentation, error identification and notification. Procedure was developed in-house based on the requirements of NQA-1-1994, Part II, Subpart 2.7 and DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplement I. It is mandatory. SQA activities are installation testing and validation.
	WIPP	WP 16-IT3117, WIPP internal, mandatory, use-dependent; WP 16-2, WIPP internal, optional, use-dependent.

2. Do these procedures comply with the following guidelines?		
DOE O 420.1	LLNL	CSG--Criticality safety software complies with DOE O 420.1 requirements.
	LANL	In part
	SNL	Yes
	SRS	Yes
	Pantex	See "Other" below.
	Rocky Flats	In Whole
	Y-12	See "Other" – Y80 Series based on DOE guidance indicated below.
	INEEL	Implemented but not mapped
	YMP/TESS	Not Applicable
	Hanford/RL	•Fluor Hanford--DOE Order 420.1 is not in the Project Hanford Management Contract (PHMC); however, the following DOE Orders and FH procedures are in compliance with them: DOE 5480.28, *Natural Phenomena Hazards Mitigation* DOE 5480.7A, *Fire Protection* DOE 6430.1A, *General Design Criteria* DOE 5480.24, *Criticality Safety* •Bechtel Hanford--DOE Order 420.1 is not included in the ERC Contract at this time. However, the ERC procedures identified above are consistent with the requirement of DOE Order 420.1 •PNNL Hanford--Not in PNNL's contract yet. Not applicable. (DOE Orders 5480.24 and 5480.7A have been implemented.)
	Hanford/ORP	•Tank Farm–The SQA program was not written to satisfy DOE O 420.1 specifically, but in that DOE O 420.1 invokes 10CFR830.120, the SQA program does comply with DOE O 420.1. Specifically, DOE O 420.1 requires design of safety structures, systems and components (SSCs) to be performed under a quality assurance program that satisfies 10 CFR830.120. Our quality assurance program satisfies 10 CFR830.120. Specifically, under design, SQA requirements are addressed to ensure that safety SSCs that are designed with the use of software are properly controlled. •Tank Waste–Under the privatization concept and under the current "bridge" design effort the cited DOE Orders are not applicable; see section V, Additional Comments.
	WIPP	Yes, compliance in whole.
DOE O 414.1	LLNL	HCD/ABS--Compliance with applicable sections of 10 CFR 830.120 — on-the-job training, peer and independent review of calculations, record keeping, approved procedures for use of codes
	LANL	In part
DOE O 414.1 cont'd	SNL	Yes

2. Do these procedures comply with the following guidelines?		
	SRS	In part
	Pantex	Mapped, see "Other" below
	Rocky Flats	In Whole
	Y-12	See "Other", based on DOE O 5700.6C
	INEEL	Implemented but not mapped
	YMP/TESS	Full compliance
	Hanford/RL	•Fluor Hanford--This Order is implemented through HNF-MP-599, *PHMC Quality Assurance Program Description*. The applicable requirements of HNF-MP-599 are implemented by HNF-PRO-2778, *IRM Application System Life Cycle Standards* and HNF-PRO-309, *Computer Software Quality Assurance Requirements*. •Bechtel Hanford--DOE Order 414.1 is not included in the ERC Contract at this time. The ERC procedures are compliant with DOE Order 5700.6C as required by the Contract. •PNNL Hanford--The "Computer Software and Database Control" subject area is compliant with this order.
	Hanford/ORP	•Tank Farm–Yes •Tank Waste--Under the privatization concept and under the current "bridge" design effort the cited DOE Orders are not applicable; see section V, Additional Comments.
	WIPP	Yes, compliance in whole.
DOE O 200.1	LLNL	HCD/ABS--Yes
	LANL	In part
	SNL	Yes
	SRS	Uncertain
	Pantex	See "Other" below
	Rocky Flats	In Whole
	Y-12	See "Other", based on DOE O 1360.1A
	INEEL	Implemented but not mapped
DOE O 200.1 cont'd	YMP/TESS	Full compliance

2. Do these procedures comply with the following guidelines?		
	Hanford/RL	•Fluor Hanford--HNF-PRO-2778, *IRM Application Software System Life Cycle Standards* implements this Order. •Bechtel Hanford--DOE Order 200.1 is not included in the ERC Contract at this time. The ERC procedures are based on the Bechtel Corporate SDMF, which is consistent with DOE Order 200.1. •PNNL Hanford–Not in PNNL's contract yet. Not applicable. (DOE Order 1330.1D has been implemented.)
	Hanford/ORP	•Tank Farm–HNF-PRO-2778 implements this Order. •Tank Waste--Under the privatization concept and under the current "bridge" design effort the cited DOE Orders are not applicable; see section V, Additional Comments.
	WIPP	Yes, compliance in whole.
DOE G 200.1-1	LLNL	HCD/ABS--Not appropriate for desktop computing software
	LANL	In part
	SNL	No
	SRS	Uncertain
	Pantex	Mapped, see "Other" below
	Rocky Flats	In Whole
	Y-12	See "Other"
	INEEL	Implemented but not mapped
	YMP/TESS	Full compliance
	Hanford/RL	•Fluor Hanford--The FH procedures comply with DOE Order 200.1. The Guide is not in the PHMC. •Bechtel Hanford--DOE Order 200.1 is not included in the ERC Contract at this time. The ERC procedures are based on the Bechtel Corporate SDMF, which is consistent with DOE Order 200.1. •PNNL Hanford–The SSEP complies.
	Hanford/ORP	•Tank Farm–Yes •Tank Waste--Under the privatization concept and under the current "bridge" design effort the cited DOE Orders are not applicable; see section V, Additional Comments.
	WIPP	No
DOE G 414.1-1	LLNL	HCD/ABS–DOE G 414.1 does not have a section 4.6.3. DOE G 414.2 *Quality Assurance Management System Guide* does have a section 4.6.3 related to the Design Process. It calls for validation of the software used in the design process. As noted above, informal validation is attained by comparison with standard output results, widespread use for exposure and dose calculations, and review and approval of output during the approval of the safety basis documents.

2. Do these procedures comply with the following guidelines?		
	LANL	In part
	SNL	No
	SRS	Uncertain
	Pantex	See "Other" below
	Rocky Flats	In Whole
	Y-12	See "Other", based on DOE AL QC-1
	INEEL	Implemented but not mapped
	YMP/TESS	Full compliance
	Hanford/RL	•Fluor Hanford--The FH procedures comply with section 4.6.3 of DOE G 414.1-2. •Bechtel Hanford--DOE Order 414.1 is not included in the ERC Contract at this time. The ERC procedures are compliant with DOE Order 5700.6C as required by the Contract. •PNNL Hanford--Was considered when developing the Integrated Assessment System within PNNL. (Note: August 1996 version does not contain a section 4.6.3)
	Hanford/ORP	•Tank Farm–Yes •Tank Waste--Under the privatization concept and under the current "bridge" design effort the cited DOE Orders are not applicable; see section V, Additional Comments.
	WIPP	Yes, compliance in whole.
ANSI/ANS-10.4-1987	LLNL	–
	LANL	In part
	SNL	No
	SRS	In part
	Pantex	See "Other" below
ANSI/ANS-10.4-1987 cont'd	Rocky Flats	Yes
	Y-12	See "Other"
	INEEL	Implemented but not mapped

