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RADCALC: AN ANALYTICAL TOOL FOR SHIPPERS OF RADIOACTIVE MATERIAL AND WASTE

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ABSTRACT

The U.S. Department of Energy (DOE) ships radioactive materials in support of its research and development, environmental restoration, and national defense activities. The Radcalc software program was developed to assist personnel working on behalf of DOE in packaging and transportation determinations (e.g., isotopic decay, decay heat, regulatory classification, and gas generation) for shipment of radioactive materials and waste.

Radcalc performs:

- The U.S. Department of Transportation determinations and classifications (i.e., activity concentration for exempt material Type A or B, effective A_1/A_2, limited quantity, low-specific activity, highway route controlled quantity, fissile quantity, fissile excepted, reportable quantity, list of isotopes required on shipping papers)
- DOE calculations (i.e., transuranic waste, ^{239}Pu-equivalent curies, fissile-gram equivalents)
- The U.S. Nuclear Regulatory Commission packaging category (i.e., Category I, II, or III)
- Dose-equivalent curie calculations
- Radioactive decay calculations using a novel decay methodology and a decay data library of 1,867 isotopes typical of the range of materials encountered in DOE laboratory environments
- Hydrogen and helium gas calculations
- Pressure calculations.

Radcalc is a validated and cost-effective tool to provide consistency, accuracy, reproducibility, timeliness, quality, compliance, and appropriate documentation to shippers of radioactive materials and waste at DOE facilities nationwide. Hundreds of shippers and engineers throughout the DOE Complex routinely use this software to automate various determinations and to validate compliance with the regulations. The effective use of software by DOE sites contributes toward minimizing risk involved in radioactive waste shipments and assuring the safety of workers and the public.

1.0 INTRODUCTION

Radcalc is a user-friendly software that may be used to automate packaging and transportation determinations for shipment of radioactive materials. Radcalc is used throughout the U.S. Department of Energy (DOE) Complex; by multiple Federal, state, and international agencies; and by public and commercial organizations. Radcalc capabilities include the following:

- Performs transportation classifications based on selected U.S. Department of Transportation (DOT) definitions and methodologies outlined in 49 CFR Chapter I, Subchapter C, "Hazardous Materials Regulations"
- Performs calculations in accordance with selected methods prescribed by the DOE, U.S. Nuclear Regulatory Commission (NRC), U.S. Environmental Protection Agency, and International Conference of Radiological Protection
- Calculates the decay heat and activity of radionuclides and their daughter products at the end of a specified time interval
- Calculates the radiolytic production of hydrogen gas in a radioactive waste matrix
- Calculates the production of helium gas due to radioactive decay.

The capability to automatically import and export data allows information to be entered, evaluated, and reported within minutes.

2.0 RADCALC 4.0

2.1 Historical Development

GEND-041, *A Calculational Technique To Predict Combustible Gas Generation in Sealed Radioactive Waste Containers*, documents an EG&G Idaho, Inc., and the Electric Power Research Institute TMI-2 Technology Transfer Office methodology developed for quantifying the concentration of hydrogen generated by radiolysis in sealed radioactive waste containers.
NP-4938, *Methodology for Calculating Combustible Gas Concentration in Radwaste Containers*, documents that the GEND-041 methodology was accepted for use in demonstrating acceptably low concentrations of hydrogen in low-level waste packages in compliance with NRC Office of Inspection and Enforcement Information Notice No. 84-72, *Clarification of Conditions for Waste Shipments Subject to Hydrogen Gas Generation* (NRC 1984).

Using the GEND-041 methodology, the Electric Power Research Institute developed a simple spreadsheet to predict hydrogen gas concentrations. Three Mile Island EPICOR[1] II resin bed measurements were used as a benchmark for the spreadsheet showing that the model predicted hydrogen gas concentrations within 20 percent of measured concentrations.

Radcalc 1.0, issued in September 1995, adapted the GEND-041 computational methodology to calculate the production of hydrogen gas in the waste packages, incorporating a FORTRAN executable code to calculate decay. Radcalc 2.0 incorporated DOT requirements and an improved user interface. Radcalc 3.0 incorporated regulatory changes; consolidated, updated, and substantially expanded the isotopic database; isolated the calculation, package, and user interfaces to facilitate independent modification; and was developed to ASME NQA-1-1994 standards. Radcalc 4.0, issued in September 2004, incorporated changes to the DOT regulations, dose-equivalent curie (DE-Ci) and helium gas calculations; and an enhanced the user interface.

