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Accession #: D196050262

Document #: SD-TP-CSWD-002

Title/Desc:

RADCALC FOR WINDOWS VOL II TECHNICAL MANUAL

2. To: (Receiving Organization) Packaging Engineering	3. From: (Originating Organization) Packaging Engineering	4. Related EDT No.: 611656
5. Proj./Prog./Dept./Div.: 84100	6. Cog. Engr.: J. R. Green	7. Purchase Order No.: NA
8. Originator Remarks: The attached document (two volumes) is being submitted for approval and release.		9. Equip./Component No.: NA
11. Receiver Remarks:		10. System/Bldg./Facility: NA
		12. Major Assm. Dwg. No.: NA
		13. Permit/Permit Application No.: NA
		14. Required Response Date: NA

15. DATA TRANSMITTED					(F)	(G)	(H)	(I)
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	Approval Designator	Reason for Transmittal	Originator Disposition	Receiver Disposition
1	WHC-SD-TP-CSWD-002 Vol I		0	Radcalc for Windows Volume I: User's Manual	SQ	1/2	1	1
2	WHC SD-TP-CSWD-002 Vol II		0	Radcalc for Windows Volume II: Technical Manual	SQ	1/2	1	1

16. KEY					
Approval Designator (F)		Reason for Transmittal (G)		Disposition (H) & (I)	
E, S, Q, D or N/A (see WHC-CM-3-5, Sec. 12.7)		1. Approval	4. Review	1. Approved	4. Reviewed no/comment
		2. Release	5. Post-Review	2. Approved w/comment	5. Reviewed w/comment
		3. Information	6. Dist. (Receipt Acknow. Required)	3. Disapproved w/comment	6. Receipt acknowledged

17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)										(G)	(H)
Reason	Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN	(J) Name	(K) Signature	(L) Date	(M) MSIN	Reason	Disp.
1/2	1	Cog. Eng.: JR Green	<i>[Signature]</i>	9/26/95	G2-02	KE Hillesland	<i>[Signature]</i>	9/26/95	H0-35	1/2	1
1/2	1	Cog. Mgr.: JG Field	<i>[Signature]</i>	9/26/95	G2-02	VE Roetman	<i>[Signature]</i>	9/26/95	H0-35	1/2	1
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1/2	1	RP Genoni	<i>[Signature]</i>	9/25/95	G2-02						

18. <i>[Signature]</i> 9/26/95 Signature of EDT Originator	19. Authorized Representative Date for Receiving Organization	20. <i>[Signature]</i> 9/26/95 Cognizant Manager Date	21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments
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RELEASE AUTHORIZATION

Document Number: WHC-SD-TP-CSWD-002, Rev. 0, Volume 2

Document Title: Radcalc for Windows Volume II: User's Manual

Release Date: 9/27/95

**This document was reviewed following the
procedures described in WHC-CM-3-4 and is:**

APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

C. WILLINGHAM

9/27/95

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SUPPORTING DOCUMENT

1. Total Pages 283

2. Title

Radcalc for Windows Volume II: Technical Manual

3. Number

WHC-SD-~~EP~~-CSWD-002

4. Rev No.

0

5. Key Words

Radcalc for Windows, hydrogen generation, radioactive waste packages, decay heat, radionuclide decay, DOT classifications

6. Author

Name: J. R. Green

Signature

Organization/Charge Code 84100/YHA09

7. Abstract

Radcalc for Windows is a user-friendly menu-driven Windows-compatible software program with applications in the transportation of radioactive materials. It calculates the radiolytic generation of hydrogen gas in the matrix of low-level and high-level radioactive waste using NRC-accepted methodology. It computes the quantity of a radionuclide and its associated products for a given period of time. In addition, the code categorizes shipment quantities as radioactive, Type A or Type B, limited quantity, low specific activity, highway route controlled, and fissile excepted using DOT definitions and methodologies, as outlined in 49 CFR Subchapter C. The code has undergone extensive testing and validation. Volume I is a User's Guide, and Volume II is the Technical Manual for Radcalc for Windows.

8. RELEASE STAMP

OFFICIAL RELEASE
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DATE Sept. 27, 1995

Station 35

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**RADCALC FOR WINDOWS VOLUME II:
TECHNICAL MANUAL**

**J. R. Green
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V. E. Roetman
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September 1995

**Prepared for the U.S. Department of Energy
by
Packaging Engineering
Transportation and Packaging
Westinghouse Hanford Company**

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ACKNOWLEDGEMENTS

The development of Radcalc for Windows was supported by the U.S. Department of Energy. Radcalc for Windows' authors would like to thank the following people for their support on this project: Jess Greenborg, Frank Schmittroth, Randy Schwarz, Reid Chesterfield, Teresa Kaufman, and Howard Harris. In addition, we would like to acknowledge the work and support of two of the original authors of the Electric Power Research Institute report: Jim Flaherty and Paul Deltete. Acknowledgement is also due to Rich Genoni and Greg Field for their effort in the development of the Excel version of the Radcalc spreadsheet.

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**RADCALC FOR WINDOWS VOLUME II:
TECHNICAL MANUAL**

**J. R. Green, K. E. Hillesland
V. E. Roetman, J. G. Field**

ABSTRACT

Radcalc for Windows is a user-friendly computer software program that has applications in the transportation and packaging of radioactive high- and low-level waste. It calculates the radiolytic production of hydrogen gas in the waste matrix of radioactive waste. In addition, Radcalc for Windows contains a robust decay algorithm that calculates the activity of a radionuclide and its associated products at a future date. Radcalc for Windows also classifies waste quantities using the U.S. Department of Transportation definitions and methodologies outlined in Title 49, Code of Federal Regulations, Subchapter C.

Documentation for Radcalc for Windows is available in two volumes. Volume I is a user's manual, which is intended as a quick reference. It will aid the user in becoming familiar with Radcalc for Windows. Volume II is the Radcalc for Windows technical manual. The technical manual contains information on the history of Radcalc for Windows, as well as the theoretical background, calculational methodology, configuration control, and verification and validation of the code.

Radcalc for Windows is sponsored by the U.S. Department of Energy. It was developed and is maintained by Packaging Engineering, Transportation and Packaging, Westinghouse Hanford Company. Copies of the software program are available by calling Packaging Engineering.

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FOREWORD

Radcalc for Windows is a software program developed and maintained by Packaging Engineering, Transportation and Packaging, Westinghouse Hanford Company, Richland, Washington, for the U.S. Department of Energy. Documentation for the software program exists in the form of *Radcalc for Windows Volume I: User's Manual* and *Radcalc for Windows Volume II: Technical Manual*. The software is available from Packaging Engineering by calling 509-376-0610 or -372-0703. Corrections and suggestions for Radcalc for Windows are welcomed.

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CONTENTS

1.0	INTRODUCTION	1
1.1	DESCRIPTION	1
1.2	BACKGROUND	1
1.3	SCOPE	2
2.0	RADCALC FOR WINDOWS METHODOLOGY	3
2.1	HYDROGEN GAS GENERATION	3
2.1.1	Theoretical Basis	3
2.1.2	Hydrogen Gas Generation Calculations	4
2.2	HYDROGEN GAS GENERATION RATE	5
2.3	TOTAL PRESSURE AND PARTIAL PRESSURE	5
2.4	DECAY HEAT	6
2.5	RADIOACTIVE DECAY CALCULATIONS	6
2.6	TRANSPORTATION CLASSIFICATION DETERMINATIONS	8
2.6.1	Definitions	8
2.6.2	Radioactive Material	9
2.6.3	Unity Fraction/Package Type Determination	9
2.6.4	LSA Determination	10
2.6.5	Limited Quantity Determination	11
2.6.6	Highway Route Controlled Quantity Determination	11
2.6.7	Fissile Excepted Determination	11
2.7	UNIT CONVERSIONS	11
2.8	PRIMARY RADCALC CALCULATION ROUTINES	12
3.0	DATABASES AND INPUT PARAMETERS USED IN RADCALC FOR WINDOWS	13
3.1	DATABASES AND INPUT PARAMETERS USED FOR HYDROGEN GAS GENERATION AND HEAT DECAY	14
3.1.1	Radionuclide Databases	14
3.1.2	Gamma Absorption Fraction Input Parameters	16
3.1.3	G Value Data	21
3.2	TRANSPORTATION DATA	22
4.0	VERIFICATION AND VALIDATION	22
4.1	SOFTWARE TEST PLAN: VERIFICATION CASES	22
4.2	RADCALC FOR WINDOWS VALIDATION	22
5.0	CONFIGURATION CONTROL	25
5.1	CONFIGURATION MANAGEMENT PLAN	26
5.2	ARCHIVAL STORAGE AND RECORDS	26
5.3	BACKUP AND RECOVERY	27
5.4	DISTRIBUTION	27
6.0	REQUIREMENTS SPECIFICATION	28
7.0	SUMMARY	28
8.0	REFERENCES	29