2. Do these procedures comply with the following guidelines?		
	YMP/TESS	Full compliance
	Hanford/RL	•Fluor Hanford–No response. •Bechtel Hanford–No. •PNNL Hanford–No response.
	Hanford/ORP	•Tank Farm–No response. •Tank Waste–No response.
	WIPP	–
NQA-1-1997	LLNL	CSG--Criticality safety software meets ANSI/ANS 8.1, Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors
	LANL	In part
	SNL	Yes
	SRS	In part
	Pantex	Mapped, see "Other" below
	Rocky Flats	Yes
	Y-12	See "Other"
	INEEL	Implemented but not mapped
	YMP/TESS	Full compliance
	Hanford/RL	•Fluor Hanford--The FH procedures comply with NQA-1-97, Subpart 2.7, *Quality Assurance Requirements of Computer Software for Nuclear Facility Application* with NQA-1-99 Addendum •Bechtel Hanford–No •PNNL Hanford–This can be applied on a project specific basis, as needed, but it is not a foundation for the entire Laboratory. For example, analysis for criticality and shielding is done using MCNP and SCALE. Control and maintenance of these codes is performed by the following procedure, PNL-MA-875 "Computer Code Maintenance Quality Assurance Manual." This manual is NQA-1 Part 2.7 Compliant.
NQA-1-1997 cont'd	Hanford/ORP	•Tank Farm–The CHG quality assurance program invokes NQA-1-89 as a consensus standard for implementing 10CFR830.120 and utilizes the FH procedures for implementing the NQA-1-89 requirements. The FH procedures comply with NQA-1-97, Subpart 2.7, Quality Assurance Requirements of Computer Software for Nuclear Facility Application with NQA-1-99 Addendum. •Tank Waste–ASME NQA-1-1994, Part II, Subpart 2.7.
	WIPP	Yes, compliance in whole, where required.

2. Do these procedures comply with the following guidelines?		
Other	LLNL	No
	LANL	QC-1, IEEE STD 730-1998, IEEE STD 730.1-1995, IEEE STD 828-1998, ASME NQA-2-1989, NQA-2a-1990, NUREG/CR-0178, NUREG/CR 6463, NUREG/CR 4640, IEEE Std. 610.12-1990
	SNL	–
	SRS	–
	Pantex	The in-house developed Software Quality Life Cycle Plant standard has been mapped to the following: ANSI/ISO/ASQC Q9001 –1994 Quality Systems, DOE/HQ Software Engineering Methodology 3/96, DOE Order 5700.6C Quality Assurance (10 CFR 830.120, Quality Assurance Requirements), ASME NQA-1 Addenda Part 2.7, DOE/AL Quality Criteria (QC-1), and the Software Engineering Institute's (SEI) Capability Maturity Model's eighteen Key Process Areas.
	Rocky Flats	–
	Y-12	The current software procedures were issued in early 1991 and revised in early 1995. The procedures have not been evaluated against the above requirements. The new Y80 Series procedures, expected to be issued end of CY2000, will address the above requirements and be in line with the current safety criteria such as those required by Integrated Safety Management (ISM) processes. The revised procedures will incorporate the latest QA, security, and software engineering requirements.
	INEEL	–
	YMP/TESS	–
Other cont'd	Hanford/RL	•Fluor Hanford–The FH procedures also comply with Office of Civilian Radioactive Waste Management (OCRWM) QA Requirements and Description, Section 3 - Design Control, Section 11 - Test Control, and Supplement 1 - Software, and with Title 10, Code of Federal Regulations, Part 830.120 - *Quality Assurance Requirements.* •Bechtel Hanford–ISO 9000. The ERC has not developed in-house computer codes for safety analysis applications. All software in use for safety analysis was developed by third parties and is either in the public domain or commercially available. The ERC specifies, procures, and validates such software consistent with our SQA program. The minimum requirements are: •A determination by the applicable functional manager that the documentation supplied by the third party includes a description of the theoretical basis for the software package, instructions in the use of the package, and that the extent of software validation and verification is adequate for the ERC application. •Confirmation that the software as delivered reproduces the results of tests conducted as part of the software validation/verification. BHI's Automation Technology group is in the process of updating the SQA program, and existing procedures are being reviewed/ revised. The plan is to adopt the following DOE documents in their entirety: DOE Order 200.1 *Information Management Program*, and DOE Guide 200.1-1 *Department of Energy Software Engineering Methodology.* •PNNL Hanford–The primary standard for the SSEP is the Software Engineering Institute's Capability Maturity Model for Software (see http://www.sei.cmu.edu/cmm/)
	Hanford/ORP	•Tank Farm–The FH procedures comply with 10CFR830.120, Quality Assurance Requirements. Subsequent to creation of the DOE Office of River Protection (ORP) and changing the Tank Farm Contractor from a subcontractor under Fluor Hanford, Inc. (FH) to a prime contractor under ORP, the Tank Farm Contractor (now CH2M HILL Hanford Group, Inc. [CHG]) and FH agreed that common use of some existing FH procedures would facilitate consistency among interfacing Hanford contractors. CHG utilizes SQA programs that were written by FH for use with the Project Hanford Management System. •Tank Waste–DOE/RW/0333P, *Quality Assurance Requirements and Description (QARD)*, Supplements I and V.

2. Do these procedures comply with the following guidelines?		
	WIPP	N/A

3.	How frequently is compliance with these procedures audited?	Are audits performed by external groups?	What is the date(s) of your last SQA audit?
LLNL	•HCD/ABS--No formal audit program •CSG--Criticality safety is audited by both LLNL ARO and DOE-Oakland Operations Office. The ARO audit is on a three-year cycle. •HWM--Multiple times per year through assessments, audits, and surveillance. Audits are directly and indirectly performed of HWM's QA Program by DOE, State of CA/DTSC, internal and external audits of the Waste Certification Program, internally by Hazards Control and Assurance Review Office. SQA has not been the main subject of an audit, but some components of SQA have been assessed as part of a audit.	•HSD/ABS –No •CSG–Yes, Criticality safety audit by LLNL Assurance Review Office, which did include external experts. •HWM--Yes, by the Assurance Review Office (ARO) and State and Federal agencies.	•HCD/ABS --N/A •CSG–Last ARO audit on Criticality safety was in January of 2000.
LANL	Varies by customer	Varies by customer	Varies by code, by as an example TWCP was audited in August 2000.
SNL	Once per Year	No – Internal Independent	January, 2000
SRS	Compliance with WSRC software and practices, and evolving WSMS procedures are audited in part every 3 to 4 years.	The audits are usually performed by external groups (WSRC, others). Occasionally, self-assessments are conducted by WSMS. The latter are mostly spot-checks of some software users and only apply to a few software packages.	Compliance has been checked once (~ 1998) since the formation of WSMS (1 October 1997). It's unclear to the degree this activity was an audit.
Pantex	As determined by the Internal Auditing department relative to the risk assessment process (Criticality Safety – annually).	Several Y2K audits were conducted by external groups.	9/00 by DOE/AAO relative to QC-1 compliance. Criticality Safety – 2/00.
Rocky Flats	Audits are conducted on various aspects of SQA and Nuclear Safety matters throughout the year according to the site Master Audit Schedule.	Yes, both actual external groups (EPA, CAO, etc.), as well as internal, but independent, groups (K-H Internal audit, Independent Safety Oversight)	June 26, 2000.
Y-12	SQA is not singled-out as a specific entity. It is integrated into the overall software control process. Therefore, an assessment just on the SQA elements of the software control program would not be performed.	The Plant Quality Assurance Organization assesses software associated with a work process when the work process is being assessed.	November 1999 (QAS-2)
INEEL	Compliance with INEEL procedures is a typical subject for facility self-assessments.	Not specified	No comprehensive sitewide audit has been performed. Flowdown review conducted in FY 99.
YMP/TESS	Monthly	Yes	8/25/2000

