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A POTENTIAL APPLICATION OF UNCERTAINTY ANALYSIS TO DOE-STD-3009-94 ACCIDENT ANALYSIS

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ABSTRACT

The objective of this paper is to assess proposed transuranic waste accident analysis guidance and recent software improvements in a Windows-OS version of MACCS2 that allows the inputting of parameter uncertainty. With this guidance and code capability, there is the potential to perform a *quantitative* uncertainty assessment of unmitigated accident releases with respect to the 25 rem Evaluation Guideline (EG) of DOE-STD-3009-94 CN3 (STD-3009). Historically, the classification of safety systems in a U.S. Department of Energy (DOE) nuclear facility's safety basis has involved how subject matter experts qualitatively view uncertainty in the STD-3009 Appendix A accident analysis methodology. Specifically, whether consequence uncertainty could be larger than previously evaluated so the site-specific accident consequences may challenge the EG. This paper assesses whether a potential uncertainty capability for MACCS2 could provide a stronger technical basis as to when the consequences from a design basis accident (DBA) truly challenges the 25 rem EG.

INTRODUCTION

Part of the work for the classification of safety systems in a U.S. Department of Energy (DOE) nuclear facility's safety basis has involved how subject matter experts qualitatively view uncertainty in the accident analysis calculations in accordance with DOE-STD-3009-94 CN3 (STD-3009) Appendix A. Specifically, the magnitude of the qualitative uncertainty in a site-specific accident scenario's consequence analysis may force a conclusion that the 25 rem Evaluation Guideline (EG) is challenged. Two recent events may help to move the assessment of STD-3009 accident analysis uncertainty to a *quantitative* technical-based methodology. The first is the development of a new DOE standard for the preparation of documented safety analysis (DSA) for transuranic (TRU) waste facilities. The second is ongoing U.S. Nuclear Regulatory Commission (NRC) sponsored improvements to MACCS2 code package, which is also part of DOE's "toolbox" of high-use safety software codes.

DOE’s TRU waste facilities in the past have often employed a variety of different controls to manage the TRU wastes even though they face similar hazards and scope of operation. The recognition of these inconsistencies has led DOE to develop a new technical standard with, in part, specific technical expectations for analyzing TRU waste hazards from which the need for controls is demonstrated. This new DOE standard also provides additional direction on whether a calculated dose for a specific scenario should be considered as “challenging” the EG, depending on the conservatism in the accident analysis.

The NRC sponsored MACCS2 code improvements includes a version of the MACCS2 code known as WinMACCS. This version of MACCS2 can operate on Windows-based personal computers via a user interface, but also can allow the entering of uncertainty distributions for most input parameters. A beta version of WinMACCS is reviewed for its potential application for aiding DOE’s accident analysis

The objective of this paper is to assess whether the combination of additional guidance from the new DOE standard and the potential improvements in a DOE toolbox consequence code has the potential to allow a quantitative uncertainty assessment of unmitigated accident releases with respect to the EG for LLNL TRU waste facilities.

SOURCES OF UNCERTAINTY IN DOE-STD-3009 ACCIDENT ANALYSES

The guiding radiation dose equation from STD-3009 compliant accident analysis has been the radioactive airborne source term five factors with an additional three consequence analysis factors.¹ These are:

$$D_{MOI} = MAR \cdot [ARF \cdot RF] \cdot DR \cdot LPF \cdot BR \cdot DCF_{ICRP72} \cdot \chi/Q \quad (\text{Eq. 1})$$

Where:

- MAR is the material-at-risk, namely the amount of radionuclides available to be acted on by a given physical stress (Curies),
- ARF·RF is the airborne release fraction times the respirable fraction (unitless),
- DR is the damage ratio or fraction of the MAR that is impacted by the postulated accident scenario (unitless),
- LPF is the leak path factor (unitless),
- BR is the breathing rate (m³/s),
- DCF_{ICRP 72} is the inhalation dose conversion factor based on International Commission on Radiological Protection 72 (rem/Curie), and
- χ/Q is the atmospheric dilution factor (s/m³).