CONTENTS (cont)

APPENDICES

A	A COMPUTER ALGORITHM FOR SOLVING THE BATEMAN DECAY EQUATIONS	A-1
B	FENDL/D-1.0	B-1
C	RESULTS OF GAMMA ABSORPTION FRACTION ANALYSIS	C-i
D	INSTALLATION TEST CASES	D-1
E	VALIDATION CASES	E-i
F	CHANGE REQUEST AND PROBLEM REPORT FORM	F-1

LIST OF TABLES

2-1	Radionuclides Identified as Daughter Products in Radcalc for Windows	10
3-1	FENDL Radionuclides With Total Recoverable Energies Differing From ORIGEN2 and Browne and Firestone	15
3-2	Dimensions of Modeled Shipping Containers	17
3-3	Index to Tables and Graphs for Each Geometry	21
4-1	Radcalc for Windows Validation Cases	23

LIST OF TERMS

Bq/s	becquerels per second
Ci/L	curies per liter
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
ENDSF	Evaluated Nuclear Data Structure File
EPRI	Electric Power Research Institute
ESOE	End System Operating Environment
eV	electronvolt
ENDF	Evaluated Nuclear Data File
FENDL	Fusion Energy Nuclear Data Library
g/cm ³	grams per cubic centimeter
HRCQ	highway route controlled quantity
ID	inside diameter
IE	Office of Inspection and Enforcement
kPa	kilopascals
LET	linear energy transfer
LLW	low-level waste
LSA	low specific activity
μCi/g	microcuries per gram
mCi/g	millicuries per gram
MeV	megaelectronvolt
MCNP	Monte Carlo N-Particle
NCAW	neutralized current acid waste
NRC	U.S. Nuclear Regulatory Commission
OD	outside diameter
ORIGEN	Oak Ridge Isotope Generation and Depletion Code
OTC	onsite transfer cask
QA	quality assurance
RIDS	Records Inventory and Disposition Schedule
SARP	safety analysis report for packaging
WHC	Westinghouse Hanford Company

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RADCALC FOR WINDOWS VOLUME II: TECHNICAL MANUAL

1.0 INTRODUCTION

1.1 DESCRIPTION

Radcalc for Windows¹ 1.0 is a Windows-compatible software program with applications in the packaging and transportation of radioactive materials. Its primary function is to calculate the generation of hydrogen gas by radiolytic production in the waste matrix of high- and low-level radioactive waste packages. It can also be used to categorize radioactive shipments into appropriate U.S. Department of Transportation (DOT) classifications. In addition, it contains a robust decay algorithm that determines the daughter products of selected radionuclides. The various functions in Radcalc for Windows can be used separately or together.

The software program requires a personal computer with a 386 or higher coprocessor and Windows Version 3.1 or later. It is written in Visual C++² using the Microsoft³ Foundation Classes and Windows Library routines. It is compiled on Microsoft Visual C++ Version 1.5. It is also written in FORTRAN using the Microsoft FORTRAN 5.10 compiler. It contains libraries of radionuclide data, G values, and A_1/A_2 values for transportation classification. The software format is similar to other Windows-compatible codes.

Volume I of the documentation of Radcalc for Windows is a user's manual. The user's manual contains installation and use instructions. This volume, Volume II, is the technical manual, which contains the theoretical and calculational basis of the program, the verification and validation of the program, and configuration control.

1.2 BACKGROUND

High-level and low-level radioactive wastes produce ionizing radiation, which may cause the radiolytic formation of hydrogen gas. A calculational technique for quantifying the concentration of hydrogen generated by radiolysis in sealed radioactive waste containers was developed in a U.S. Department of Energy (DOE) study conducted by EG&G Idaho, Inc., and the Electric Power Research Institute (EPRI) TMI-2 Technology Transfer Office. The study resulted in report GEND-041, *A Calculational Technique To Predict Combustible Gas Generation in Sealed Radioactive Waste Containers* (Flaherty et al. 1986). The study also resulted in a presentation to the

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²Visual C++ is a trademark of Microsoft Corporation.

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U.S. Nuclear Regulatory Commission (NRC) which gained acceptance of the methodology for use in ensuring compliance with NRC Office of Inspection and Enforcement (IE) Information Notice No. 84-72 (NRC 1984) concerning the generation of hydrogen within packages.

NRC IE Information Notice No. 84-72, "Clarification of Conditions for Waste Shipments Subject to Hydrogen Gas Generation," applies to any package containing water and/or organic substances that could radiolytically generate combustible gases. The NRC requires the following over a period of twice the expected shipment time.

- o The hydrogen gas concentration is less than 5% by volume (or equivalent limits for other inflammable gases) of the secondary container gas void.
- o The secondary container and cask cavity must be inerted to ensure that oxygen is limited to 5% by volume in those portions of the package that could have hydrogen concentrations greater than 5%.

If the material being shipped classifies as low specific activity (LSA) and if it is shipped within ten days after venting, the above requirements do not apply. Notice No. 84-72 is pertinent to shipments of resins, binders, waste sludge, and wet filters. The notice requires compliance by tests or measurements of a representative package. However, in April of 1985, the NRC accepted the calculational method presented in report GEND-041 to confirm the absence of hydrogen in low-level waste (LLW) packages (Deltete 1987).

Subsequently, EPRI developed a simple computer program in a spreadsheet format utilizing the GEND-041 calculational methodology to predict hydrogen gas concentrations. The computer code was extensively benchmarked against TMI-2 (Three Mile Island) EPICOR II resin bed measurements. The benchmarking showed that the model developed predicted hydrogen gas concentrations within 20% of the measured concentrations. The computer code has since been dubbed Radcalc and is still accepted today by the NRC for Certificates of Compliance for shipping casks containing materials that may result in the radiolytic formation of hydrogen gas. Radcalc for Windows utilizes the computational methodology outlined in GEND-041 to calculate the production of hydrogen gas in the waste matrix of packages.

1.3 SCOPE

Radcalc for Windows calculates the production of hydrogen gas in the waste matrix of 14 commonly used radioactive material container types. It contains a radionuclide library of approximately 260 radionuclides. The library is utilized by the hydrogen gas generation algorithms and can also be used to determine daughter products of selected radionuclides. The G value database (molecules of H_2 formed per 100 eV of energy absorbed) has been widely researched and includes a large number of material types.

In addition, the code categorizes packages as radioactive, Type A, Type B, limited quantity, low specific activity, highway route controlled

quantity, and fissile excepted, employing 49 CFR 173.403 definitions. The A₁/A₂ database used by the code for these determinations is based on 49 CFR 173.435. Radcalc for Windows also calculates decay heat and pressure buildup due to hydrogen.

The Radcalc for Windows calculational methodology is outlined in Chapter 2.0. Chapter 3.0 presents the data that support the software. Chapter 4.0 gives the verification and validation documentation for the code. Configuration control is located in Chapter 5.0. Requirement specifications are summarized in Chapter 6.0, and Chapter 7.0 gives a summary.

2.0 RADCALC FOR WINDOWS METHODOLOGY

2.1 HYDROGEN GAS GENERATION

2.1.1 Theoretical Basis

Hydrogen gas generation occurs in radioactive waste materials through two main mechanisms. One of these mechanisms, the one that is addressed in Radcalc for Windows, is the release of hydrogen through radiolysis. The other mechanism is the release of hydrogen from the oxidation of metals immersed in water, and it is not included in Radcalc for Windows.

Radiolysis is the chemical change that occurs in materials as a result of ionizing radiation. The majority of radiolysis that occurs in radioactive waste materials is due to interactions initiated by alpha particles, beta particles, and photons (gamma rays and x-rays). As ionizing radiation travels through a medium, the atoms and molecules within the trajectory of the particle or photon will absorb energy and be ionized or left in an excited state. The initiating interacting radiation creates a track of excited ions and molecules. Freed electrons can, in turn, create secondary tracks or spurs branching off from the primary track. The length of the tracks and the distance traveled by the ionizing radiation will depend upon the energy and type of radiation and the chemical and physical properties of the medium. The species resulting from the interactions will depend upon the chemical structure of the absorbing medium and will, for the most part, be the same for different types of ionizing radiation. The quantity of the species formed will depend upon the amount of radiation energy absorbed within the material, the proximity of the different species formed (which will affect the chances of species recombination), and, in some part, the chemical nature of the different components.