3.	How frequently is compliance with these procedures audited?	Are audits performed by external groups?	What is the date(s) of your last SQA audit?
Hanford/RL	•Fluor Hanford--There isn't a set frequency; however, audits have occurred approximately annually. •Bechtel Hanford--Comprehensive compliance audits, as referred to here, are not routinely scheduled. Audits for software licensing are performed annually. •PNNL Hanford--Assessment for Laboratory compliance to the subject area has not been conducted. However, there is a SSEP assessment program that focuses on projects performed by IS&E and for the ISE product line.	•Fluor Hanford--Yes, audit groups include: Fluor Corporate Auditors, DOE-RL Auditors, IG Auditors, DNFSB Auditors, OCRWM Auditors, and other oversight agencies. The frequency and schedule of audits are not known until an audit notification is sent. •Bechtel Hanford-No •PNNL Hanford--The SSEP assessments are performed by representatives from the Quality organization.	•Fluor Hanford--1997 - Fluor Corp (97-001-1), General and Applications Controls Audit; June, 1999 - DOR-AUD-PAD-99-021, Software Quality Assurance; July, 2000 - IA2000-06, Software Acquisition/Development •Bechtel Hanford--The last documented SQA audit was performed in February 1996. •PNNL Hanford--SSEP assessments are performed continually. There are currently several in progress. In FY00 Internal Auditing performed an audit on General Information Systems Controls, which included looking at the subject area and SSEP, but did not cover them in depth or specifically focus on them.
Hanford/ORP	•Tank Farm–Specific frequencies for audits of the SQA program are not set. However, as a program implementing quality assurance requirements, the implementation of these requirements are required to be audited on an annual basis. •Tank Waste–No frequency is established; however, audits have been performed approximately annually. In addition, management assessments and surveillance have been performed more frequently.	•Tank Farm–CHG has performed no audits on SQA since October 1,1999. Prior to October 1, 1999, the SQA program was under FH and was audited by internal and external groups. •Tank Waste–Yes. Audit groups included DOE/RL-Regulatory Unit, DOE-Office of River Protection	•Tank Farm–June 1999 •Tank Waste–External audit: 11/4/99; internal audit: 2/16/00
WIPP	Periodically.	Sometimes external, sometimes internal.	External, Environmental Protection Agency, March 1999 --WWIS Programmatic Audit; Internal, WID QA, November 2000 -- WWIS Programmatic audit to NQA-2A; Each Software Quality Assurance plan (per WP 16-IT3117) is reviewed and approved by WID QA.

4. To what degree are safety-related decisions on facility operation, or the safety analysis process itself based on the output of one or more computer codes?	
LLNL	•HCD/ABS --Chemical hazard classification and risk assessments are based on these codes. •HWM--HWM Codes such as HOTSPOT, ALOHA, and EPI are used by FS&C safety analysts in the performance of safety analyses. Results are used in HWM SARs.
LANL	Codes have a large impact on safety-related decisions. Computer codes effect functional requirements of some safety systems and therefore directly impact facility operations. Safety analysis process for Category 2 nuclear facilities is highly dependent on computer codes.
SNL	*Safety Analysis Process:* •Reactor Kinetics – High degree–The safety analysis using reactor kinetics codes can produce TSR requirements and design requirements for instrumentation (safety-significant SSCs). •Thermal Hydraulic and Heat Transfer – High degree – The safety analysis using thermal hydraulic and heat transfer codes is used to develop reactor power and fuel temperature limits for TSRs and to identify potential safety-significant SSCs. •Neutronics (for Reactor configuration) – High degree – The safety analysis using neutronic codes can produce TSRs and safety-significant SSCs. •Accident Analysis – High degree – The safety analysis of dose consequences from radiological material release using downwind dose calculations can result in safety-class SSC determination and TSRs. *Facility Operation:* •Control console (ACRR) contains computer software that assists operator in manipulating rods to maintain continuous power or to place the reactor on a positive or negative period. The software also plays a role in sequencing interlocks that prohibit reactivity insertion during some stages of the operation.
SRS	•In most cases for Category 2 facilities, the overall safety case for a facility is built on several layers of analysis. For example, the layers can be thought to consist of: the Hazard Analysis, the Accident & Consequence Analysis, the Functional Classification and determination of Technical Safety Requirements, and Defense-in-Defense analysis (as the key pieces). While one of these layers (Accident Analysis) is heavily computationally oriented, most of the work is engineering calculation-based. Accident phenomenology and source term codes are usually not emphasized to properly conduct this work. The next layer is the dispersion and consequence analysis. In most cases, this will be a code such as MACCS to provide a 95th percentile dose. (Note that WSMC still applies MACCS vs. MACCS2 because of the SQA pedigree concerns.) •Other segments of this analysis are not as computer model intensive. Hazard analysis, functional classification, and defense-in-depth phases of safety analysis are qualitatively driven (although some decisions rest on quantitative output from previous steps). •Thus, while a computer code can be applied for this stage of analysis, the actual robust safety case rarely relies on the dose or other code outcome as the sole measure to determine ultimate safety of a facility. Several counter-examples may be cited, but these are typically heavily reviewed in this case by independent parties. For example, if fire issues are critical to a facility a number of fire computer model calculations may be requested, performed, and documented. However, a thorough review is normally performed by DOE and other reviewers. •Category 3 and lower facilities are much less likely to base their safety case on a computer model-based analysis. Preset spreadsheet estimates can be used for the hazard analysis, but again, other work is used to document the safety case. In other words, there is less reliance on the "numbers" from a code, and more likely the "big picture" of walk downs, qualitative hazard binning, and other techniques are applied to build a complete safety case.
Pantex	The majority of authorization basis controls at Pantex are derived through hazard and accident analysis methods that do not rely on computer models. However, various computer models, as noted above, are used to support the safety analysis process and the derivation of preventative and mitigative controls. For example, (a) computer dispersion models are relied upon for quantifying consequences and deriving appropriate mitigative controls for unmitigated radiological release scenarios that exceed DOE evaluation guidelines (EGs), and (b) fire modeling is used to determine separation distances between combustibles and high explosive. Emergency Management requires computer models to determine protective action recommendations at various receptor points.
Rocky Flats	The codes provide input to the decision-making process with specific and necessary information, but the results from the codes are evaluated against other information (Internal Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/ Doc(95) 03/I) as decisions are formulated.
Y-12	•Facility Safety: The main software used in support of safety-related decisions on facility operations is software used in nuclear criticality safety evaluations and software used in evaluating accidents postulated in the Authorization Basis (AB) documents. The results from these codes may indicate that safety related controls are required and whether these controls are Safety Class or Safety Significant. •Nuclear Criticality Safety: Extensively. In making a determination of nuclear criticality safety, the criticality safety analyst bases determining the "limits and conditions of operations" for maintaining subcriticality on a number of calculations, as well as, on industry standards, administrative guidance, and professional judgement.

