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**DEFENSE NUCLEAR FACILITIES
SAFETY BOARD**

Washington, DC 20004-2901



August 24, 2022

The Honorable Jennifer M. Granholm
Secretary of Energy
US Department of Energy
1000 Independence Avenue, SW
Washington, DC 20585-1000

Dear Secretary Granholm:

Twenty years ago, the Defense Nuclear Facilities Safety Board (Board) issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software*. As the Board noted in its Recommendation, “DOE and its contractors use many codes to evaluate the consequences of potential accidents. Safety controls and their functional classifications are often based on these evaluations...The robustness and reliability of many structures, systems, and components (SSCs) throughout DOE’s defense nuclear complex depend on the quality of the software used to analyze and to guide these decisions, the quality of the software used to design or develop controls, and proficiency in use of the software.”

As an important part of its response, the Department of Energy (DOE) created the Safety Software Central Registry, which provides enhanced assurance of the quality of commonly used safety software. Since then, DOE has struggled to maintain this software registry, leading to the use of outdated software for safety-related calculations. DOE’s use of outdated safety software reduces the assurance that calculations provide reliable results.

DOE is aware of this challenge and is considering changes to the Central Registry. As part of this effort, DOE solicited and recently received input from the Energy Facility Contractors Group regarding possible changes to the Central Registry. The Board encourages DOE to make improvements in a timely manner while being mindful of the overall purpose of the Board’s Recommendation 2002-1, which is still pertinent. In particular, the Board advises DOE to continue a centralized approach, while enacting changes to make the software registry more sustainable.

Pursuant to 42 United States Code § 2286b(d), the Board requests a briefing by the end of January 2023 that addresses DOE's plans for the Central Registry, how those plans will promote quality assurance for software used in safety analysis, and how they will address the safety concerns laid out in the enclosed report.

Sincerely,


Joyce L. Connery
Chair

Enclosure

c: Mr. Joe Olencz

DEFENSE NUCLEAR FACILITIES SAFETY BOARD

Staff Report

April 2, 2022

Review of DOE's Safety Software Central Registry

Summary. A team from the Defense Nuclear Facilities Safety Board's (Board) staff performed a safety review of the Department of Energy's (DOE) Safety Software Central Registry. The Central Registry is a collection of safety-related software that DOE recommends its contractors use for safety analysis. An overall goal of the Central Registry is to provide enhanced assurance of the quality of commonly used safety software. DOE's contractors use the safety software for analyzing hazards and estimating the consequences of potential accident scenarios. Such consequence estimates inform decisions regarding whether to implement safety-significant or safety-class controls to prevent or mitigate accident scenarios.

DOE has struggled to maintain the Central Registry, and as a result, DOE contractors sometimes use outdated versions of software for safety calculations. This situation is problematic because older versions of software may contain errors that have since been addressed by the code developers. Historically, DOE identified at least one such error in a Central Registry code [1]. While the staff team is not aware of any specific safety calculations that are currently erroneous due to software issues, the use of outdated software leads to decreased assurance that calculations are reliable. Further, DOE created guidance for using the software in the Central Registry, and this guidance has also become outdated. In some cases, DOE contractors have decided to use versions of the codes that are newer than what is in the Central Registry. New versions sometime introduce new features for which there is no DOE guidance; the use of such features could lead to inconsistencies across DOE sites.

DOE is aware of its challenges with the Central Registry and is currently considering changes. This report details the staff team's findings, along with topics for DOE's consideration as it develops its path forward. In the staff team's perspective, DOE should retain some centralized aspects of the Central Registry (the identification of recommended codes, the evaluation of those codes, and guidance for using those codes), while making the program more sustainable.

Background. The DOE Safety Software Central Registry is a collection of safety-related software codes (also called the "toolbox" codes). DOE's contractors use these safety codes to perform calculations that support the safety analyses for DOE nuclear facilities. DOE encourages, but does not require, its contractors to use the toolbox codes. The Central Registry currently consists of the following eight codes, grouped by topic:

- **Plume dispersion and accident consequences:** ALOHA, EPIcode, GENII, Hotspot, MACCS,
- **Fire:** CFAST,

- **Health physics:** IMBA, and
- **Leak path factor:** MELCOR¹

DOE created the Central Registry in response to the Board’s Recommendation 2002-1, *Quality Assurance for Safety-Related Software* [2]. The Board issued this recommendation and an associated technical report [3] after finding deficiencies in software quality assurance (SQA) for codes related to the safe operation of DOE facilities. In particular, the Board recommended that DOE should:

- “Identify software that would be recommended for use in performing design and analyses of SSCs [structures, systems, and components] important to safety, and for analysis of expected consequences of potential accidents.”
- “Identify an organization responsible for management of each of these software tools, including SQA, technical support, configuration management, training, notification to users of problems and fixes, and other official stewardship functions.”