A chemical response initiated by ionizing radiation can cause a large number of intermediary reactions. For instance, in the radiolysis of water, Spinks and Woods (1990) identifies 16 additional major reactions that follow as a result of the initial reactions caused by ionizing radiation. The formation of intermediary species and excited molecules can lead to the production of free radicals and in some cases to the formation of a flammable gas, such as hydrogen.

The types of species produced radiolytically depend upon the chemical structure of the material through which the radiation is traveling. The major products in the radiolysis of water are:

The addition of substances such as nitrates to the water will change the chemical components produced and the quantities of these components. Some of the gases identified from the radiolysis of cation exchange resins are H_2 , CO_2 , CO , SO_2 , O_2 , and CH_4 and from the radiolysis of anion exchange resins: H_2 , CO_2 , CO , N_2 , N_2O , and NO .

In order to relate the quantity of a species produced radiolytically to the amount of energy absorbed, a term arbitrarily called the *G value* was defined (Burton 1952). The *G value* of a material is defined as the number of molecules formed or disassociated per 100 eV energy absorbed. *G values* are species and material specific; that is, $G(\text{H}_2)$ refers to the *G value* for the production of hydrogen gas and will differ for different absorbing media. *G values* are also radiation specific and depend upon the linear energy transfer (LET) of the radiation type. For instance, alpha particles have a much higher LET than beta particles and the *G value* will be correspondingly greater.

Using the *G value* concept, the production of hydrogen can be calculated by multiplying the total decay heat or energy produced over a specified period of time of radiation type *j* for radionuclide *i* by the fraction of decay heat or energy absorbed in the medium for that radiation type by the medium specific *G value* for the *j*th radiation type. Summing this product for all radiation types and radionuclides in the material and multiplying by the mass of the medium and a conversion factor will result in the quantity of hydrogen produced.

2.1.2 Hydrogen Gas Generation Calculations

The hydrogen gas volume is calculated as

$$H(t) = K \sum_{ij} G_j D_i(t) Z_{ij} \quad , \quad (2-1)$$

where:

- i* = Index for radionuclide type
- j* = Index for radiation type. Radiation types are:
 - j* = α (hereafter referred to as "heavy particle"), which are decays of heavy, charged particles, such as alpha and spontaneous fission, as well as delayed neutrons,
 - j* = β (hereafter referred to as "beta-type"), which are all electron-related radiation, such as electrons, positrons, conversion-electrons, and Auger electrons, and
 - j* = γ (hereafter referred to as "gamma"), which includes all electromagnetic radiations, such as gamma rays, x-rays, annihilation radiation, and internal bremsstrahlung.
- G* = Hydrogen *G value* for the given radiation type (molecules/100 eV)

$D_i(t)$ = Total number of disintegrations for the radionuclide over time t
 $\mathcal{E}_{ij}$ = Total energy absorbed per disintegration
 K = Conversion factor from molecules to volume for an ideal gas at 20° C and standard pressure (101.325 kPa).

For known discrete gamma radiation, the total energy absorbed is calculated as follows:

$$\mathcal{E}_{i\gamma} = \sum_k E_{i\gamma k} A_{i\gamma k} F(\rho, E_{i\gamma k}) + \overline{E'_{i\gamma}} ,$$

k = Index for each discrete gamma
 $E_{i\gamma k}$ = k th discrete gamma energy
 $A_{i\gamma k}$ = Fraction of decays exhibiting the k th gamma
 $F(\rho, E_{i\gamma k})$ = Fraction of energy absorbed in the waste matrix, as discussed in Chapter 3.0
 $\overline{E'_{i\gamma}}$ = Electromagnetic radiation not accounted for amongst the known discrete gammas, usually very low energy x-rays.

$\overline{E'_{i\gamma}}$ is calculated from

$$\overline{E'_{i\gamma}} = \overline{E_{i\gamma}} - \sum_k E_{i\gamma k} A_{i\gamma k} .$$

where $\overline{E_{i\gamma}}$ is the total average gamma radiation.

For heavy particle and beta-type radiation the total energy absorbed is simply the average recoverable decay energy for the given disintegration type per disintegration. E_{ii} , $E_{i\gamma k}$, and $A_{i\gamma k}$ data are taken from the Fusion Energy Nuclear Data Library (FENDL)/D-1.0 database discussed in Chapter 3.0.

2.2 HYDROGEN GAS GENERATION RATE

The hydrogen gas generation rate is calculated over the time that the container is sealed. It is calculated by dividing the volume of hydrogen gas produced during the seal time by the seal time duration.

2.3 TOTAL PRESSURE AND PARTIAL PRESSURE

Using van der Waals' reduced equation of state for ideal gases and assuming ideal gas conditions at constant temperature and volume, the total pressure due to the buildup of hydrogen gas is found from the original pressure times the ratio of the final total molecules to the initial total molecules. The partial pressure of the hydrogen gas is calculated from the original pressure times the ratio of the hydrogen molecules generated to the initial molecules.

2.4 DECAY HEAT

The decay heat calculated by Radcalc for Windows is conservatively assumed to be equal to the total recoverable energy. The decay heat for a given radionuclide indexed by i is calculated as follows:

$$H = K \sum_i A_i E_i .$$

H = Decay heat rate in Watts at the start of shipment (seal time)
 E_i = Total recoverable energy per disintegration of the i th nuclide in eV
 A_i = Activity in curies of the i th nuclide at the beginning of shipment
 K = Conversion factor of $5.93E-9$ W/(Ci-eV), derived from conversion factors listed in the student edition of the 72nd edition of the *Handbook of Chemistry and Physics* (Lide 1991).

The total recoverable energy for a disintegration of each nuclide is calculated in RADCALC as follows:

$$E_i = E_{\alpha} + E_{\beta} + E_{\gamma} .$$

$E_{i\alpha}$ is the average energy per decay for all heavy charged particles and delayed neutrons for the i th nuclide. $E_{i\beta}$ is the average recoverable energy per decay for beta-type radiation for the i th nuclide. $E_{i\gamma}$ is the average energy per decay for all gamma radiations for the i th nuclide. $E_{i\alpha}$, $E_{i\beta}$, and $E_{i\gamma}$ originate from the FENDL/D-1.0 database, as discussed in Chapter 3.0.

2.5 RADIOACTIVE DECAY CALCULATIONS

Given a starting inventory and a time period for decay, Radcalc for Windows will calculate the radionuclide inventory at the end of the decay time and the time-integrated disintegrations of each radionuclide during the decay time.

The decay equations can be expressed as follows:

$$\frac{dn_i}{dt} = \sum_{j=1} \alpha_{ij} n_j - \beta_i n_i ,$$

where:

i = Index for daughter radionuclides
 j = Index for parent radionuclides
 n_i = Amount of the i th radionuclide
 t = Time
 n_j = Amount of the j th parent
 α_{ij} = Decay constant for decay from radionuclide j to radionuclide i
 β_i = Decay constant for depletion of radionuclide i .

Appendix A, written by F. Schmittroth, shows a solution to the decay equation and demonstrates how it is implemented. The technique outlined in

Appendix A was adopted in Radcalc for Windows. The amount, v_i , of the i th radionuclide produced from its immediate parent is given by

$$v_i = \sum_j e^{-\beta_j t} \sum_{r=0}^{\infty} c_{jr}^{(i)} t^r . \quad (2-2)$$

The second sum represents a polynomial in t with constants $c_{jr}^{(i)}$. The method for calculating $c_{jr}^{(i)}$ is documented in Appendix A. The v_i are summed over all decay-chain branches to find the total amount, n_i , of radionuclide i .