4. To what degree are safety-related decisions on facility operation, or the safety analysis process itself based on the output of one or more computer codes?	
INEEL	Computer codes developed and maintained here at the INEEL, as well as software developed elsewhere and used here, are employed to perform the following functions important to nuclear safety: •Thermal hydraulic primary coolant calculations and neutron physics calculations for the Advanced Test Reactor (ATR) core and experiment loops, to establish reactor operating limits and safety system trip settings to ensure protection of fuel integrity throughout anticipated and unlikely reactor upsets. •Calculation of radionuclide inventories in reactor fuels to determine source terms for postulated accidents in SARs. •Radiological dose consequence calculations for postulated abnormal events and accident scenarios for identification of safety class and safety significant SSCs and TSR-level controls in nuclear facility SARs, and in support of establishing emergency planning zones (EPZ) in emergency preparedness documents. •Calculational software for on-line control of the New Waste Calcining Facility (NWCF) rapid shutdown system, for prevention of an explosion involving the in-bed combustion heating system in the NWCF calciner vessel.
YMP/TESS	At this stage of the Project (Site Characterization) little use is made of computer codes in the performance of safety analyses. No nuclear material is stored on-site and facility operations consist of drilling, mining and scientific data collection to determine the suitability of Yucca Mountain as a Mined Geologic Repository for spent nuclear fuel.
Hanford/RL	•Fluor Hanford--Computer codes are used to quantify the consequences of operational accidents, natural phenomena events, and external events that have been selected for accident analyses. They are used to estimate the radiological or other hazardous material source terms for these accidents by: (1) estimating physical facility damage to the facility; (2) providing the basis for assigning material-at-risk quantities; and (3) establishing the basis for material release and respirable fractions or release rates. Then codes are used to estimate dose and exposure profiles considering variables such as meteorological conditions, time dependent characteristics, activity, and release rates or duration for radioactive or other hazardous materials that could be released to the environment. Thus computer codes are a significant input to safety-related decisions but not a sole factor. Decisions also have to consider economics, schedules, duration and type of missions and good common sense engineering judgement. •Bechtel Hanford--The facilities in the ERC work scope do not involve inventories of hazardous chemicals that exceed the threshold quantities in 29 CFR 1910.119 and 40 CFR 68.130. Many ERC facilities do not involve inventories of radioactive materials that exceed the Category 3 threshold quantities in DOE-STD-1027-92. The material in ERC facilities with radiological inventories in excess of the Category 3 threshold quantities is not readily dispersible. Consistent with this work scope, ERC decisions on facility operation, or the safety analysis process, do not rely greatly on the output from computer codes. The safety analysis for ERC facilities includes evaluation of the bounding consequences from airborne releases of radioactive materials and exposures to direct radiation. The consequences from airborne releases use computer generated atmospheric dispersion coefficients; the consequences from direct exposures are computer generated. These evaluations support the final hazard classification of the facility and serve to confirm the qualitative consequence assessments that are part of the hazard analysis process. These results are also compared to evaluation guidelines and are used in developing emergency action levels. ERC facilities do not include safety class systems, structures, and components (SSCs), and the safety significant SSCs in ERC facilities are so designated based on defense-in-depth considerations. Given the ERC work scope, this is not expected to change. Accordingly, the ERC does not rely on computer code output to establish performance requirements for SSCs, to assess the performance of SSCs under evaluation basis accident conditions, or to establish the bases for technical safety requirements (TSRs). •PNNL Bechtel–continued on following page
	•PNNL Bechtel–With specific application to Radiochemical Processing Laboratory (RPL) (the only PNNL category 2 nuclear facility)there are three codes of primary interest (GENII, SCALE, and MCNP) that are used in developing and maintaining the authorization basis (i.e., used in performance of safety analysis). All of these codes are distributed through the Radiation Safety Information Computational Center (RSICC) managed by ORNL (http://epicws.epm.ornl.gov/rsic.html). Most if not all of the documentation needed to pedigree the use of these codes for RPL can be found in the Safety Basis documentation (http://wwwi.pnl.gov/operating/reports/cmp.stm). The safety analysis is done using GENII version 1.485. The analysis is done by staff in Risk Analysis & Health Protection. Control of the code and training and qualification of the analysis staff is under the group's purview. The information at http://wwwi.pnl.gov/operating/pdf/rplsar4.pdf provides great insight into how this is done. The Hanford and Environmental Dose Overview Program was established to standardize dose calculations between all contractors. Procedures were established to define how the calculations were to be done. During the last review of the RPL Safety Basis Authorization, the code was used and standard review procedures were implemented for the results. There were no specific QA requirements imposed on the effort. GENII was developed and released in 1988, during which time consideration was given to NQA-1 SQA requirements and the QA Program in place was an NQA-1 based program. Training on GENII was conducted informally by the lead developer. Analysis for criticality and shielding is done using SCALE and MCNP. This analysis is done by staff in Materials & Engineering Analysis. Control of the code and training and qualification of the analysis staff is under the group's purview. PNL-MA-875 is used as the manual for SQA. This manual is NQA-1, Part 2.7 compliant. Training on SCALE and MCNP is done via formal courses with the developers and with on the job training with experienced users.

4. To what degree are safety-related decisions on facility operation, or the safety analysis process itself based on the output of one or more computer codes?	
Hanford/ORP	•Tank Farm–Computer codes are used to determine release quantities and consequences of hypothetical accidents. The results of these analyses, along with other considerations such as economics, duration and type of the associated mission, and engineering judgement, are used to determine operational controls. Computer codes provide input in this process, but are not the sole factor for determining operational controls. •Tank Waste–Computer codes are verified and validated using predetermined input standards that have known results. To qualify as acceptable, the test results of a computer code must meet predetermined acceptance criteria. When used in design to determine k-effective for neutron criticality, shielding thickness, or dose rates, these computer codes are fun by experienced engineers who set up computer models to simulate the physical conditions of the design. These experienced and qualified engineers apply their knowledge and experience to judge whether the output of each computer run is reasonable when compared to the input data. If the output is judged to be unreasonable when compared to the input, the model is examined and/or revised and the code is rerun until the output is reasonable. The results are then compared to the design criteria. If the results are within the acceptable window of tolerances for the design criteria, the results of the computer run or series of runs are relied on for design application. If the results do not fall within the acceptable window of tolerance for the design criteria, the work is subject to redesign until it meets the design criteria. Having met the criteria, calculations using the results of the computer code are checked by another experienced and qualified engineer. The checker reviews the entire calculation including the computer runs. Using a predetermined checklist, the checker ensures that the computer model was appropriate, the computer inputs were correct and appropriate to the model and that the results were reasonable when compared to the input data and that the results meet the criteria within acceptable tolerances. When the above conditions are judged acceptable by the author, the checker, and management, the results are approved for design application.
WIPP	For safety-related decisions on facility operations -- very little. For the safety analysis process itself -- dose assessment relies on output of computer codes.

Appendix C. APAC Working Group Recommendations (1996 – 1998)
(Accident Phenomenology and Consequence)

Source Term Generation and In-Facility Transport Model Recommendations

The Fire Working Group (FWG) concluded that FIRAC/FIRIN was the best overall computer model of the five fire analysis models reviewed for DOE safety analysis applications, based on its ability to calculate not only the fire characteristics but also the potential radioactive and fire by-product source terms. However, because of the many limitations and errors identified in FIRIN, and the better fire compartment modeling capabilities of CFAST, a combination of CFAST/FIRAC, if developed, would be an optimized tool. FPETool was found readily applicable to applications in which no source term calculations are needed, but in which first order-of-magnitude estimates are adequate. This computer model is useful in the context of supporting fire hazard analyses in compliance with regulatory requirements. The FWG determined that while CFAST was the best code for implementing the mass and energy conservation equations within a compartment or zone, it had limitations in its ability to model mechanical ventilation systems. Table C.1 summarizes a "first-order" assessment of the applicability of the evaluated fire models in meeting DOE fire hazard requirements by consequence locations, specifically, local, collocated workers and the general public, and facility impacts.