For LLNL TRU waste facilities, the prior experience has been to apply the currently available version of the MACCS2 code package to determine the three right-hand factors on a unit value basis, namely the $BR \cdot DCF_{ICRP 72} \cdot \chi/Q$ factors as a unit source term-to-dose conversion factor in rems per plutonium-239 equivalent curies (PE-Ci) for the particular type of radiological releases being examined in accident analysis section of the documented safety analysis (DSA)

(i.e., ground release or fire with plume rise). Because MACCS2 applies the DCFs from Federal Guidance Report (FGR) 11 and FGR 12 (Reference # MACCS2 manual), it is LLNL's practice to apply an additional scaling factor to modify the MACCS2-obtained unit source term-to-dose conversion factor to a FGR 13-based value.²

Recently, DOE completed a new standard through the RevCom process that provides guidance, in part, on how and why the source term five factors will be expected to be set for each anticipated accident scenario being considered in a TRU waste DSA.³ For radiological consequence modeling, the new DOE standard requires the following dispersion attributes:

- The values of χ/Q used for radiological and chemical consequence analysis are generated using MACCS2 Computer Code (see DOE-EH-4.2.1-MACCS2-Code Guidance, MACCS2 Computer Code Application Guidance for Documented Safety Analysis). Use of other DOE-approved Toolbox Codes, or site-specific codes that have undergone appropriate validation and verification in accordance with DOE O 414.C requirements on software quality assurance, must be technically justified.
- Worst case meteorological assumptions (i.e., 95th percentile based on local site data) for onsite radiological and chemical releases (see DOE-STD-3009, Appendix A for offsite evaluations)
- Dry deposition velocity must be used at a value of 1 cm/s for all unfiltered, non tritium, non-noble gas species.
- Wet deposition must not be modeled.
- A surface roughness value of 3 cm must be assumed for radiological and chemical releases.
- Building wake effects must not be credited (modeled) unless shown to yield more conservative or bounding results.
- Plume buoyancy may only be used when modeling fires that are outdoors or venting through a large breach in the facility (use of plume buoyancy should not be credited in a non-conservative manner).
- The breathing rate value, as specified in the DOE Toolbox Codes, is $3.3 \times 10^{-4} \text{ m}^3/\text{s}$. This value corresponds to the light activity breathing rate for adults and must be used in consequence assessment.
- Inhalation dose conversion factors for the maximally exposed offsite individual (MOI) evaluation must be consistent with ICRP 72, Age-dependent Dose to Members of the Public from Intake of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients, and optionally may use ICRP 68, Dose Coefficients for Intakes of Radionuclides by Workers, for the collocated worker evaluation.

The new DOE standard also outlines the known sources of uncertainty for each source term and consequence analysis factors. Based on the information provided in the new DOE standard, there are only, at most, the DR and χ/Q terms that require consideration for an uncertainty analysis. All others should be bounded or conservative.³ This can be reduced to one factor if the accident analysis assumptions and selections of the DR for each scenario are properly developed (i.e., bounding or conservative for the scenario). Therefore, for TRU waste facilities, the uncertainty analysis could concentrate on assessing the atmospheric dilution factor, χ/Q , for demonstrating whether there is the potential for challenging the EG.