The time-integrated disintegrations for n_i , designated as D_i , can be obtained from

$$D_i = \beta_i \int_0^t n_i(t') dt' . \quad (2-3)$$

The result, d_i , corresponding to the single decay-chain branch represented by v_i , can be calculated by inserting equation 2-2 into 2-3 above.

$$d_i = \beta_i \sum_j \sum_{r=0}^{\infty} c_{jr}^{(i)} \int_0^t t'^r e^{-\beta_j t'} dt' .$$

This can be rewritten as

$$d_i = \beta_i \sum_j \sum_{r=0}^{\infty} c_{jr}^{(i)} t^r \frac{1}{\beta_j} H_r(x_j) .$$

where the unitless variable $x_j = \beta_j t$. The function $H_r(x)$ is defined as

$$H_r(x) = \frac{1}{x^r} \int_0^x e^{-x'} x'^r dx' .$$

Radcalc for Windows uses two forms to evaluate the above integral. For $x < 1$,

$$H_r(x) = e^{-x} \sum_{n=0}^{\infty} \frac{r! x^n}{(r+n)!} .$$

For $x \geq 1$,

$$H_r(x) = \frac{r!}{x^r} - e^{-x} \sum_{n=0}^r \frac{r!}{(r-n)! x^n} .$$

As for the v_i , the d_i are summed over all decay chain branches to find the total time-integrated disintegrations of radionuclide i , designated D_i above.

2.6 TRANSPORTATION CLASSIFICATION DETERMINATIONS

Definitions, quantity calculations, and the A_1/A_2 database used in Radcalc for Windows are taken from 49 CFR Subchapter C, "Hazardous Materials Regulations." This section contains the definitions and calculations used in Radcalc for Windows.

2.6.1 Definitions

Definitions are taken from 49 CFR 173.403.

"§ 173.403 Definitions

In this subpart:

- (a) A_1 means the maximum activity of special form radioactive material permitted in a Type A package.
- (b) A_2 means the maximum activity of radioactive material, other than special form or low specific activity radioactive material, permitted in a Type A package
-
- (j) Fissile material means any material consisting of or containing one or more fissile radionuclides. Fissile radionuclides are plutonium-238, plutonium-239, plutonium-241, uranium-233 and uranium-235. Neither natural nor depleted uranium are fissile material. . . .
-
- (l) Highway route controlled quantity means a quantity within a single package which exceeds:
 - (1) 3000 times the A_1 value of the radionuclides as specified in §173.433 for special form radioactive material;
 - (2) 3000 times the A_2 value of the radionuclides as specified in §173.433 for normal form radioactive material; or
 - (3) 30,000 curies, whichever is least.
- (m) Limited quantity of radioactive material means a quantity of radioactive material not exceeding the materials package limits specified in § 173.423 and which conform with requirements specified in §173.421.
- (n) Low specific activity (LSA) material means any of the following:
 -
 - (4) Material in which the radioactivity is essentially uniformly distributed and in which the estimated average concentration of contents does not exceed:
 - (i) 0.0001 millicurie per gram of radionuclides for which the A_2 quantity is not more than .05 curie;
 - (ii) 0.005 millicurie per gram of radionuclides for which the A_2 quantity is more than .05 curie; but not more than 1 curie; or
 - (iii) 0.3 millicurie per gram of radionuclides for which the A_2 quantity is more than 1 curie.
-
- (s) Normal form radioactive material means radioactive material which has not been demonstrated to qualify as special form radioactive material.

- (t) **Package** means, for radioactive materials, the packaging together with its radioactive contents as presented for transport.
- (u) **Packaging** means, for radioactive materials, the assembly of components necessary to ensure compliance with the packaging requirements of this subpart. It may consist of one or more receptacles, absorbent materials, spacing structures, thermal insulation, radiation shielding, and devices for cooling or absorbing mechanical shocks. The conveyance, tie-down system, and auxiliary equipment may sometimes be designated as part of the packaging.
- (y) **Radioactive material** means any material having a specific activity greater than 0.002 microcuries per gram ($\mu\text{Ci/g}$) (see definition of specific activity).
- (aa) **Specific activity** of a radionuclide, means the activity of the radionuclide per unit mass of that radionuclide. The specific activity of a material in which the radionuclide is essentially uniformly distributed is the activity per unit mass of the material.
- (cc) **Type A package** means a Type A packaging together with its limited radioactive contents. A Type A package does not require competent authority approval, since its contents are limited to A_1 or A_2 .
- (dd) **Type B package** means a Type B packaging together with its radioactive contents."

2.6.2 Radioactive Material

The content of a package is classified as radioactive material if the specific activity is greater than 0.002 $\mu\text{Ci/g}$. Radcalc for Windows divides the total activity in the material by the total mass of material to evaluate this criteria.

2.6.3 Unity Fraction/Package Type Determination

The unity fraction is used to determine Type A or Type B classification. It is calculated as follows:

$$\text{Unity Fraction} = \sum_i \frac{R_i}{A}$$

where:

- i = Index for radionuclides in the material
- R_i = The activity of radionuclide i in curies
- A = The A_1 value for the radionuclide for material designated as "special" or the A_2 value for material designated as "normal."

If the unity fraction is less than or equal to 1, the payload is defined as Type A. If the unity fraction is greater than 1, the content is a Type B package.

2.6.3.1 Daughter Products in Radcalc for Windows. Radcalc for Windows uses the criteria outlined in 49 CFR 173.433(b)(2) for identifying daughter products in unity fraction calculations. That is: a single radioactive decay chain is considered to be a single radionuclide when no daughter radionuclide has a half-life either longer than ten days or longer than that of the parent radionuclide. Radcalc for Windows has identified 36 radionuclides that are usually shipped as by-products of a parent radionuclide. If the radionuclides have undergone processing and are shipped in quantities other than that produced by natural decay, then the user can input a value for the daughter. If, however, the radionuclide quantity is a product of the natural decay of a parent isotope, the user can input a 30-day or longer decay time value, and Radcalc for Windows will decay all products to their equilibrium quantities.

For instance, in the case of ^{90}Sr and ^{90}Y , the user can input a value for ^{90}Sr and input a 30-day decay time, and the program will automatically calculate the equilibrium value for ^{90}Y . If, however, ^{90}Y is to be shipped as a medical isotope, the user can input this value directly, ignoring the "daughter" label next to the radionuclide. In most instances the user should input parent radionuclides and a 30-day (or longer) decay time and allow Radcalc for Windows to bring the radionuclides into a state of equilibrium.

Table 2-1 provides a list of daughter products that Radcalc for Windows will bring into equilibrium with a 30-day (or longer) decay period.

Table 2-1. Radionuclides Identified as Daughter Products in Radcalc for Windows.*

^{47}Sc	$^{99\text{m}}\text{Tc}$	^{127}Te	$^{144\text{m}}\text{Pr}$	^{214}Pb	^{214}Po
^{69}Zn	$^{103\text{m}}\text{Rh}$	^{129}Te	^{194}Ir	^{210}Bi	^{215}Po
^{90}Y	^{106}Rh	^{132}I	^{207}Tl	^{211}Bi	^{218}Po
$^{91\text{m}}\text{Y}$	^{108}Ag	$^{137\text{m}}\text{Ba}$	^{209}Pb	^{212}Bi	^{217}At
$^{95\text{m}}\text{Nb}$	$^{113\text{m}}\text{In}$	^{140}La	^{211}Pb	^{213}Bi	^{221}Fr
^{97}Nb	^{126}Sb	^{144}Pr	^{212}Pb	^{214}Bi	^{224}Ra

*Windows is a trademark of Microsoft Corporation.

2.6.4 LSA Determination

The LSA limit for radionuclides is based on the A_2 value as follows:

$$\begin{aligned} A_2 &\leq 0.05 \text{ Ci} && \rightarrow 0.0001 \text{ mCi/g limit} \\ 0.05 &< A_2 \leq 1.0 \text{ Ci} && \rightarrow 0.005 \text{ mCi/g limit} \\ A_2 &> 1.0 \text{ Ci} && \rightarrow 0.3 \text{ mCi/g limit} \end{aligned}$$

where mCi/g is the mCi of the radionuclide per gram of the material. The material is considered to have low specific activity if

$$\sum_i \frac{S_i}{L_i} \leq 1$$

where:

- i = Index for radionuclides in the material
- S_i = mCi of radionuclide i per g of material
- L_i = LSA limit for radionuclide i as specified above.

In addition, as defined in 49 CFR 173.403(n), the radioactivity in the material must be uniformly distributed. The user should note that Type A and Type B classifications are distinct from LSA determination. An LSA material may also be a Type B quantity.

2.6.5 Limited Quantity Determination

The material is considered limited quantity if the following criteria are met:

Solid: Unity fraction ≤ 0.001 (contents $\leq 10^{-3} A_1$ or A_2)

Liquid: Unity fraction ≤ 0.0001 (contents $\leq 10^{-4} A_2$)

Tritiated water:

Total specific activity < 0.1 Ci/L and total curies ≤ 1000 Ci

or

Total specific activity of 0.1 to 1.0 Ci/L and total curies ≤ 100 Ci

or

Total specific activity of > 1.0 Ci/L and total curies ≤ 1 Ci.