Table C.1. Fire Model "First-Order" Assessment

Computer Model	Zone (Z) Field (F) Model	Local Worker Consequences	Collocated Workers, General Public, and Environmental Consequences	Facility (or Mission) Impacts
FIRAC/FIRIN	Z	YES	YES	YES
FPETool	Z	YES (Note 1)	NO	YES (Note 4)
COMPBRN III	Z	YES (Note 2)	NO	YES
CFAST	Z	YES (Note 3)	NO	YES
VULCAN	F	NO	NO	YES

Note 1. Excludes radiological consequences
Note 2. Has very limited capabilities
Note 3. User must manually input initial airborne source terms and energy functions within the fire room.
Note 4. Must input compartment dimensions, vent locations, fire load, and fire load density.

The Explosions and Energetic Events (EEE) Working Group concentrated on methodology recommendations over computer model preferences. This was done in part due to the complexity of the phenomenon[12] and its impact on scenario development, resource limitations on the project, the focused needs at most DOE sites, and also in recognition that the many special-purpose methodologies that have been developed would demand more time to thoroughly investigate than was allotted in the APAC program. A survey of DOE Complex hazards and historical data indicated that the Working Group should devote most of its time to methods amenable to treating solid-phase detonation, gas-phase detonation, gas-phase deflagration, and stored-energy releases.

[12] Explosions can lead to combustion products, and toxicological and radiological source terms, that are important in the overall determination of consequences for safety basis documentation. However, detonation and deflagration events can also cause blast wave overpressures, thermal radiation, the generation of debris and projectiles, and potentially knock-on effects.

The EEE Working Group recommended using a model that is consistent with the level of sophistication required in the analysis and for the facility in question. Methodologies reviewed included simple handbook-prescribed engineering calculations to sophisticated hydrodynamic/computational fluid dynamics models. It was the consensus of working group members that engineering calculations provide the safety analyst with sufficient information to assess the potential consequences associated with explosions and energetic events in DOE facilities. Engineering calculational methods could be applied to all levels in the graded approach for assessing facility hazards, with the possible exception of some cases involving high hazard facilities and specialized analysis needs, where computational fluid dynamic codes may be required. Table C.2 lists recommended modeling approaches for specific explosion types.

Table C.2. Explosion Model Guide

Explosion Type	Modeling Guidance
Condensed-Phase Explosion (TNT-type)	-Use TNT Model with a yield factor of 1, and no limit placed on near field overpressure. -Use the hydrodynamic codes, if necessary.
Physical Explosion	-Compute the "stored energy" and select TNT, Baker-Strehlow, or TNO model to calculate the explosion overpressure effects. -Use the hydrodynamic codes, if necessary
BLEVE	-See "Physical Explosion" guidance above. -Use fire modeling to calculate the thermal radiation effects of BLEVEs of vessels containing flammable material.
Confined Explosion	-Use discharge and dispersion models to calculate the mass of material in the cloud. Use the TNT, Baker-Strehlow, or TNO model to calculate the explosion overpressure effects. Use of TNO, and Baker-Strehlow methods is particularly appropriate. -As necessary, use the hydrodynamic codes.
Vapor Cloud Explosion	- Use discharge and dispersion models to calculate the mass of material in the cloud. Use the TNT, Baker-Strehlow, or TNO model to calculate the explosion overpressure effects. -As necessary, use the hydrodynamic codes.

The Spills Working Group recommended that more sophisticated models were generally more applicable for scenarios in facilities with higher hazards. The recommended models are identified in Table C.3, and are listed according to spill type and the facility hazard category to which they most reasonably apply. In general, the Working Group concluded that engineering calculations and look-up tables are advised over computer models for most simple problems. Hand calculations may be particularly useful for phenomena such as resuspension, where only a limited number of codes are available. For radiological spills, the SWG recommended use of the DOE Source Term Handbook, DOE-HDBK-3010-94 (DOE, 1994b).

The In-Facility Transport Working Group performed confined their review to CONTAIN, KBERT, and MELCOR codes from Sandia National Laboratories (SNL), and to FIRAC and GASFLOW from Los Alamos National Laboratory (LANL). Based on the evaluation performed, the Working Group concluded that there were not any advantages of CONTAIN over MELCOR for analysis of in-facility transport problems. Therefore, the WG recommends that MELCOR be used for applications in which agglomeration of aerosols is an important phenomenon. It was found that the aerosol models in MELCOR have been assessed and validated against experimental data and can provide a benchmark for aerosol models in codes such as GASFLOW that do not include agglomeration. GASFLOW is also recommended in modeling situations where multidimensional effects are important. Examples of the latter are: (1) when concentration profiles are of interest in one or more rooms under varying states of ventilation function; and (2) when lower flammability limits (LFLs) are required versus cell-average flammability limits.

KBERT was advised in analyses supporting functional classification, and in particular for in-facility worker assessment. However, the safety analyst must input time-varying flow rates in scenarios where the ventilation status is changing.

Table C.3. Spills Working Group Model Recommendations

Facility Hazard Category	Liquid Chemical Spills and Evaporation	Pressurized Liquid/Gas Releases	Solid Spills and Resuspension/ Sublimation	Resuspension of Material from Spilled Liquids
Low/ Category 3	Tscreen ADAM ALOHA	TScreen ALOHA	HOTSPOT KBERT	HOTSPOT
Moderate/ Category 2	ADAM ALOHA CASRAM HGSYSTEM	ALOHA CASRAM HGSYSTEM	HOTSPOT KBERT	HOTSPOT
High/ Category 1	CASRAM HGSYSTEM	CASRAM HGSYSTEM	HOTSPOT KBERT	HOTSPOT

Note 1. Excludes radiological consequences

Atmospheric Dispersion and Consequence Analysis

The Radiological Dispersion/Consequence Working Group evaluated MATHEW/ADPIC (ARAC System) as the best overall computer model from the 15 considered, with MACCS/MACCS2, COSYMA, and TRAC RA/HA grouped in the next best ranking. However, of these four models, only MACCS/MACCS2 has the proven requisite availability, performance record, and portability attributes required for consequence analysis at most DOE sites. While it was concluded that these four models cover most dispersion and dose modeling needs, only MACCS/MACCS2 has sufficient application experience. The Working Group ranked highest the following models in terms of the major evaluation categories:

1. Software Quality Assurance/User Interface: MACCS, RSAC-5, MATTHEW/ADPIC
2. Technical Model Adequacy: MATHEW/ADPIC, COSYMA, TRAC RA/HA
3. Source Term Applicability: MATHEW/ADPIC, MACCS2, GENII.
4. Overall Use Recommendations: MATHEW/ADPIC, MACCS, GENII

Table C.4 lists the Working Group recommendations for source term types, specifically, detonations/deflagrations, fires, momentum/buoyancy-driven, spills/evaporation, criticality, and tritium-based releases. The ordering of models is based on the overall ranking and in general, identifies those codes that can adequately represent the initial input and transport conditions associated with the release type.

Table C.4. Radiological Consequence Model by Source Term Type

Explosions	Fires	Momentum/ Buoyancy-Driven	Spills/Evaporation	Criticality	Tritium-Based
ERAD	MACCS2	MATHEW/ ADPIC*	MATHEW/ ADPIC*	MACCS2	UFOTRI
MATHEW/ ADPIC*	COSYMA**	BNLGPM*	GXQ	HOTSPOT	COSYMA**
HOTSPOT	MATHEW/ ADPIC*	GXQ	AXAIRQ*	RSAC 5	AXAIRQ*
	HOTSPOT UFOTRI***	RSAC-5	COSYMA** MACCS2 TRAC RA/HA**		HOTSPOT MACCS2 MATHEW/ ADPIC*

* Portability limits availability of computer model.
** Limited experience with computer model in the U.S.
*** Fire-driven source terms containing tritium only.