UNCERTAINTY IN DISPERSION MODELS

Addressing uncertainty is widely recognized as a key part of dispersion modeling, especially in light of hazard analysis moving toward probabilistic results as a valuable tool for decision-making and optimizing the use of resources. There have been many papers and journal articles over the years addressing various issues revolving around the determination of uncertainty in dispersion models. The purpose of this paper is not to revisit this subject. Rather, two articles are recommended for those wishing to understand the sources of uncertainty and for an example of recommendations in characterizing the uncertainty in dispersion models. The articles are by K. Shankar Rao entitled “Uncertainty Analysis in Atmospheric Dispersion Modeling” and by John S. Irwin and Steven R. Hanna entitled “Characterizing Uncertainty in Plume Dispersion Models”.^{4,5}

FUTURE UNCERTAINTY ANALYSIS CAPABILITIES WITHIN MACCS2

MACCS2 has been designated as part of a DOE "toolbox" of high-use safety software codes.⁶ A Windows-based version of MACCS2, known as WinMACCS, is under development that provides a graphical user interface to MACCS2. WinMACCS would allow for a more intuitive and efficient manner to create or modify MACCS2 input files, run the code, evaluate results, and to support uncertainty analysis.^{7,8,9} A beta version of WinMACCS is used in this paper only as an initial tool to help develop a quantitative uncertainty analysis process of the χ/Q consequence analysis factor.

A number of uncertainty distribution types (up to thirty) may be available for uncertainty analysis of up to approximately 147 input parameters among all four modules (ATMOS, EARLY, CHRONC, and COMIDAC2). A Latin Hypercube Sampling (LHS) routine randomly determines an input parameter's value from its uncertainty distribution for each MACCS2 run/simulation performed during the uncertainty analysis. An analyst should also be able to correlate dependent input parameters to each other so the LHS routine does not produce combinations of unphysical values between the correlated input parameters. Additionally, once the NRC-sponsored MACCS2 development work is complete later this year, a user manual and/or modeling document may be available that further outlines the sources of uncertainty with technical guidance on assigning uncertainty distributions within the MACCS2 code package.

PROPOSED METHOD FOR ASSESSING UNCERTAINTY

In developing a proposed method for assessing the χ/Q uncertainty, the following will need to be evaluated:

1. Determine which MACCS2 modules are applied for the site-specific accident analysis,
2. Verify the input parameters for the MACCS modules of concern, which can be included in the uncertainty analysis or removed from the uncertainty assessment based on DOE guidance, the specific scenario assumptions, and/or by site-specific conditions,

3. For the remaining input parameters, establish their uncertainty distribution type and associated input values,
4. Determine if the selected input parameters are dependent (i.e., they have a relationship that must be accounted for during the LHS step of the uncertainty analysis) and, if so, establish their “Correlation Coefficients,” and
5. Perform necessary MACCS2 runs/simulations and document the results.

These steps are proposed to focus the uncertainty analysis to those MACCS2 input parameters that should truly affect the uncertainty. To demonstrate their use, they will be applied to a previous MACCS2 calculation performed at LLNL.

LLNL SITE-SPECIFIC EXAMPLE

The previous LLNL safety calculation applying MACCS2 that will be applied as the test case for this study is an aircraft crash with an ensuing fire involving 90 gallons of gasoline.¹⁰ The MOI for this case is at the LLNL fenceline at a distance of approximately 150 m. The MACCS2 input values from this calculation were entered into a WinMACCS input deck and run for the baseline case. The resulting baseline consequence dose from a 1 PE-Ci source term to the MOI at the nearest fence line (0.1 to 0.2 km in the NE direction) is a 95th percentile value of 1.12E-1 Sv, or 11.2 rem/PE-Ci.

Using this calculation as the example, the proposed steps of the uncertainty analysis are as follows:

1. Selection of the MACCS2 Modules to Include in the Uncertainty Analysis

Because the guidance in DOE-STD-3009 for accident analysis specifically concerns short-term radiological exposure to the MOI via the inhalation pathway, only the input parameters for the ATMOS and EARLY modules need to be evaluated in the uncertainty analysis.

2. Identifying the Potential Input Parameters for Uncertainty Analysis

WinMACCS displays whether an input parameter can have an uncertainty distribution if the “Make Uncertain” button is activated. For the LLNL example, there are a total of forty input parameters between the ATMOS and EARLY modules as shown in Table 1 that could have uncertainty distributions assigned to them.