The unity fraction calculation is discussed in Section 2.6.3. Total specific activity is calculated by dividing the total activity in the material by the volume of the material. If the material consists of tritiated water and other radionuclides the sum of the fractions must be less than or equal to 1.

2.6.6 Highway Route Controlled Quantity Determination

A package contains a highway route controlled quantity if the quantity within the package exceeds 3,000 times the A_1 or A_2 value or 30,000 Ci, whichever is least. In the case of mixed radionuclides, a unity fraction is calculated by summing the ratios of the activity of each radionuclide to 3,000 times the A_1 or A_2 value or 30,000 Ci, whichever is least.

2.6.7 Fissile Excepted Determination

Radioactive material is considered fissile excepted under 49 CFR 173.453 if the total mass of the following isotopes is less than or equal to 15 g: ^{238}Pu , ^{239}Pu , ^{241}Pu , ^{233}U , and ^{235}U . The other fissile excepted criteria listed in 49 CFR 173.453 are not applied in Radcalc for Windows.

2.7 UNIT CONVERSIONS

The user may input quantities in English units (e.g., inches, feet, pounds) or in units in the Systeme International (e.g., centimeters, meters, grams). Radcalc for Windows will display the input quantities in terms of the

units used when entered, as well as in terms of centimeters and grams, which are the units used internally for the calculations. All unit conversion factors and physical constants; e.g., Avogadro's number, are standard and were taken from the student edition of the 72nd edition of the *Handbook of Chemistry and Physics* (Lide 1991).

2.8 PRIMARY RADCALC CALCULATION ROUTINES

ExecuteMain (execute.cpp)

When the user selects the "calculate" button, the program calls subroutine ExecuteMain found in source file execute.cpp. ExecuteMain first performs some variable initialization, including the conversion of user input quantities to units convenient for use in the calculations. ExecuteMain then calls subroutine decayit1 for the decay calculation up until seal time and calc1 to calculate quantities relevant at the beginning of shipment. If the user has specified time of the container sealed, ExecuteMain then calls decayit2 for the decay calculation while the container is sealed and calc2 to calculate quantities relevant at the end of the shipment. If, on the other hand, the user has specified a target percent hydrogen, ExecuteMain will call the subroutine iterate.

iterate (execute.cpp)

When the user specifies a target hydrogen percent, iterate will make a series of iterations to find the seal time required to reach or come close to the target percent specified. The volume required to reach the specified percent is first calculated. For the first try, iterate chooses five years. Extrapolation is used for each successive guess based on up to two previous results. The iteration stops without errors when (1) the time to the target volume will be less than one hour, (2) the time to the target volume will be greater than 36,500 days, (3) ten iterations have been made, or (4) the result is found for a volume between 95 and 100% of the target volume.

decayit1 (decayit.cpp)

The decay calculations for the time period before the container is sealed are conducted by decayit1. Decayit1 calls the FORTRAN subroutine decay2, supplying conversions of the data, as necessary, before and after the call. Decayit1 returns the radionuclide inventory at the start of seal time.

decayit2 (decayit.cpp)

The decay calculations for the time period during which the container is sealed are conducted by decayit2. Decayit2 calls the FORTRAN subroutine decay2, supplying conversion of the data, as necessary, before and after the call. Decayit2 returns the radionuclide inventory at the end of seal time and the total number of disintegrations for each radionuclide during seal time.

calculate1 (calc.cpp)

Quantities relevant at the beginning of shipment (seal time) are calculated by calculate1. These quantities are:

- Decay heat
- Unity fraction for type determination
- Type determination
- Unity fraction for LSA determination
- LSA determination
- Fissile mass for fissile excepted determination
- Fissile excepted determination
- Limited quantity determination
- Highway route controlled quantity determination
- Radioactivity determination.

calculate2 (calc.cpp)

Quantities relevant at the end of shipment (end of seal time) are calculated by calculate2. These quantities are:

- Hydrogen volume generated
- Percent hydrogen in the void volume
- Partial pressure of hydrogen
- Total pressure of hydrogen and air
- Total hydrogen generation rate (total hydrogen volume divided by total seal time).

DECAY2 (decay2.for)

This routine receives a list of initial radionuclides in terms of initial curies and converts to gram-atoms. It then calls DKSolv, which returns a list of final radionuclides, final gram-atoms, and final disintegrations for each radionuclide. DECAY2 converts the gram-atoms into curies before returning to the calling routine (decayit1 or decayit2).

Disin (disin.for)

Calculates number of disintegrations for each radionuclide.

Evaln (evaln.for)

Calculates amount of each radionuclide in terms of gram-atoms.

3.0 DATABASES AND INPUT PARAMETERS USED IN RADCALC FOR WINDOWS

Radcalc for Windows uses databases for hydrogen gas and heat generation calculations and for transportation classification determinations. The following sections discuss the databases and document their origins.

3.1 DATABASES AND INPUT PARAMETERS USED FOR HYDROGEN GAS GENERATION AND HEAT DECAY

The volume of generated hydrogen gas is calculated by summing the product of decay energy, absorption fraction, and G value over all radionuclides present and all decay types. Radcalc for Windows uses radionuclide information, calculated gamma absorption fractions for selected container types, and G values to complete these calculations. Decay heat is also dependent upon radionuclide information.

3.1.1 Radionuclide Databases

Radionuclide information for hydrogen gas generation and decay heat calculations is taken from the FENDL/D-1.0⁴ database. Decay calculations use the Oak Ridge Isotope Generation and Depletion Code (ORIGEN)2⁵ database.

3.1.1.1 FENDL/D-1.0 Database. Radcalc for Windows utilizes the FENDL/D-1.0 database. The FENDL/D-1.0 database is the Evaluated Nuclear Data File (ENDF)/B-VI decay database library supplemented by experimental data from the Evaluated Nuclear Data Structure Data File (ENDSDF). See Appendix B for more information on FENDL/D-1.0. The required data was extracted from FENDL using a FORTRAN code and was reformatted for use in Radcalc for Windows. The following is a list of radionuclide parameters taken from FENDL/D-1.0 and the values they are used to calculate.

Radionuclide half-lives are used in calculating specific activity, which is used to determine LSA and fissile excepted classifications.

Average heavy particle, beta-type radiation, and gamma radiation energies per disintegration are used in decay heat and hydrogen gas generation calculations.

Discrete gamma energies and abundances are used in hydrogen gas generation calculations.

3.1.1.2 ORIGEN2 Database. Radcalc for Windows uses the ORIGEN2 database for decay calculations. ORIGEN2 is managed and distributed by Oak Ridge National Laboratory and is widely accepted and used in national laboratories and the nuclear industry. The decay algorithms calculate the activity of the user-specified source and daughter products over a specified period of time and the total number of disintegrations accumulated over this same time interval for each radionuclide. Parameters relevant to these calculations include atomic mass, atomic number, and state. These parameters are used for radionuclide identification and conversions. The decay constant and the branching ratios for decay modes are also used in the decay algorithms.

⁴ FENDL/D Version 1, January 1992, is a decay data library for fusion (and other) applications. Summary documentation by A. B. Pashchenko. Index No. IAEA-NDS-167 in Index to the IAEA-NDS-Documentation Series.

⁵ Croff, A. G., 1980, A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, ORNL-5621, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3.1.1.3 FENDL/D-1.0 Verification. The data extracted from FENDL/D-1.0 and used by Radcalc for Windows were checked against the ORIGEN2 database by comparing recoverable energy. The total recoverable energy for a disintegration of each radionuclide is calculated in Radcalc for Windows as follows:

$$E_{\text{total}} = E_{\alpha} + E_{\beta} + E_{\gamma}$$

E_{α} is the average energy per decay for all heavy particles. E_{β} is the average recoverable energy per decay for all beta-type radiation. E_{γ} is the average energy per decay for all gamma radiations. For more detailed definitions of E_{α} , E_{β} , and E_{γ} , see Section 2.1.2. E_{α} , E_{β} , and E_{γ} values originate from the FENDL/D-1.0 database.

The total recoverable energy per disintegration for each radionuclide was calculated using the values found in FENDL/D-1.0 and the results compared to those reported in the ORIGEN2 decay library. Those cases with greater than 20% difference were also checked against Browne and Firestone's *Table of Radioactive Isotopes* (Browne and Firestone 1986). In most of these cases, the FENDL numbers agreed with Browne and Firestone, and the energy values were not changed. Those that agreed with neither ORIGEN2 nor Browne and Firestone (1986) are listed in Table 3-1. The radionuclides listed in Table 3-1 rarely occur, and the values from the FENDL database were used without alteration. However, the average beta energy for I-133 (not shown in Table 3-1) was found to be erroneous in the FENDL database and was replaced by the average beta energy reported in Browne and Firestone (410.5 keV).