The recommendations of the Chemical Dispersion and Consequence Assessment (CDCA) Working Group are summarized in Table C.5. In arriving at these recommendations, the Working Group cited the need to apply a graded modeling approach in chemical dispersion modeling in support of safety basis documentation. The CDCA made their determinations based on review and evaluation of each of the Tier I and II codes, as well as the insights gained from the Tier I test scenarios.

EPIcode (Homman and Associates) was noted favorably in terms of widespread use and capabilities but was not selected because it is a proprietary computer model.

Table C.5. Chemical Dispersion & Consequence Assessment WG Model Recommendations

Conditionally Recommended*	Conditionally Recommended for Special Purpose Safety Basis Applications	Conditionally Recommended for Further Evaluation	Not Recommended for Safety Basis Applications
ALOHA **DEGADIS** **HGSYSTEM** **SLAB**	**ADAM** CALPUFF **FEM3C** INPUFF **TSCREEN**	CASRAM-SC HOTMAC/RAPTAD SCIPUFF	**VLSTRACK**

* Codes in boldface have dense gas modeling capabilities.

Appendix D. Scoring of Codes with Quantitative Criteria

Computer Code	Threshold Criteria		Quantitative Criteria							
	Usage	Meets Minimum Requirements	Capability and Versatility of Code	Number of Code Users	APAC Recommended Code	SQA Status	User Interface	Origin	Code Sponsor	Total
	>=2 =1	Yes = 1	0 – 40	5-10-15-20	10	10	10	5	5	
Radiological Dispersion and Consequence Analysis										
MATHEW/ADPI C	0	1	40	5	10	10	5	5	5	80
MACCS MACCS2	**1**	**1**	**36**	**20**	**10**	**5**	**5**	**5**	**5**	**86**
GENII	**1**	**1**	**24**	**10**	**10**	**5**	**10**	**5**	**5**	**69**
HOTSPOT	**1**	0	**24**	**15**	0	5	10	**5**	5	64
UFOTRI	0	1	**12**	**5**	10	0	5	0	0	32
Chemical Dispersion and Consequence Analysis										
ALOHA	**1**	**1**	**30**	**20**	**10**	**5**	**10**	**0**	**0**	**75**
DEGADIS	0	1	30	0	10	5	5	0	0	50
HGSYSTEM	0	1	30	**10**	10	5	**5**	5	2	67
SLAB	0	1	30	0	10	5	10	2	2	59
EPIcode	1	1	25	20	5	5	10	0	0	65
Fire (Zone Models)										
CFAST	**1**	**1**	**30**	**15**	**5**	**5**	**10**	**0**	**0**	**65**
FIRAC/FIRIN	0	1	35	0	10	10	5	5	5	70
FPETool	0	1	30	0	5	0	5	0	0	40
In-Facility Transport										
CONTAIN	0	1	20	5	0	5	5	5	0	40
MELCOR	**1**	**1**	**35**	**15**	**10**	**5**	**10**	**5**	**0**	**80**
GASFLOW	0	1	35	0	10	5	5	5	5	65

Computer Code	Threshold Criteria		Quantitative Criteria							
	Usage	Minimum Requirements	Capability and Versatility of Code	Number of Code Users	APAC Recommended Code	SQA Status	User Interface	Origin	Code Sponsor	
	>=2 = 1	Yes = 1	0 – 40	10-15-20	10	10	10	5	5	
Chemical Release & Spills										
ALOHA	**1**	**1**	**30**	**15**	**10**	**5**	**10**	**0**	**0**	**70**
CASRAM	0	1	30	0	10	0	5	5	0	50
EPIcode	**1**	**1**	**25**	**10**	**5**	**5**	**10**	**0**	**0**	**65**
HGSYSTEM	0	1	30	0	10	5	5	5	2	57
Other Special Purpose										
FLUENT	1	N/A	35	10	N/A	5	5	0	0	See Text.

Appendix E. Recommendations to Improve Models and Subsequent Applications

Each Accident Phenomenology and Consequence (APAC) Working Group (WG) identified recommendations for its specific subject area.

Although improvements have been made in accident analysis, source term, atmospheric dispersion and dose/chemical concentration models for over 25 years, this area warrants continued, but targeted work. Table E.1 lists the recommendations from the three source term and in-facility transport groups indicating by Working Group specific priorities.

Table E.2 categorizes the chief issues that merit consideration to cost-effectively review, evaluate, and develop models, achieve consistency, and maintain useful guidance for atmospheric dispersion analysis of radiological and chemical releases. It represents an integrated recommendation list from WG 5 and WG 6.

Table E.1. Recommendations from Fire, Explosions and Energetic Events, Spills, and In-Facility Transport WGs

Areas	WG#1 Fire	WG#2 Explosions/ Energetic Events	WG#3 Spills	WG#4 In-Facility Transport
1. Model reviews.	Add more models, including proprietary and NFPA-, CCPS sponsored.	Initialize model evaluation of DOE, DoD, and NATO models; include blast effects and fragment loading	Add more models to review, including private sector codes. Address source and accompanying dispersion needs.	Include EPA, other non-DOE agencies' models.
2. Conduct Systematic Model Performance Evaluations Using Field and Laboratory Data	Not discussed.	Assess accuracy/uncertainty in model estimates with standard set of stat. performance measures & field data	Evap. pool models; Multicomponent chemical mixture behavior;	Not addressed.
3. Database Requirements or Expansion	No extensive data programs recommended. Fire characteristics and source terms: NUREG-1320, NFPA Handbook, and DOE-HDBK-3010-94	Add to EEE database on airborne release of material due to shock and blast effects from explosions	Chemical spill data ref. should be established for DOE analysts ~ DOE-HDBK-3010-94	None recommended.
4. Model Development	Enhance CFAST: a. Model burning rad. material (liqs. & solids) b. Simulate compartment failures c. Model fire effects on equipment d. Model aerosol depletion mechanisms Continue to support VULCAN field model.	Develop post-processor for pressure and velocity output as a function of distance and barrier strength coupled with development of a database of release fractions; Develop explosion effects analysis code for safety analysis source term estimates	1. Flash fraction formation; 2. Aerosol gen. & entrainment 3. Liq. evap. in-facility; 4. Water reactive database link to model; 5. Resuspension process during evaporation phase of spilled liq. containing dissolved/suspended solid material; 6. Chemical mixtures Subseq. chem. rxns.	FIRAC - Update software documentation & troubleshoot to correct transient completion problem. GASFLOW -Add source-term capability to address fires involv. liqs/sols. Aerosol models, esp. agglom. KBERT - improve availability; benchmark vs. expt'l data; add flow-solver. MELCOR - Add GUI.
5. Consolidate technical peer working groups	Integrate fire/EEE, possibly in-facility	Combine EEE and Fire WGs	Chemical Dispersion & Consequence Assessment WG	Consolidate with one or more of source term WGs
6. Establish and maintain Workshops.	Conduct on annual frequency basis; Suggest in coordination with EFCOG Safety Analysis Working Group workshop.			
7. Establish an APAC safety analysis	An AB safety analysis internet WWW page should be established to serve as a clearinghouse to response to issues raised by contractor safety analysts on the selection and application of analysis methodologies. Input files, guidance on particular models			

Internet Web page	and modeling problems should be maintained

Table E.2. Radiological and Chemical Dispersion Working Group Recommendation by Technical Area