General assumptions or requirements from accident analysis guidance or by site-specific conditions in the scenario set the values for many input parameters.^{1,3} Such input parameters would be removed from further consideration in the uncertainty analysis. Examples from Table 1 of these input parameters are:

- Breathing Rate (BRRATE): The new DOE standard sets this input parameter specifically to 3.3E-4 m³/s and excludes all other values.³

- Boundary Weather Rain Rate (BNDRAN): Wet deposition beyond the specified distances is defined; however, all wet deposition is excluded from DOE accident analysis.¹
- Particle Size Distribution (PSDIST): The parameter only involves monodisperse particulate of concern.¹⁰

Table 1 MACCS2 Input Parameters under Consideration for Uncertainty Analysis

No	Module	Section	Sub-Section	Parameter	Definition	
1	ATMOS	Deposition	Dry Deposition	VDEPOS	Dry Deposition Velocities	
2		Dispersion	Dispersion Function	CYSIGA	Linear Coefficient - σ_y (6 Classes)	
3				CYSIGB	Exponential Term - σ_y (6 Classes)	
4				CZSIGA	Linear Coefficient - σ_z (6 Classes)	
5				CZSIGB	Exponential Term - σ_z (6 Classes)	
6				Scaling Factors	YSCALE	Scale Factor- Horizontal Dispersion
7					ZSCALE	Scale Factor - Vertical Dispersion
8		Plume Specs	Time of Releases	PDELAY	Plume Release Times	
9			Plume Meander Data	TIMBAS	Time Base - Plume Expansion	
10				BRKPNT	Breakpoint Time - Plume Meander	
11				XPFAC1	Base Time - Meander Expansion	
12				XPFAC2	Breakpoint - Expansion Factor	
13			Plume Rise Data	SCLCRW	Scaling Factor - Critical Wind Speed	
14				SCLADP	Scaling Factor - A-D Plume Rise	
15				SCLEFP	Scaling Factor - E-F Plume Rise	
16			Wake Effect Data	BUILDH	Reactor Building Height	
17				SIGYINIT	Initial Value of σ_y	
18				SIGZINIT	Initial Value of σ_z	
19		Release Description	Release Info	OALARM	Off-Site Alarm Time	
20			Plume Parameters	REFTIM	Plume Reference Time Point	
21			Particle Size Distrib.	PSDIST	Particle Size Distribution by Group	
22			Inventory Scale Factor	CORSCA	Linear Scaling Factor-Core Inventory	
23			Plume Segment Release Fractions	RELFRC	Release Fractions of the Source Term	
24		Weather	Boundary Conditions	BNDMXH	Boundary Weather Mixing Layer Ht.	
25				BNDRAN	Boundary Weather Rain Rate	
26				BNDWND	Boundary Weather Wind Speed	
27			Samples per Day	NSMPLS	Number of Weather Samples per Bin	
28	EARLY	Model	Population Data	POPDEN	Average Regional Population Density	
29		Basis	Shielding and Exposure	CSFACT	Cloudshine Shielding Factor	
30				PROTIN	Inhalation Protection Factor	
31				BRRATE	Breathing Rate	
32				SKPFAC	Skin Protection Factors	
33				GSHFAC	Groundshine Shielding Factor Table	
34		Emergency Phase Resuspension	RESCON	Resuspension Conc. Coef.		
35			RESHAF	Resuspension Conc. Half-Life		
36		Emergency Scenario 1	Duration of Early Phase	ENDEMP	Duration of the Early Phase	
37			Hot Spot Reloc. Time	TIMHOT	Hot Spot Relocation Time	
38			Hot Spot Reloc. Dose	DOSHOT	Normal Relocation Dose Threshold	
39			Normal Relocation	TIMNRM	Normal Relocation Time	
40		DOSNRM		Hot-Spot Relocation Dose Threshold		

The remaining input parameters are examined to determine if they should have an uncertainty distribution. A description of each MACCS2 input parameter and their use in the code is provided in the DOE Toolbox document for MACCS2.¹¹ In some cases, the recommendation is to maintain at a set value in all cases. After further review, only a small number of input parameters remained for further evaluation in the uncertainty analysis and are highlighted in Table 1.