In response, DOE established the Central Registry. DOE stated it would “Identify safety analysis ‘toolbox’ codes that are commonly used across the Department, upgrade the codes to a prescribed qualification, and establish a Central Registry to facilitate maintenance, technical support, configuration management, training, and notification to users of problems and revisions to these codes” [4]. As part of this effort, DOE evaluated the toolbox codes against its SQA requirements, and provided guidance to its contractors on how to use the codes. These SQA requirements are currently documented in DOE Order 414.1D, *Quality Assurance* [5], with additional details provided in a related DOE guide² [6]. DOE intended for the Central Registry to be a sustainable effort, stating that it would provide “for the long-term maintenance and control of the safety analysis ‘toolbox’ codes” [4]. DOE’s Office of Environment, Health, Safety, and Security (EHSS) is responsible for the Central Registry.

Discussion. To ensure that the underlying safety issues from the Board’s Recommendation 2002-1 continue to be addressed by DOE, the staff team finds that DOE should revitalize and reform the Central Registry. DOE initially put substantial effort into creating the Central Registry, but its approach has not been sustainable over time. DOE has struggled to keep the Central Registry up to date.

Outdated Software and Guidance in the Central Registry—DOE evaluates a specific version of a code and puts that specific version into the Central Registry. Code developers frequently issue new versions of codes to add features or to address issues. DOE does not automatically incorporate the code revisions into the Central Registry; rather it first evaluates them against its SQA requirements. DOE has struggled to evaluate these revisions to the codes, so the version of a code in the Central Registry tends to be older than the latest release from the developer.

¹ While MELCOR has other uses, the scope covered by the Central Registry is focused on leak path factor.

² As a result of the Board’s recommendation, DOE revised Order 414.1 to include content on SQA and developed the related guide.

As a result, DOE contractors sometimes use outdated versions of codes for safety-related calculations (see Appendix A for further detail). The use of old versions can be problematic in cases where the code developer has identified issues with the older versions of a code, and subsequently addressed those issues in revisions³. Historically, DOE has identified at least one such issue in a toolbox code [1]. It should be noted that the staff team is not aware of any safety calculations that are currently erroneous due to issues with the toolbox codes, though the scope of the team’s review did not include systematically searching for any such errors. Nevertheless, unless DOE either updates the Central Registry or maintains awareness of issues that code developers are identifying, there will be decreased assurance that the toolbox codes provide reliable results.

DOE is aware of the challenges it has faced with updating the Central Registry and its sustained implementation of the Board’s Recommendation 2002-1. In 2008, DOE stated, “Over time, these codes have been updated and the newer versions have not been evaluated for inclusion in the Central Registry...it is important to establish a cost-effective way, based on need, for updating the existing toolbox codes to newer versions” [7].

More recently, DOE commissioned an assessment of the Central Registry [8]. The resulting report, completed in 2018, concluded that the Central Registry “as it is currently being implemented, does not meet the intent of the DOE IP [Implementation Plan] for DNFSB recommendation 2002-1.” One reason for this conclusion was the “lack of timeliness in including later versions of the toolbox codes in the CR [Central Registry].”

The assessment report also discussed the extended timelines involved when DOE has attempted to evaluate a newer version of a code for inclusion in the Central Registry. In the cases examined in the assessment report, the process took between about 1.5 and 5 years, from start to finish. The assessment report identified factors that contributed to the timelines, including “the amount of time review team members can devote,” the “quality and completeness of the documentation provided by the code developer,” and the time needed for the code developer to implement any improvements recommended by DOE (e.g., improved documentation). In some cases, the code developer had competing priorities.

Personnel from EHSS informed the staff team that they intend to make changes to the Central Registry. Previously, they were attempting to implement the recommendations from the 2018 assessment but paused that effort when they decided that more fundamental changes to the Central Registry were warranted. In 2021, EHSS requested a team of contractors from the Energy Facility Contractors Group (EFCOG) to identify options for addressing the challenges with the Central Registry. The EFCOG team recently presented options for DOE’s consideration [9]. The options include models where contractors would evaluate the Central Registry software instead of DOE, as well as an option where the Central Registry would be eliminated.