2.2 DOT Determinations

Radcalc provides the following DOT determinations for radioactive material shipments:

- Radioactive
- Type A or Type B
- Effective A_1 or A_2 for mixture
- Limited quantity
- Low specific activity-I, -II, or -III
- Highway route controlled quantity
- Fissile quantity
- Fissile excepted
- Reportable quantity.

Radcalc also provides a list of isotopes that are required for shipping papers and labels (95 percent of the total A_1/A_2 values). Radcalc has a transportation library including all isotopes identified in 49 CFR 173, "Shippers—General Requirements for Shipments and Packagings," 173.435, "Table of A_1 and A_2 values for radionuclides."

2.3 NRC Determination

Radcalc categorizes radioactive contents as Category I, II, or III in accordance with NRC Regulatory Guide 7.11, *Fracture Toughness Criteria of Base Material for Ferritic Steel Shipping Cask Containment Vessels With a Maximum Wall Thickness of 4 inches (0.1 m).*

2.4 DOE Determinations

Radcalc categorizes waste using selected DOE requirements including the following:

- Transuranic waste classification in accordance with the DOE Manual M435.1-1, Chg. 1, *Radioactive Waste Management Manual*
- ^{239}Pu-equivalent activity in accordance with Appendix B of DOE/WIPP-02-3122, *Contact-Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant*
- ^{239}Pu fissile gram equivalent calculations in accordance with Section 3.1.2 of the *TRUPACT-II Authorized Methods for Payload Control (TRAMPAC)* (WTS 2003).

2.5 DE-Ci

Radcalc calculates DE-Ci values in accordance with FGR11/EPA-520/1-88-020, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*. In addition, Radcalc calculates DE-Ci values in accordance with ICRP 71, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 4 Inhalation Dose* Coefficients, and ICRP 72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients*.

2.6 Radioactive Decay

Radcalc uses a decay data library of 1,867 isotopes to calculate the activity and decay products over a specified period. Radcalc also calculates the decay heat of the nuclear material in a package. The Radcalc nuclear database is based on a combination of the *Fusion Evaluated Nuclear Data Library (FENDL)* (IAEA 1988) and the *Joint Evaluated File (JEF)* (OECD 1993). The Radcalc atomic mass database is based on "The NUBASE Evaluation of Nuclear and Decay Properties" (Audi 1997). Users may input source term in grams, becquerels, or curies and

convert between units; multiply the source term by a factor to increase or decrease activity; and import data from or export data to other Radcalc files or spreadsheet files.

2.7 Hydrogen and Helium Gas Calculations

Radcalc can calculate the radiolytic production of hydrogen gas in packages containing radioactive material and hydrogenous material or, alternatively, calculate the $G_{effective}$ value for a specified hydrogen gas generation rate. Radcalc calculates percent hydrogen in a specified period or will iterate the time needed to reach a specified hydrogen gas concentration.

Radcalc calculates the production of helium gas due to alpha decay. This calculation utilizes the total number of alpha decays from the decay algorithm and assumes that each alpha decay produces one atom of helium gas.

2.8 Pressure Calculations

Radcalc calculates package pressurization associated with hydrogen, oxygen, and helium generated in the package using the ideal gas law. The package is assumed sealed at atmospheric pressure and at 0 °C. Atmospheric pressure and temperature changes are ignored. Pressure is calculated for cases where the hydrogenous material is or is not primarily water. Water is assumed to yield 1 mole of H_2 gas and ½ mole of O_2 gas per mole of water. Other materials are assumed to produce only H_2 gas.

2.9 Limitations

Users are responsible to account for the limitations described below. Users must:

- Understand, interpret, and implement regulations and associated guidance documents
- Verify that Radcalc source documents are appropriate and current for the user's calculations
- Understand the purpose and limits of the reference material selected
- Evaluate both numeric and non-numeric requirements established in the regulations
- Understand the terminology, methodologies, and limitations of hydrogen gas calculations
- Review limitations described in the User's Manual and Read Me First file
- Regularly review known problems and limitations published on the website.