Areas	Radiological Dispersion/Consequence WG	Chemical Dispersion and Consequence Assessment WG
1. Expand and update model reviews.	a. Expand candidate evaluations to foreign and proprietary codes b. Evaluate COSYMA, TRAC RA/HA, and new ARAC II module	a. Include proprietary models available to Chemical Processing Industries. b. Identify models that treat other, important phenomena (e.g. BLEVE)
2. Conduct a Systematic Model Performance Evaluation Using Field and Laboratory Data	a. Reach consensus on standards or criteria for model performance b. Benchmark detonation/deflagration models with earlier test data	a. Assess model performance against newly available dense gas data b. Reach consensus on standards or criteria for model performance
3. Develop and Improve Models	a. Improve building wake effect models for treating aerodynamic effects of buildings and surrounding terrain on ground-level, near-field releases b. Implement fast-running algorithm for short-duration releases and better accountability for downwind diffusion c. Account for spatial and temporal changes in meteorological changes and wind field d. Improve dispersion parameter selection and spatial growth options e. Add more realistic dry deposition capability f. Implement detonation/deflagration front end to primary codes	a. Identify better data/algorithms for modeling enhanced dispersion around DOE facilities b. Improve building wake effect models for treating aerodynamic effects of buildings and surrounding terrain on near-surface releases c. Improve short duration release estimates. d. Improve aerosol physics model for vapor source term and dispersion calculations.
4. Establish Internet Reference Points	a. Support development of internet site for user query on data and appropriate models, and experience log b. Safety analysis homepage for executable models	a. Support development of internet site for user query on data and appropriate models, and experience log b. Safety analysis homepage for executable models
5. Establish and maintain Dispersion/Consequence Workshops	a. Conduct modeling/application workshop (Special purpose and/or EFCOG SAWG Workshop)	a. Conduct modeling/application workshop (Special purpose and/or EFCOG SAWG Workshop)
6. Consolidate Working Groups to Develop Joint, Integrated Solutions	a. Identify core group to work through Accident and Consequence Analysis issues as integrated team	a. Consolidate Spills/Chemical Dispersion/Consequence Assessment tech. group to jointly address issues

Appendix F. IEEE Guidance on Software Engineering Methods (Excerpt from E7 Manual, Procedure 5.03 and other sources)

IEEE Standard 730	IEEE Standard for Software Quality Assurance Plans
IEEE Standard 730.1	IEEE Guide for Software Quality Assurance Planning
IEEE Standard 828	IEEE Standard for Software Configuration Management Plans
IEEE Standard 830	Software Requirements Specifications
IEEE Standard 1008	Software Unit Testing
IEEE Standard 1012	IEEE Standard for Software Verification and Validation
IEEE Standard 1012a	EEE Standard for Software Verification and Validation – Supplement to 1012
IEEE Standard 1063	IEEE Standard for Software User Documentation
IEEE Standard 1074	IEEE Standard for Developing Software Life Cycle Processes
IEEE/EIA Standard 12207.0	Industry Implementation of International Standard ISO/IEC 12207 Standard for Information Technology – Software Life Cycle Processes
IEEE/EIA Standard 12207.1	Industry Implementation of International Standard ISO.IEC 12207 Standard for Information Technology – Software Life Cycle Processes – Life Cycle Data
IEEE/EIA Standard 12207.2	Industry Implementation of International Standard ISO.IEC 12207 Standard for Information Technology – Software Life Cycle Processes – Implementation Considerations

Appendix G. Summary Listings of DOE SQA Survey Inputs

1. **Phase of Safety Analysis**

2. **Phenomenological Area**

Review of Survey Inputs: Safety Analysis Software Group

Computer Codes Used at the Various Sites by Phase of Safety Analysis

1. Focus on Accident Analysis Area	MACCS/MACC	PD	5
	ALOHA	NOAA	4
2. Public Domain (PD)	ERAD	PD	4
	EPIcode	Pr	4
3. Proprietary (Pr)	GENII/GXQ	PNNL	~4

	LLNL	LANL	SNL	SRS	PANTEX	RFETS	Y-12	INEEL	YMP/TESS	YMP/RSIS	HANFORD Fluor	HANFORD PNNL	HANFORD Bechtel Hanf.	HANFORD Tank Farm Ops	HANFORD Waste Treatment	WIPP
Hazard Analysis	*HCD,ABS: ChemTrack*	*HA Tables via*	*ORIGEN 2,1*	*RADScreen*	ALOHA,	-	*Facility Safety: -*	RSAC-5	CAFTA	No	None.	Not Applied	N/A	None	EXCEL,	Excel Spreadsheet
	HWM: ChemTrack	Excel/Word	Microshield 4	(MACCS based)	HOTSPOT,ARAC		Nuclear Crit. Safet	MICROSHIELD	ANSYS						MATHCAD	
	& TWMS databases						EM: HOTSPOT98	QAD-FN							Guidance:-3010	
							NARAC; CHARM;	ALOHA							NUREG/CR-6410	
							EPIcode;									
Accident Analysis	HCD, ABS; HWM:	MACCS2	Reactor Kinetics	EXCEL spreadsh.	BLASTX	RADIDOSE (MACCS2	FAST 3.1, HASS 7.2	RSAC 5	GENII-S	No	CAFTA	GENII	GXQ	AA: GOTH, HSC	HADCRT	GXQ Version 4.0
	EPIcode	ERAD	Code;	Mathematica	SHOCK, FRANG	Basis)	PIPE2000	ORIGEN	ANSYS		FLUENT	1.4B5	EPICode	HSC Chemistry	GXQ	Excel Spreadsheet
	HOTSPOT	ALOHA, EPIcode,	MACCS2	CONTAIN	MUDEMIMP		HGSYSTEM		LS-DYNA		HADCRT		GENII	HMS/TRAC	Microshield	for doses
	ALOHA	QCRR	downwind dose	FLUENT;	ANSYS,AUTODYN		HEATING7.3		SCALE		CFAST		MicroShield	ORNATE		
			database	CFAST2/FastLite	MCNP,		M.C./PATHAN		RELAP		HANSF			POOLFIRE,SPRAY		
				MACCS; ALOHA	MAX2 MHC		M.C. THERMAL				GENII			ESP, FLUENT		
					ERAD		EM: HOTSPOT98				GXQ			ORIGEN2,		
					HOTSPOT		NARAC; CHARM;				SPRAY			HADCRT,		
					MELCOR, ALOHA		EPIcode;				MICROSHIELD			HSC Chemistry		
											ISO-PC			CFAST (FHAs)		
											MCNP			CA: GENII,GXQ,		
														Mircoshield,MCNP		
														Microskyshine		
Selection of Controls	HCD, ABS; HWM:	-	None	N/A	BLASTX	-	-	ATR T/H, hot-ch.,	CAFTA	No	CAFTA	Not Appl.	N/A	Results from	None identified.	N/A
	EPIcode				SHOCK, FRANG			reactor kinetics	GENII-S		FLUENT			abpve used for		
	HOTSPOT				MUDEMIMP			ABAQUS			HADCRT			Control sets.		
	ALOHA				ANSYS,AUTODYN			RSAC-5			CFAST					
					MCNP,						HANSF					
					MAX2 MHC						GENII					
					ERAD						GXQ					
					HOTSPOT						SPRAY					
					MELCOR, ALOHA						MICROSHIELD					
											ISO-PC					
											MCNP					
Emergency Action Levels & EPHAs	HCD, ABS; HWM:	MIDAS	N/A	HOTSPOT	HOTSPOT	Emergency Action	-	ALOHA	N/A	No	CAFTA	Em. Prep.	HUDU	HUDU, EPICode	Waste- Not	GXQ
	EPIcode			ALOHA	EPIcode	Level Planning:		RSAC-5			FLUENT	GENII 1.485	EPICode	ALOHA, GENII	Yet Built	CAP88
	HOTSPOT			are primary work-		TRAC		CONWEP			HADCRT	EALs from				EXCEL SPREADSHEET
	ALOHA			horse codes				CHEMIX			CFAST	HA - no code				
											HANSF					
			Reactor Oper.								GENII					
			Characteristics								GXQ					
			Reactor Oper.								SPRAY					
			Reactor Kin., T/H								MICROSHIELD					
			and MCNP codes								ISO-PC					
											MCNP					
											HUDU	HUDU				
											EPIcode	EPIcode				
											ALOHA					