The staff team is encouraged that DOE is taking the initiative to evaluate and reform the Central Registry. The team notes that DOE should identify and implement improvements in a

³ There may be other practical challenges with using older codes, such as lack of full support from the code developer, difficulties in running codes on modern computers, and cybersecurity vulnerabilities.

timely manner. Although DOE has been aware of challenges with the Central Registry for several years, DOE still has no clear schedule for its current efforts.

The staff team has identified the following topics that DOE should consider as it develops its path forward:

Clear Identification of DOE's Goals for the Central Registry—As DOE develops its path forward, it is important for DOE to determine the purpose and goals of the Central Registry. While DOE is changing its approach based on experience, the overall intent of Recommendation 2002-1 is still relevant.

The primary goals of the Central Registry are achieving assurance that safety-related calculations using commonly used software will have reliable results, and assurance that the analysis is performed in a manner that is consistent with relevant DOE standards (e.g., DOE Standard 3009). Such assurance is important for supporting safety in the design and operation of defense nuclear facilities. The staff team accordingly finds that DOE should continue the Central Registry, with modifications to make it more sustainable.

Benefits of Centralization—Centralization is a defining feature of the Central Registry. While some aspects of the Central Registry may change, the staff team finds that continued centralization would be beneficial for meeting SQA goals, in line with the Board's 2000 analysis [3]. Most of the codes in the Central Registry are relevant to the analysis of accidents. Accident analysis is an important part of safety analysis for many DOE facilities. While some details vary between different facilities and sites, these calculations share many similarities. It thus remains appropriate for DOE to identify the codes it recommends for commonly performed calculations. The use of a standardized set of software also facilitates DOE's review of its contractors' analyses. Further, it is important for DOE to continue providing guidance on the use of such codes, as discussed further below.

DOE is considering options where contractors will evaluate software against SQA requirements, instead of DOE. If DOE pursued such an option, the staff team finds it would be beneficial for those evaluations to be centralized. A centralized process could enable a more rigorous safety evaluation by drawing on a group of qualified personnel from DOE contractors or an external center of excellence, and it could be more efficient than multiple duplicative evaluations by individual site contractors. In any case, given that DOE is struggling to evaluate new versions of software, it should recognize that another entity brought in to evaluate software could also face similar challenges. If DOE chooses to have contractors evaluate software against SQA requirements, it would be important for DOE to perform rigorous oversight over that process.

Clear Roles and Responsibilities—The Central Registry involves three types of organizations: code developers who create the software, DOE personnel who evaluate the software and provide guidance, and DOE contractors who use the software and follow the DOE guidance. As DOE reforms the Central Registry, it is important to clearly define the roles and responsibilities of these groups. This section discusses some challenges that have arisen in the current implementation of the Central Registry.

EHSS evaluates the software according to the SQA requirements it has identified [5, 10]. This role is unusual for DOE; typically, DOE contractors evaluate the software they use against DOE's requirements. EHSS personnel informed the Board's staff that evaluating software is resource-intensive, and that EHSS does not have dedicated staff for that task. As mentioned above, this lack of resources is one reason why DOE has had challenges in completing evaluations in a timely fashion. This situation suggests that DOE should explore a different approach for the evaluation of safety software in the Central Registry. DOE is considering options where contractors would perform the evaluations for the Central Registry, instead of DOE.

When evaluating software, DOE sometimes identified gaps where the code developer should make improvements. However, in many cases the code developers are not sponsored by DOE. Thus, DOE is typically not able to direct the developer to make those changes on a schedule determined by DOE. DOE could develop a memorandum of understanding with the code developers to try and provide greater influence when it comes to making essential software improvements to ensure safety at defense nuclear facilities.

When formulating the Central Registry, DOE stated that the personnel evaluating the software would be "an independent reviewer...who is not affiliated with the code developing organization" [10]. However, DOE's assessment report [8] mentioned one case where the DOE evaluators assisted the software developer in generating the documentation that DOE then evaluated. Regardless of who evaluates a code (DOE or DOE contractor), any expectations of independence should be clearly stated.

EHSS personnel emphasized to the staff team that DOE's evaluation does not relieve its contractors from meeting quality assurance requirements under DOE Order 414.1D [5]. That order states that "Safety software must be acquired, developed and implemented using ASME NQA-1...*Quality Assurance Requirements for Nuclear Facility Applications*...or other national or international consensus standards that provide an equivalent level of quality assurance requirements." The staff team notes that DOE standards and directives contain ambiguous language on the obligations of DOE contractors who use toolbox codes. DOE Standard 3009-2014 refers to codes in the Central Registry as having "pre-approval." DOE Guide 414.1-4 [6] describes them as a "safe harbor" methodology, and states that "analysts using these codes do not need to present additional defense as to their qualification...." DOE directives should be clear about what DOE's contractors are required to do to demonstrate compliance with DOE Order 414.1D.