Table 3-1. FENDL Radionuclides With Total Recoverable Energies Differing From ORIGEN2 and Browne and Firestone.*

Radionuclide	Recoverable energy		Ratio of ORIGEN2/ FENDL values	Decay type of concern	Energy from decay type	
	FENDL	ORIGEN2			FENDL	Browne and Firestone
^{58m} Co	5.23 MeV	24.7 keV	212	γ	5.2 MeV	2 keV
⁶⁷ Cu	6.08 MeV	271 keV	22	γ	5.9 MeV	115 keV
¹⁰³ Pd	19.5 keV	64.5 keV	0.3	β ⁻	5 keV	59 keV
¹³¹ Ba	1.06 MeV	515 keV	2	γ	1.02 MeV	458 keV
¹³⁹ Ce	687 keV	192 keV	3.6	γ	613 keV	160 keV
¹⁹¹ Os	125 keV	245 keV	0.5	γ	40 keV	169 keV
²²⁸ Ra	9.4 keV	13 keV	0.7	β ⁻	8.93 keV	No Data

*Browne, E., and R. B. Firestone, 1986, *Table of Radioactive Isotopes*, John Wiley & Sons, Inc., New York, New York.

β⁻ = beta.

γ = gamma.

FENDL = Fusion Energy Nuclear Data Library.

3.1.2 Gamma Absorption Fraction Input Parameters

Radcalc for Windows uses the total energy emitted by heavy particle and beta-type decay in calculating the volume of hydrogen produced. However, only a percent of gamma energy will be absorbed in the package and waste. The original spreadsheet (Flaherty et al. 1986) developed to calculate hydrogen gas generation uses fitted curves for four container types to calculate the absorbed gamma dose in the waste material. The four container types are a 55-gallon drum, a 4x4 liner, a 5x5 liner, and a 6x6 liner. The absorbed gamma dose is a function of energy, waste density, material type, and geometry. The spreadsheet uses curve fits for each of these containers for densities ranging from 0.6 to 2.0 g/cm³ and energies ranging from 0.4 to 2.0 MeV. The material inside the container is assumed to be water. The data for these fits were generated using the QAD-FN computer code (Flaherty et al. 1986).

For use in Radcalc for Windows, these same four curve fits have been recalculated using the Monte Carlo N-Particle (MCNP) transport code (Breisemeister 1993, Carter 1994). Along with the four original containers included in the Radcalc spreadsheet, ten additional containers have been added. The new containers are used in the DOE complex for the transportation of radioactive waste materials.

3.1.2.1 Calculation of Absorbed Gamma Dose. The original spreadsheet calculates the fraction of gamma energy absorbed in the waste material, which is assumed to be water, as a function of energy, density, and geometry. An independent fit is used for each individual container geometry. Each of these fits is a function of density and energy.

The fit is of the form:

$$F(\rho, e) = a_1 \rho e + a_2 \rho \sqrt{e} + a_3 \sqrt{\rho} e + a_4 \rho \\ + a_5 \sqrt{\rho} e + a_6 e + a_7 \sqrt{\rho} + a_8 \sqrt{e} + a_9 \quad (3-1)$$

where $F(\rho, e)$ is the fraction of energy absorbed, ρ is density in g/cm³, and e is the emitted energy in MeV.

For Radcalc for Windows new data were generated using a volumetric source of unity source strength (1 Bq/s) for each container. MCNP runs were made for energies varying from 0.4 to 5.0 MeV and densities ranging from 0.6 to 3.0 g/cm³. A UNIX⁶ version of Mathematica⁷ (Wolfram Research, Inc. 1993) was used to perform least-squares fits from the MCNP data generated. The resulting coefficients for the 14 different geometries are contained in an array in the computer code. When calculating hydrogen gas generation, Radcalc for Windows calculates the gamma absorption fraction for the corresponding density and discrete gamma energy.

⁶UNIX is a trademark of Novell, Inc.

⁷Mathematica is a trademark of Wolfram Research, Inc.

3.1.2.2 Container Geometry. The four original container geometries are reproduced with the same dimensions (Flaherty et al. 1986), and the 55-gal drum is reproduced with additional, more exact dimensions. The new container geometries are based on dimensions reported in their respective safety analysis reports for packaging (SARP). The model for each container has its interior volume completely filled with water, representing an upper bound in the calculation of the absorption fraction. Both English and metric units are given for each container's dimensions. The first set of numbers given represents the original units used for the container in the document referenced for dimensions. The interior and exterior dimensions and interior volume of each container are given in Table 3-2.

Table 3-2. Dimensions of Modeled Shipping Containers.*

Container	Geometry	Inside modeled dimensions (diameter x height)	Outside modeled dimensions	Internal volume
55-gal drum	Cylinder	22.5 in. x 33.25 in. (57.2 cm x 84.46 cm)	22.6 in. x 33.41 in. (57.40 cm x 84.86 cm)	7.65 ft ³ (2.17E5 cm ³)
4x4 liner	Cylinder	120 cm x 120 cm (47.24 in. x 47.24 in.)	NA	47.9 ft ³ (1.36E6 cm ³)
5x5 liner	Cylinder	140 cm x 140 cm (55.12 in. x 55.12 in.)	NA	76.1 ft ³ (2.16E6 cm ³)
6x6 liner	Cylinder	180 cm x 180 cm (70.87 in. x 70.87 in.)	NA	162 ft ³ (4.58E6 cm ³)
30-gal drum	Cylinder	18 in. x 28 in. (45.72 cm x 71.12 cm)	18.1 in. x 28.1 in. (45.97 cm x 71.37 cm)	4.12 ft ³ (1.17E5 cm ³)
85-gal drum	Cylinder	26 in. x 37.9 in. (66.04 cm x 96.27 cm)	26.13 in. x 38.03 in. (66.37 cm x 96.60 cm)	11.6 ft ³ (3.30E5 cm ³)
Doorstop sample carrier	Cylinder	4.5 in. x 5.625 in. (11.43 cm x 14.29 cm)	6.38 in. x 11.38 in. (16.21 cm x 28.91 cm)	0.0518 ft ³ (1,470 cm ³)
Ion exchange column	Cylinder	17.5 in. x 69 in. (44.45 cm x 175.3 cm)	18 in. x 69.5 in. (45.72 cm x 176.5 cm)	9.60 ft ³ (2.72E5 cm ³)
LR-56	Cylinder	140 cm x 320 cm (55.12 in. x 126.0 in.)	338 cm x 518 cm (133.1 in. x 203.9 in.)	174 ft ³ (4.93E6 cm ³)
Neutralized current acid waste	Cylinder	3.375 in. x 40.2 in. (8.573 cm x 102.1 cm)	3.75 in. x 48.88 in. (9.53 cm x 124.2 cm)	0.208 ft ³ (5,890 cm ³)
Onsite transfer cask	Cylinder	2.375 in. x 42.75 in. (6.033 cm x 108.59 cm)	5.505 in. x 45.87 in. (13.98 cm x 116.51 cm)	0.110 ft ³ (3,104 cm ³)
PAS-1	Cylinder	18 in. x 21.88 in. (45.72 cm x 55.58 cm)	32.5 in. x 40 in. (82.55 cm x 101.6 cm)	3.22 ft ³ (91,300 cm ³)
Sample Pig carrier	Cylinder	2.06 in. x 4.875 in. (5.23 cm x 12.38 cm)	6.71 in. x 9.275 in. (17.04 cm x 23.56 cm)	9.40E-3 ft ³ (266 cm ³)
Single pass fuel cask	Box	35.25 in. x 37.50 in. x 46.625 in. (89.54 cm x 95.25 cm x 118.4 cm)	57 in. x 59.25 in. x 69 in. (144.8 cm x 150.5 cm x 175.3 cm)	35.7 ft ³ (1.01E6 cm ³)

*The first dimensions shown for a container are in the original units of the referenced work.