3. Establish the Selected Input Parameters' Uncertainty Distributions

The next step is to determine the input parameter's respective uncertainty distributions and related input values must be determined and set. This needs to be technically justified, defensible, and retrievable.

A potential user error is to define distributions that lead to illegal values (e.g., a negative value for a parameter that must be greater than zero) or results in a LHS value outside the allowed input range. Either the run fails during input validation or an unphysical situation is calculated (i.e., the angle of the plume spread becomes greater than 180 degrees) causing the run to fail.

From this step, the following input parameters are selected for further analysis with the following uncertainty distributions:

Dry deposition rate:	Loguniform distribution from 2.7e-6 to 0.025 m/s ^{12, 13}
Dispersion scaling factors:	Uniform distribution from 1.0 to 2.51 for vertical dispersion (ZSCALE) ¹¹
Plume rise scaling factors:	Uniform distribution from 0.1 to 10 (SCLADP & SCLEFP)

While, it would be desirable to include the dispersion function input parameters (CYSIGA, CYSIGB, CZSIGA, and CZSIGB), an uncertainty distribution could not be found that also satisfactorily completed MACCS2 input validation. Once the NRC-sponsored MACCS2 improvements have been completed and published, these input parameters will be revisited.

4. Correlating One Input Parameter Related to Another

For the case where one input parameter is related to another, the beta version of WinMACCS allows for assigning a correlation coefficient that then can force the LHS routine to sample each parameter in the same manner to avoid unphysical combinations (for example, one value is selected from the low end of the uncertainty distribution while the other is selected from the high end). For this example, the plume rise scaling factors were correlated to each other (SCLADP to SCLEFP) for consistency in sampling.

5. Perform and Document the Uncertainty Analysis

The above sets of input parameter's uncertainty distributions and values were entered into the baseline MACCS2 input deck. Each input parameter set was run separately along with a combined run when all uncertainty distributions were applied. Twenty MACCS2 runs/simulations were performed for each uncertainty run. Graphical plots of the 95th quantile

peak dose for the 0.1 to 0.2 km sector from each run were generated (see Figures 1 through 4, note that baseline value was 1.12E-1 Sv for 1 PE-Ci or 11.2 rem/PE-Ci).