Review of Survey Inputs: Safety Analysis Software Group

Revision 1

Computer Codes by Source Term / Phenomenological AreasUsed at the Various Sites

	LLNL	LANL	SNL	SRS	PANTEX	RFETS	Y-12	INEEL	YMP/TESS	YMP/RSIS	Hanford Fluor	Hanford PNNL	Hanford Bechtel Han.	Hanford Tank Farm Ops	Hanford Waste Treatment	WIPP
Explosion	HCD,ABS*: Breeze Haz 3.2.3 HWM: EPIcode, HOTSPOT	BLAST-X	Use Hand Calcs	EXCEL, Mathematica, At-Risk, FLUENT; Guidance: DOE-HDBK-3010-94 Facility doc. on MAR	OSH*: ALOHA, HOTSPOT Blast Analysts: DOE/TIC-11268; TM5-1300; TM5-855 Dispersion: ERAD Emerg. Man. HOTSPOT Guidance: -3010 & DOE G 151-1	Chico SOLVER (similar to Mathematica)	Guidance: DOE-HDBK-3010-94	RSAC-5, for airborne rad. disp. and dose calcs.	N/A	N/A	FLUENT SPRAY & DOE- HDBK- 3010-94	GENII 1.485 Guidance: DOE-HDBK- 3010-94	Guidance: DOE-HDBK- 3010-94	FLUENT, HADCRT HMS/TRAC SHMS Database	Guidance: DOE-HDBK- 3010-94	Guidance: DOE-STD-3009-94
Fire	HCD,ABS/HWM: EPIcode HOTSPOT	CFAST	DOE-HDBK-3010-94 used for inputs to hand calcs.	EXCEL, Mathematica, At-Risk, FLUENT; Guidance: DOE-HDBK-3010-94 Facility doc. on MAR Fire Risk & Fire hazard: FASTLITE/CFAST2	Fire Protection Engr. CFAST Dispersion: MAX2_MHC Emerg. Man. HOTSPOT Guidance: -3010 & DOE G 151-1	RADIDOSE (MACCS2 Basis)	Guidance: DOE-HDBK-3010-94	RSAC-5, for airborne rad. disp. and dose calcs.	N/A	N/A	CFAST DOE- HDBK- 3010-94	CFAST GENII 1.485 Guidance: DOE-HDBK- 3010-94	CFAST Guidance: DOE-HDBK- 3010-94	CFAST HSC Chemistry ORNATE POOLFIRE Safety Analysis Database	Guidance: DOE-HDBK- 3010-94 Data from Proprietary Datab.	Guidance: DOE-STD-3009-94 Guidance: DOE-STD-1066-99
Criticality	CSG: MCNP, COG SCALE, VIM, TART	MCNP	MCNP	Source Term: ORIGEN Scaling of prev. results; Guidance: DOE-HDBK-3010-94 Facility doc. on MAR	MCNP	SCALE, MCNP, ORIGEN2	Guidance: DOE-HDBK-3010-94	RSAC-5, for pr. fiss. prod. inv. and dispersion doses	SCALE RELAP	N/A	DOE- HDBK- 3010-94	GENII 1.485 Guidance: DOE-HDBK- 3010-94	MCNP	MCNP SCALE	MCNP	SCALE: KENO V.A
Spill	HCD/ABS: EPIcode, ALOHA, HOTSPOT HWM: EPIcode, ALOHA, HOTPSOT, GENII, CHARM, MACCS2	HCs**	3010 and NUREG-1320 used for inputs to scoping calculations MACCS2 Downwind Dose Database	EXCEL, Mathematica, At-Risk, FLUENT; Guidance: DOE-HDBK-3010-94 Facility doc. on MAR	OS&H & Dispersion: ALOHA	N/A	Guidance: DOE-HDBK-3010-94	None	N/A	N/A	DOE- HDBK- 3010-94	GENII 1.485 Guidance: DOE-HDBK- 3010-94	Guidance: DOE-HDBK- 3010-94	GOTH SPRAY ALOHA EPICode PC-SACS data	Guidance: DOE-HDBK- 3010-94	Guidance: DOE-STD-3009-94
Chemical Release	HCD,ABS;HWM: EPIcode, ALOHA HOTSPOT	-	MACCS2 for X/Q	ALOHA, EPIcode; HCs EXCEL, Mathematica, At-Risk, FLUENT; Guidance: DOE-HDBK-3010-94 Facility doc. on MAR	OS&H & Dispersion: ALOHA	ALOHA	Guidance: DOE-HDBK-3010-94	ALOHA/CAMEO	N/A	N/A	DOE- HDBK- 3010-94	N/A	Guidance: DOE-G- 151.1-1	ESP, ALOHA, EPICode	Guidance: EPA RMP	Guidance: DOE-STD-3009-94
In-Facility Transport	HCD,ABS;HWM: Hand Calculations	MELCOR	Hand Calculations; Use inputs from -1320 and -3010	CONTAIN; MELCOR Mathematica Guidance: DOE-HDBK-3010-94; Facility doc. on MAR	MELCOR	N/A		RSAC-5	No	No	Occasional FLUENT	N/A	CFAST	FLUENT	HADCRT	No.
Atmospheric Dispersion Analysis																
Radiological	HCD,ABS;HWM: "Gaussian Plume"	MACCS2	MACCS2-based single-Ci for accid. spreadsheet	General purpose: MACCS1.5.11.1 Explosion: ERAD occas Tritium: UFOTRI Guidance: RG1.145; App.A to -3009	OSH/EM: HOTSPOT and ARAC Dispersion Analysts: ERAD and MAX2_MHC	RADIDOSE; Occasional use of MACCS2	1. HOTSPOT 2. NARAC	RSAC-5 Hismler-Gifford<15m Markee>15m-80m	N/A	N/A	GXQ GENII SPRAY HADCRT FLUENT ORIGEN2 3010	GENII	GXQ HUDU	GXQ, GENII	GXQ, RG 1.145 Guidance: DOE-HDBK- 3010-94	GXQ Version 4.0 CAP88
Chemical	HCD,ABS;HWM: "Gaussian Plume"	ALOHA, EPIcode, QCRR	MACCS2 for X/Q	ALOHA, EPIcode; Occas. HGSYSTEM MACCS for X/Q	OSH: ALOHA/ARAC; Dispersion: ALOHA EM: EPIcode & ARAC	ALOHA	1. CHARM 2. EPICode	ALOHA/CAMEO	N/A	N/A	SPRAY HADCRT FLUENT DOE- HDBK-	N/A	EPICode	GXQ	Guidance: EPA RMP	GXQ Version 4.0
Other		FLOW3D NIST 3-D Fire Simulation Tool	ORIGEN 2.1 to develop MAR for reactor fuel element		EM uses NBC Warning and BLAST Also, HPAC/Hascal	TRAC		None	N/A	N/A	3010-94	N/A		None.	None.	None.

CSG=Criticality Safety Group
** Hand Calculations
*OSH=Occup. Safety & Health