3.1.2.3 55-Gal Drum. Two different cylinder sizes were used in the analysis of the 55-gal drum. The first uses the same size source volume as the original QAD-FN calculations, with a diameter of 60 cm (23.62 in.) and a height of 90 cm (35.43 in.). The second model consists of a source volume with a diameter of 22.5 in. (114.4 cm) and a height of 33.25 in. (84.46 cm) (Kelly 1994). The source is encapsulated in 14 gauge steel (U.S. Standard, 0.0781 in./0.1984 cm) on top and bottom, and 18 gauge steel (U.S. Standard, 0.0500 in./0.1270 cm) on the side.

3.1.2.4 4x4 Liner. The model for the 4x4 liner is based on the dimensions used in creating the fit in the original spreadsheet. It consists only of the source volume, 120 cm (47.24 in.) in diameter and 120 cm (47.24 in.) tall.

3.1.2.5 5x5 Liner. The model for the 5x5 liner is based on the dimensions used in creating the fit in the original spreadsheet. It consists only of the source volume, 140 cm (55.12 in.) in diameter and 140 cm (55.12 in.) tall.

3.1.2.6 6x6 Liner. The model for the 6x6 liner is based on the dimensions used in creating the fit in the original spreadsheet. It consists only of the source volume, 180 cm (70.87 in.) in diameter and 180 cm (70.87 in.) tall.

3.1.2.7 30-Gal Drum. The model for the 30-gal drum is based on the DOT Specification 7A Type A Packaging (Kelly 1994). The interior of the 30-gal drum is modeled as 18 in. (45.72 cm) in diameter with a height of 28 in. (71.12 cm). The source volume is encapsulated in 18 gauge steel (U.S. Standard, 0.0500 in./0.1270 cm).

3.1.2.8 85-Gal Drum. The model for the 85-gal drum is also based on DOT 7A Type A Packaging Specification (Kelly 1994). The interior of the 85-gal drum is modeled with a diameter of 26 in. (66.04 cm) and a height of 37.9 in. (96.27 cm). The source volume is encapsulated in 16 gauge steel (U.S. Standard, 0.0625 in./0.1588 cm).

3.1.2.9 Doorstop Sample Carrier. The model for the doorstop sample carrier is based on the doorstop sample carrier SARP (WHC 1993b) and WHC drawing H-2-32514 (WHC 1982). The doorstop interior has a diameter of 4.5 in. (11.43 cm) and a height of 5.625 in. (14.29 cm). The outside dimensions are 6.38-in. (16.21-cm) diameter and 11.38-in. (28.91-cm) height. The shielding material is steel.

3.1.2.10 Ion Exchange Column. The model for the ion exchange column is based on the Big Bertha SARP (WHC 1991). The Big Bertha is the package currently used to transport ion exchange columns on the Hanford Site, Richland, Washington. The ion exchange column is modeled as a 69.5-in.- (176.5-cm-) long (exterior) section of 18-in. schedule 10 pipe (18-in./45.72-cm outside diameter [OD]) capped on each end with a thickness equal to that of the sides (0.25 in./0.635 cm). The total interior length is 69 in. (175.3 cm).

3.1.2.11 LR-56. The model for the LR-56 is based on the *Packaging Design Criteria for the LR-56 Cask System* (WHC 1994a). The interior of the LR-56 is a cylinder 320 cm (126.0 in.) long with a diameter of 140 cm (55.12 in.). The primary containment vessel is made from 8-mm- (0.315-in.-) thick steel. There is a 20-mm (0.787-in.) air gap and a 6-mm (0.236-in.) steel secondary confinement vessel. The shielding consists of an additional 35 mm (1.38 in.)

of lead and 30 mm (1.18 in.) of steel. There are also layers of wood and a final steel outer casing, which are left out of the model, as they would have negligible effect in the calculation.

3.1.2.12 Neutralized Current Acid Waste (NCAW) Cask. The model for NCAW cask is based on the SARP for the NCAW Packaging System (Khojandi 1992). The inner dimensions of the NCAW cask are a 3.375-in. (8.573-cm) diameter and a 40.2-in. (102.1-cm) height. The side shielding consists of a 3.75-in.- (9.53-cm-) OD pipe, which is 0.375 in. (0.953 cm) thick and is inside a 16-in. schedule 40 pipe (16-in./40.64-cm OD) with the annulus filled with lead. The top of the model uses a 2.68-in. (6.81-cm) steel plug and the bottom a 6-in. (15.24-cm) steel plug.

3.1.2.13 Onsite Transfer Cask (OTC). The model for the OTC is based on the SARP for the OTC (WHC 1992a). The inner dimensions of the OTC are a 2.375-in. (6.0325-cm) diameter and a 42.75-in. (108.59-cm) height. The radial shielding consists of a 0.065 in. (0.165 cm) steel shell, 1 in. (2.54 cm) of lead, and another 0.5 in. (1.27 cm) of steel. The bottom shielding consists of 0.065 in. (0.165 cm) of steel, 1.55 in. (3.94 cm) of lead, and another 0.5 in. (1.27 cm) of steel. The top is capped by 1 in. (2.54 cm) of steel.

3.1.2.14 PAS-1 Cask. The model for the PAS-1 cask is based on the *Packaging Design Criteria for PAS-1 Cask* (WHC 1993a). The interior of the PAS-1 cask has a height of 21.88 in. (55.58 cm) and a diameter of 18 in. (45.72 cm). The OD is 32.5 in. (82.55 cm) and the height is 40 in. (101.6 cm). There is 5.1 in. (12.95 cm) of lead shielding in the model. A layer of steel surrounding the interior volume is 1.5 in. (3.81 cm) thick on the top, 1 in. (2.54 cm) thick on the bottom, and 2.15 in. (5.46 cm) thick on the side. The steel on the side was calculated from the assumptions for the inside diameter (ID) and OD of the cask and the 5.1-in. (12.95-cm) lead shielding.

3.1.2.15 Sample Pig Carrier. The model for the sample Pig carrier came from the sample Pig SARP (WHC 1992b). The ID is 2.06 in. (5.23 cm), and the interior length is 4.875 in. (12.383 cm). The inner cavity is surrounded by 0.125-in. (0.318-cm) steel and 1.95-in. (4.95-cm) lead. There is also an outer steel cover 0.25 in. (0.635 cm) thick on the side and 0.125 in. (0.318 cm) thick on top and bottom.

3.1.2.16 Single Pass Fuel Cask. The model for the single pass fuel cask is based on the SARP for the cask (WHC 1993c). The single pass fuel cask is a box with outside dimensions of 57 in. (144.8 cm) x 59.25 in. (150.5 cm) x 69 in. (175.3 cm). The inner cavity is encased on the sides and bottom by a $\frac{1}{4}$ -in. (0.952-cm) steel inner shell, 10 in. (25.4 cm) of lead, and a $\frac{1}{2}$ -in. (1.27-cm) steel outer shell. The lid is made of 10 in. (25.4 cm) of lead encased in $\frac{3}{4}$ -in. (1.905-cm) steel. The outermost layer of steel was left out of the model, as it would not have a significant effect on the calculation.

3.1.2.17 Results of Gamma Absorption Fraction Analysis. The gamma absorption fraction analysis was originally presented in WHC-SD-TP-RPT-014 (WHC 1994b), and data for all figures and tables can be found in that document. The results presented in that work are discussed in the following text, and the corresponding figures and tables are available in Appendix C. Table 3-3 provides an index to the figures and tables found in Appendix C.

There are two 55-gal drum MCNP models. The first model, referred to as the simple model, is identical to the model used in the original QAD-FN work (Flaherty et al. 1986). In Appendix C, Figure C-1 shows a comparison of the data and fit generated in the original work to a parallel calculation using MCNP. The MCNP simple model gives up to a 5% higher absorption fraction for higher energies than QAD-FN, and up to 8% lower absorption fraction for lower energies. In general, however, the fits are similar enough so that the accuracy of absorbed dose calculations in Radcalc will not be altered. The data point at 1.5 g/cm³, 2.0 MeV for the QAD-FN is apparently reported incorrectly in Flaherty et al. (1986).

Figure C-2 is a comparison of the MCNP simple model and the more detailed model. It shows the effects of modeling a smaller volume with shielding. The more detailed model gives absorption fractions that are up to 3% lower than the MCNP simple model, due to the reduced volume.

Figure C-3 shows the difference between a curve fit to data points from densities up to 2.0 g/cm³ and a curve fit to data points for densities up to 3.0 g/cm³. The figure shows data fits for three different energy levels. There is less than 1% difference in the range of 0.6 to 2.0 g/cm³ between the two curves. When the fit created from data up to 2.0 g/cm³ is extrapolated to 3.0 g/cm³, there is a difference of as much as 4% between it and the line generated from actual MCNP data for densities between 2.0 and 3.0 g/cm³. The curve fit to actual data points up to 3.0 g/cm³ is considered to be more accurate than the extrapolated curve and will be used in Radcalc for Windows.