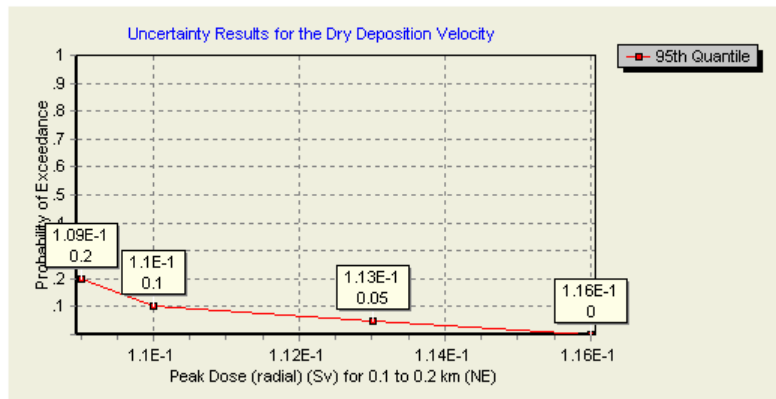


Figure 1 Impact of the Dry Deposition Velocity on Uncertainty

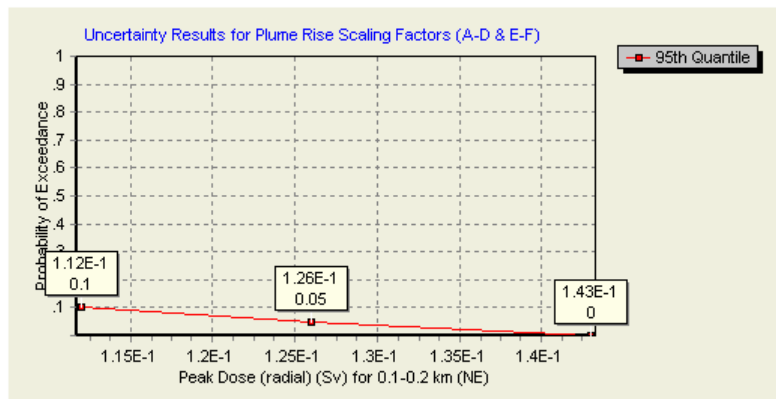


Figure 2 Impact of the Plume Rise Scaling Factors for Stability Classes A-D and E&F on Uncertainty

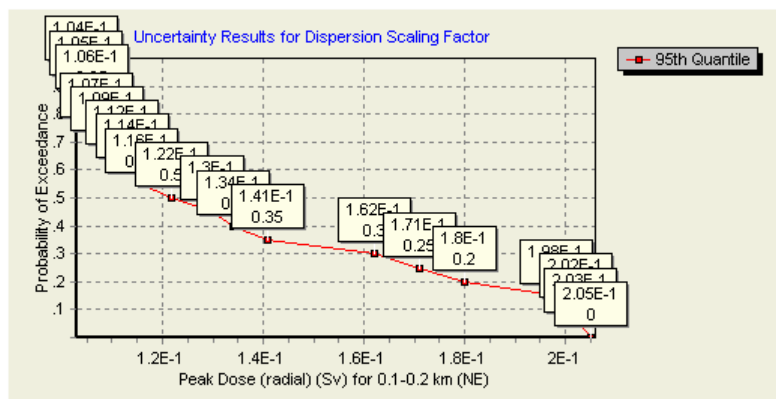


Figure 3 Impact of the Dispersion Scaling Factor on Uncertainty

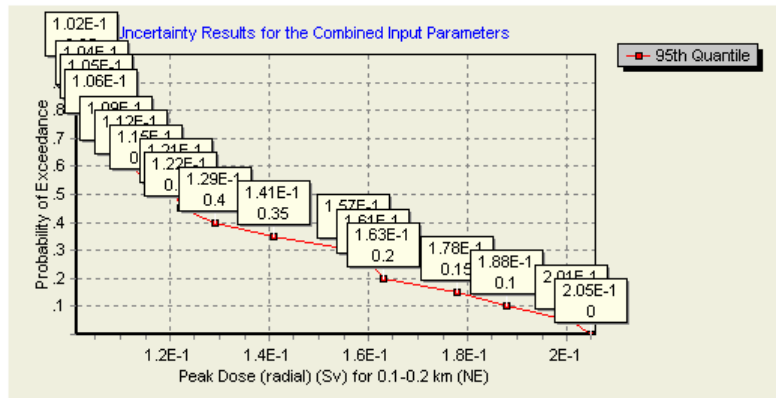


Figure 4 Impact of All Evaluated Input Parameters on Uncertainty

The results demonstrate the dry deposition and plume rise scaling factors only have a small impact on the MOI consequence dose ratio (majority of the runs at the lowest two values and the highest values no more than a factor of 1.3 times greater than the baseline value). However, the deposition scaling factor, ZSCALE, could result in a range in uncertainty of the consequence dose ratio of approximately 0.9 to 1.8 times the baseline value. The overall uncertainty from all input parameters combined is also ranges from approximately 0.9 to 1.8 times the baseline value where approximately 65% of the values are greater than the baseline value. While a limited case, this example is well within the new DOE standard's predicted uncertainty for the χ/Q term.