EHSS personnel stated that DOE can find it difficult to evaluate safety software when it is not aware of all the circumstances surrounding how its contractors will use the codes. When DOE evaluates safety software (or oversees that evaluation), the scope of the evaluation should cover the methods that DOE deems appropriate for safety at defense nuclear facilities. If a contractor chooses to use safety software in a way that goes beyond DOE's evaluation, it should be incumbent upon that contractor to independently evaluate the use of that software to

demonstrate its use meets DOE's SQA requirements. DOE should provide oversight by performing a review of the contractor's evaluation and ensuring that the methodologies are consistent with relevant DOE standards.

Guidance for Safety Software—As stated in Recommendation 2002-1, one important facet of software quality assurance is ensuring that “computer codes are properly and consistently executed by analysts.” Hence, the DOE implementation plan included an action to “Issue code-specific guidance reports on the use of ‘toolbox’ codes identifying applicable regimes in accident analysis, default inputs, and special conditions for use.”

The resulting guidance that DOE created is an important aspect of the Central Registry. This guidance is another aspect of the Central Registry that is becoming outdated. For example, the DOE guidance report for the MACCS code dates to 2004, when DOE created the Central Registry [11]. That guidance report provides recommended default values for deposition velocity, which is a parameter used in plume dispersion models. Since that time, DOE has found that these default values may be non-conservative (i.e., lead to lower estimates of the consequences of accidents), and has updated its guidance [12, 13]. However, DOE has not revised its report on MACCS, resulting in inconsistencies between the various DOE documents that provide guidance on this topic.

Several codes in the Central Registry are used to estimate the consequences of potential accidents. Per DOE standards, those estimated consequences are compared to threshold values to determine whether more robust and reliable controls (safety controls) should be considered or are required. However, the codes typically involve a multitude of input parameters, allowing a wide range of possible consequences to be estimated for a given accident scenario. It is thus important for DOE to provide its contractors with guidance and expectations on how these calculations should be performed, both in general (i.e., in standards and handbooks) and in code-specific guidance. Code-specific guidance supplements the more general guidance in standards to help ensure proper implementation of the standards. Such DOE-specific content will typically not be found in the documentation provided by the code developer.

In addition, in some cases, DOE contractors are using newer versions of the codes, and not the toolbox version. New versions may have substantial new features that can significantly affect the results; this is particularly the case with MACCS. Given that DOE has not issued guidance on the newer versions, it is not clear whether and how contractors should be using new features. This situation further illustrates the importance of updated guidance from DOE. In the staff team's perspective, it remains important for DOE to provide guidance on the appropriate usage of toolbox codes, including the various input parameters and versions.

Sustainable Methods for Updating the Central Registry—As stated above, the Central Registry contains outdated versions of some codes. As a result, DOE contractors sometimes use these outdated versions, which may have issues that have been addressed in later releases. Further, when a contractor elects to use a newer version of a code, it is unclear if new features in the code are acceptable to DOE.

DOE recognizes that it has struggled to update the Central Registry, and this recognition is part of why DOE is evaluating options for reforming the Central Registry. As DOE selects a new model for implementing the Central Registry, that new model should be sustainable regarding updates of the toolbox codes. It would also be beneficial to have a process for adding or removing codes from the Central Registry, as warranted.

To help manage updates to the Central Registry, EHSS personnel have discussed options where the code developers would be evaluated and then considered to be “qualified suppliers.” Under that model, every single update to the codes would not be comprehensively evaluated before inclusion in the Central Registry. Instead, there would be periodic audits of the developer. If DOE pursues such a model, DOE should consider developing tailored processes for minor and major updates to the codes. A streamlined process may be appropriate for minor updates, but major updates should be evaluated by DOE or its supporting contractors. DOE should also set criteria for periodic evaluations, considering the time elapsed and the number of minor updates since the previous evaluation. In the case of major updates, it may also be appropriate for DOE to update the guidance it provides on the appropriate use of the codes.

One facilitating tool that DOE could consider is the creation of DOE-specific test cases for the various codes. If a software update led to different results for the test cases, DOE and its contractors could seek to understand the reason for the different behavior in the updated software. While code developers typically maintain test cases, DOE could benefit from maintaining DOE-specific test cases as well. Also, as an interim measure, DOE could consider reviewing the revision histories of the codes to determine whether there are known issues in the toolbox versions; such a step would improve confidence in the current toolbox codes.