2.10 Quality Assurance

Energy*Solutions* Federal Services, Inc., maintains Radcalc on behalf of the DOE Office of Transportation. Energy*Solutions* work is performed under contract to DOE using a quality assurance (QA) program documented in FS-WO-QAPP-001, *Federal Services Hanford Quality Assurance Program Plan*, which is based on the following:

- 18 Basic Requirements prescribed in 10 CFR 71, "Packaging and Transportation of Radioactive Materials," Subpart H, "Quality Assurance"
- 10 CFR 72, "Licensing Requirements for the Independent Storage of Spent Nuclear Fuel, High-Level Radioactive Waste, and Reactor-Related Greater than Class C Waste," Subpart G, "Quality Assurance"
- 10 Criterion prescribed in 10 CFR 830, "Nuclear Safety Management," and 830.122, "Quality assurance criteria"

- DOE Order 414.1B, *Quality Assurance*
- 18 Basic and Supplement Requirements of American Society of Mechanical Engineers (ASME) NQA-1-1994 (and NQA-1-2000), *Quality Assurance Requirements for Nuclear Facilities*.

Implementation of the program described in FS-WO-QAPP-001 is accomplished through written, approved procedures documented in FSWO-QAP-001, *Quality Assurance Procedures*. Radcalc is a Level-1 software (software used in safety class or safety-significant applications) as defined in those procedures.

The *Software Quality Plan* (8/24/04) (DTS 2004); DTS-SQA-006, *Radcalc Software Requirement Specification*; and DTS-SQA-008, *Radcalc Software Design Description and Implementation Document*, document the QA requirements and technical content incorporated in Radcalc 4.0. DTS-VV-021, *Radcalc 4.0 Verification and Validation Test Plan*, documents the process by which the applicable QA requirements have been implemented. DTS-VV-023, *Radcalc 4.0 Verification and Validation Test Report*, documents that the software has been fully verified and validated in accordance with the QA program.

2.11 User Support

Radcalc is currently available free to users as a service of the DOE Office of Transportation. The software can be downloaded from the Radcalc website on DOE's Consolidated Business Center server (http://www.radcalc.energy.gov). Software documentation is available to registered users. Radcalc is distributed with a database viewer that allows users to access the Radcalc nuclear, transportation classification, and G value database values on an isotope-by-isotope basis.

User-funded training in the use of Radcalc's transportation and hydrogen gas modules is available periodically when sufficient students express interest. Training may be provided at facilities in Richland, Washington, or may be arranged at sites convenient to the user.

A list containing known issues with Radcalc will be maintained on the Radcalc website. User input is encouraged.

Questions may be directed by E-mail or phone to the following individuals:

Bill Willis	WLWillis@energysolutions.com	(509) 375-9532	Technical issues/training
Aaron Schatz	ALSchatz@energysolutions.com	(509) 375-9555	Distribution/web page

3.0 RADCALC 4.1

Radcalc is revised periodically to reflect changes in the regulations and customer requirements. Radcalc is in the process of being updated to correct errors, incorporate new regulatory interpretations, and implement other changes identified by DOE, users, and the technical staff. Current plans anticipate that Radcalc 4.1 will be published in June 2008. A new web interface with enhanced security will be implemented at that time.

Future initiatives may include:

- Migrating to a web-based application to facilitate more timely updates
- Developing web-based training modules
- Updating nuclear database and physical constants consistent with the current information
- Updating calculational methods and values consistent with revised source documents

- Developing means to integrate Radcalc functionality with other software applications, such as the Automated Transportation Management System, Solid Waste Information and Tracking System at the Hanford Site, and RH-TRUCON Maintenance Application at the Waste Isolation Pilot Plant
- Incorporating changes to regulations consistent with harmonization with International Atomic Energy Agency regulations.

4.0 CONCLUSIONS

Radcalc is a validated and cost-effective tool to assist in assuring consistency, accuracy, reproducibility, timeliness, quality, compliance, and appropriate documentation to shippers of radioactive materials and waste at DOE facilities nationwide. Hundreds of shippers and engineers throughout the DOE Complex routinely use this software to automate various determinations and to validate compliance with the regulations.

5.0 ACKNOWLEDGMENTS

The authors would like to recognize the many who have contributed to development of the Radcalc software and its predecessors over the years and the dedicated technical staff who continue to support and improve the application.

6.0 REFERENCES

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Radcalc website Radcalc website (http://www.radcalc.energy.gov)

[1] EPICOR is a trademark of the Epicor Software Corporation, Irvine, California.