CONCLUSION

For TRU waste facilities, the ability to quantitatively assess the uncertainty in an accident analysis may become available in the near future. First, the new DOE standard must be formally approved and released. This, in combination with site-specific scenario initial conditions, would allow for focusing the uncertainty analysis to a small number of key MACCS2 input parameters. Additionally, an uncertainty factor of two in the dispersion analysis is very small in comparison to conservatism on orders of magnitude in the ARF and RF from DOE-HDBK-3010 that is being set in the new DOE standard. Second, the NRC-sponsored improvements to MACCS2 must be completed and published. If similar to other NRC-sponsored codes, this should include a probabilistic MACCS2 user guide with technical recommendations for the selection and entering of the uncertainty distributions for the key MACCS2 input parameters. However, the improvements to MACCS2 are to support NRC efforts for probabilistic assessments to support a performance or risk-informed regulatory framework. Thus, further assessment would be necessary to ensure this may be directly transferable to DOE accident analysis methodology. To this end, this study should be considered an initial demonstration of the usefulness of such an uncertainty analysis capability in the beta version of WinMACCS.

REFERENCES

1. U.S. Department of Energy, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Documented Safety Analyses*, DOE-STD-3009 CN3, March 2006.

2. Fisher, D.K. of Lawrence Livermore National Laboratory, Safety and Environmental Protection Directorate Letter to C. Yuan-Soo Hoo, "Transition to Dose Conversion Factors in FGR13 for Accident Analysis," November 13, 2003.
3. U.S. Department of Energy, *Preparation of Safety Basis Documents for Transuranic (TRU) Waste Facilities*, DOE-STD-5506, tentative date of April 2007.
4. Rao, K. Shankar, "Uncertainty Analysis in Atmospheric Dispersion Modeling," *Pure and Applied Geophysics*, Birkhauser Verlag, Basel, Volume 162, Number 10, Pages 1893-1917, October 2005.
5. Irwin, John S. and Steven R. Hanna, "Characterizing Uncertainty in Plume Dispersion Models," *Int. J. Environment and Pollution*, Vol. 25, Nos. 1/2/3/4, Pages 16-24, 2005.
6. U.S. Department of Energy, Office of Health, Safety, and Security, Software Quality Assurance, "Safety Software Quality Assurance - Central Registry," April 17, 2007, <http://www.hss.energy.gov/csa/csp/sqa/central_registry.htm>, Accessed April 18, 2007.
7. Bixler, Nathan, K. L. McFadden, and J. E. Cash, "Future Plans for MACCS2," Fourth International MACCS Users Group (IMUG) Meeting, Brookhaven National Laboratory, Technical Report W-6139-4 10-31 -02, Principality of Monaco, September 8, 2002.
8. Bixler, Nathan, Katherine L. McFadden, and C. W. Morrow, "Current Status of the MACCS2 and WinMACCS Codes," LA-UR-05-9037, 2005 Safety Analysis Working Group Workshop, Santa Fe, New Mexico, April 30 to May 5, 2005.
9. Bixler, Nathan, et al., "Recent Improvements to the WinMACCS Code Suite," Fifth International MACCS Users Group (IMUG) Meeting, U. S. Nuclear Regulatory Commission, ADAMS Accession No. ML062760511, Rockville, Maryland, March 10, 2006.
10. Yang, Joong, M., "Aircraft Crash Consequence Analysis," HC/AB-B696-0302, Lawrence Livermore National Laboratory, Livermore, California, May 2003.
11. U.S. Department of Energy, "MACCS2 Computer Code Application Guidance for Documented Safety Analysis," .DOE-EH-4.2.1.4, June 2004.
12. Randerson, Darryl, Editor, *Atmospheric Science and Power Production*, DOE/TIC-27601, U.S. Department of Energy, 1984.
13. LePoire, D., et al., *Probabilistic Modules for the RESRAD and RESRAD-BUILD Computer Codes: User Guide*, NUREG/CR-6692, U.S. Nuclear Regulatory Commission, November 2000.