Better Methods to Notify Users of Code Issues—One of DOE’s original goals with the Central Registry was to “facilitate...notification to users of problems and revisions to these codes” [4]. However, DOE has not met this goal because it does not have a consistent and reliable method of notifying users of issues. DOE has attempted various mechanisms such as a Safety Software Communication Forum, but EHSS personnel informed the staff team that this forum is currently not functional.

EHSS has recently attempted to address this challenge by using a newer web forum on DOE’s Organizational Excellence website, as well as using communications to the contractor community through the Energy Facility Contractors Group. While the forum is a worthwhile initiative for encouraging collaboration, information posted there may not reliably reach DOE users of Central Registry codes. The operating experience program could be helpful in this regard, and in fact, DOE historically used the operating experience program to disseminate information about particularly important software issues [14, 15].

Further, DOE does not maintain any single location where all known issues with a software code are compiled. Such a compilation would help DOE contractors avoid problems with the codes. For example, in 2009, DOE released a safety advisory [1] about an issue with MACCS. In certain situations, MACCS provided “erroneous” and “unrealistic” results, but “did not issue a warning message or stop execution.” The Central Registry webpage does not

mention this issue, nor link to the safety advisory. Thus, a new user of MACCS may not be aware of the issue.

Notification is an area where the code developer also plays a role, but code developers do not necessarily send notices regarding issues to a list of users. As noted in DOE's assessment report [8], in some cases "it is up to the code user to periodically check the [code developer's] website for announcements." The staff team acknowledges this is a challenging topic, but it is still important to address.

Evaluation of Best Practices from Other Organizations—DOE could evaluate the methods that other organizations use when faced with similar challenges. For example, the Nuclear Regulatory Commission (NRC) sponsors some of the software in the Central Registry, and it maintains databases of safety-related software packages (e.g., the Radiation Protection Computer Code Analysis and Maintenance Program, RAMP). There are key differences between the DOE Central Registry and the NRC's programs, but there is still a benefit from examining the NRC's practices.

Evaluation of Challenges Beyond the Central Registry—The scope of this staff review was limited to the Central Registry. However, DOE's experience with the Central Registry shows that evaluating software can be difficult. A rigorous evaluation using DOE Order 414.1D may be resource-intensive and may require personnel with specialized qualifications. The evaluation may also be difficult if the code developer does not have a mature SQA program or does not maintain documentation that meets DOE's expectations. Such challenges may also be applicable to software that is outside the Central Registry. It is thus relevant to consider how DOE contractors evaluate software for use in safety applications, and how they ensure that they use the software in an appropriate and reliable manner. DOE's Office of Enterprise Assessments is conducting a broad assessment of SQA practices (including, but not limited to, the Central Registry), and it is encouraging that DOE is emphasizing these areas.

Conclusion. DOE's Safety Software Central Registry contains outdated versions of safety-related software. As a result, DOE contractors sometimes use these outdated versions of the software, which may contain errors that have subsequently been identified and addressed by the code developers. While the staff team is not aware of any calculations that are actually erroneous due to issues with the Central Registry codes, there is reduced confidence that the software is reliable. DOE's guidance on the use of these safety codes is also becoming outdated.

DOE should revitalize and reform the Central Registry. DOE should retain some centralized aspects of the Registry (the identification of recommended codes, the evaluation of those codes, and guidance for using those codes), while making the program more sustainable. The team understands that DOE is studying the situation and is considering changes to the Central Registry.

Appendix A: Versions of Software in the Central Registry

The staff of the Defense Nuclear Facilities Safety Board conducted a review of DOE’s Safety Software Central Registry. Table A-1 shows the codes currently in the Central Registry (also known as the “toolbox” codes), including version number.

Table A-1. *Versions of the Software in the Central Registry* [16]

Code	Toolbox Version (and year evaluated by DOE)
ALOHA	v5.4.4 (2014)
CFAST	v7.1.1 (2017)
EPIcode	v7.0 (2004)
GENII	v2.10.1 (2013)
HotSpot	v2.07.01 (2010)
IMBA	DOE Edition v.4.0.28 (2006)
MACCS	v1.13.1 (2004)
MELCOR	v1.8.5 (2004)

For some of the codes (EPIcode, MACCS and MELCOR), the version in the toolbox is still the version that DOE originally evaluated when it established the Central Registry in 2003-2004. In the case of MACCS, the current version (v4.1) was released in 2021, so the toolbox version is 17 years behind the current release. In other cases (e.g., ALOHA, CFAST, GENII), DOE updated the Central Registry to incorporate a newer version of the code. However, that process took a protracted amount of time, and in some of those cases, the toolbox version is again out-of-date.

References

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