Figure C-4 shows a comparison of the original spreadsheet fit and final detailed MCNP fits for three different energies. The discrepancy between the two models is greatest at low energies and low densities where the MCNP fit is lower by up to 6%.

For the 55-gal drum, fits were developed for energies between 0.4 and 2.0 MeV and energies between 2.0 and 5.0 MeV. Figure C-5 is a graph of the absorption fractions versus energy. It shows the final fit for densities between 0.6 and 3.0 g/cm³ and energies between 0.4 and 5.0 MeV. Table C-1 gives the original and final coefficients for the respective fits. The coefficients are the coefficients in the fit in the form of equation 3-3. The coefficients were developed using a least-squares fitting algorithm in Mathematica. Although there appears to be a large discrepancy in the fitting coefficients between those used in the original spreadsheet and those developed here, the fits themselves are quite good, as can be seen in Figures C-4 and C-5.

Figures C-6 through C-21 show final fits and comparisons for all other containers. Each container has a graph which shows the final fit from 0.6 to 3.0 g/cm³ and 0.4 to 5.0 MeV. For the containers already included in the original spreadsheet, graphs have been developed comparing the original fits to the final fits for densities between 0.6 and 2.0 g/cm³ and energies between 0.4 and 5.0 MeV. Table 3-3 lists the appropriate graphs and tables for each container. Tables C-1 through C-14 show the coefficients used for the fits. These coefficients are stored in an array in Radcalc for Windows and are accessed whenever absorption fractions are calculated.

Table 3-3. Index to Tables and Graphs for Each Geometry.

Container	Table of coefficients in fits	Graph of final fits	Graph comparing original and final fits
55-gal drum	Table C-1	Figure C-5	Figure C-4
4x4 liner	Table C-2	Figure C-7	Figure C-6
5x5 liner	Table C-3	Figure C-9	Figure C-8
6x6 liner	Table C-4	Figure C-11	Figure C-10
30-gal drum	Table C-5	Figure C-12	NA
85-gal drum	Table C-6	Figure C-13	NA
Doorstop sample carrier	Table C-7	Figure C-14	NA
Ion exchange column	Table C-8	Figure C-15	NA
LR-56	Table C-9	Figure C-16	NA
Neutralized current acid waste	Table C-10	Figure C-17	NA
Onsite transfer cask	Table C-11	Figure C-18	NA
PAS-1 cask	Table C-12	Figure C-19	NA
Sample Pig carrier	Table C-13	Figure C-20	NA
Single pass fuel cask	Table C-14	Figure C-21	NA

3.1.3 G Value Data

The G value is defined as the number of molecules formed or disassociated in a medium per 100 eV of absorbed energy (molecules/100 eV). G values were extensively researched and a list of published conservative G values is presented in document WHC-SD-TP-RPT-014 (WHC 1994b). Radcalc for Windows uses a condensed version of that list. When maximum G values are cited for a material, the G value is used for all radiation types. When G values are missing for a radiation type, they are calculated on the basis of $G_{\beta} = G_{\gamma}$ and $G_{\alpha} = 4 * G_{\gamma}$. This is in keeping with G value information given in *An Introduction to Radiation Chemistry* (Spinks and Woods 1990).

The user can indicate a weight or fraction for selected materials and Radcalc for Windows will calculate a weighted-average G alpha, G beta, and G gamma. Alternatively, the user can input G values of their own choosing.

3.2 TRANSPORTATION DATA

Radcalc for Windows uses A_1 and A_2 values to determine Type A, Type B, limited quantity, low specific activity, and highway route controlled quantity classifications. The A_1 and A_2 values are taken from 49 CFR 173.435 table of A_1 and A_2 values for radionuclides. When A_1 and A_2 values were not available, they were calculated using the methodology outlined in 49 CFR 173.433. All gases are assumed to be uncompressed and the corresponding A_2 value for uncompressed gas was used. The data was extensively checked to verify input values. All limits and definitions used in the transportation algorithms are taken from 49 CFR Subchapter C.

4.0 VERIFICATION AND VALIDATION

4.1 SOFTWARE TEST PLAN: VERIFICATION CASES

Radcalc for Windows is accompanied by verification examples for benchmark problems to be run on a system following installation. The verification problems are available in the verify subdirectory of the floppy disk containing the Radcalc for Windows executable files. The test files are automatically installed in the verify subdirectory following successful completion of the Radcalc for Windows setup routine. The verification documentation of the benchmark problems is given in Appendix D. These verification problems test the various models incorporated in Radcalc for Windows and ensure the proper installation of Radcalc for Windows on a computer system. Following installation of Radcalc for Windows, running the verification examples should yield identical results as those shown in Appendix D, thus verifying the installation. See the User's Guide for more information on running the test files.

4.2 RADCALC FOR WINDOWS VALIDATION

Test cases were designed to exercise the various routines and models programmed into Radcalc for Windows. These test cases are divided into the three components incorporated in the code: (I) hydrogen gas generation; (II) decay calculations; and (III) transportation classification determinations. In addition, section IV tests other aspects of the code, such as unit conversions and time algorithms. The tests were constructed to verify the performance of Radcalc for Windows. Table 4-1 lists the test cases with a brief description of each case and the method of verification and results. Test cases are presented in Appendix E. Each test case includes (1) a discussion of the case and conclusion, (2) independent check results, and (3) Radcalc for Windows results.

Table 4-1. Radcalc for Windows Validation Cases. (3 sheets total)

Case	Description	Method of validation	Results
I	Hydrogen gas generation		
A	Comparisons to Radcalc spreadsheet		
1	55-gal drum--dewatered resin	Radcalc spreadsheet	OK
2	55-Gal drum--solidified concentrates	Radcalc spreadsheet	OK
3	55-gal drum--cartridge filter	Radcalc spreadsheet Analytical Resources, Inc.	OK OK
4	4x4 liner--dewatered resin	Radcalc spreadsheet	OK
5	4x4 liner--solidified concentrates	Radcalc spreadsheet Analytical Resources, Inc.	OK OK
6	4x4 liner--cartridge filter	Radcalc spreadsheet	OK
7	5x5 liner--dewatered resin	Radcalc spreadsheet Analytical Resources, Inc.	OK OK
8	5x5 liner--solidified concentrates	Radcalc spreadsheet	OK
9	5x5 liner--cartridge filter	Radcalc spreadsheet	OK
10	6x6 liner--dewatered resin	Radcalc spreadsheet	OK
11	6x6 liner--solidified concentrates	Radcalc spreadsheet	OK
12	6x5 liner--cartridge filter	Radcalc spreadsheet	OK
B	Gamma absorption fractions for various container types		
1	30-gal drum	Excel spreadsheet	OK
2	Single pass fuel cask	Excel spreadsheet	OK
3	Sample Pig carrier	Excel spreadsheet	OK
4	LR-56 container	Excel spreadsheet	OK
C	Use of G values		
1	G values selected from Radcalc's database, using a single absorbing material and a beta/gamma source	Excel spreadsheet	OK
2	G values selected from Radcalc's database, using two absorbing materials and an alpha source	Excel spreadsheet	OK
3	G values entered directly, with all G values equal	Excel spreadsheet	OK
4	G values entered directly, using only a G-beta value	Excel spreadsheet	OK
5	G values entered directly, using only G-beta and G-gamma values	Excel spreadsheet	OK
D	Percent hydrogen		
1	Percent hydrogen using direct entry of interstitial void volume	Excel spreadsheet	OK
2	Percent hydrogen using a calculation of interstitial void volume	Excel spreadsheet	OK

Table 4-1. Radcalc for Windows Validation Cases. (3 sheets total)

Case	Description	Method of validation	Results
E	Hydrogen generation rate	Excel spreadsheet	OK
II	Decay algorithms		
A	Activity as a function of time		
	1 Simple decay	Excel spreadsheet	OK
	2 Parent-daughter decay	Excel spreadsheet	OK
	3 Complex decay chain	FORTTRAN program	OK
B	Integrated disintegrations over time		
	1 Simple decay	Excel spreadsheet	OK
	2 Parent-daughter decay	Excel spreadsheet	OK
	3 Complex decay chain	FORTTRAN program	OK
IIIA	Transportation calculations		
	1 Type classification for a normal form material	Excel spreadsheet	OK
	2 Type classification for a special form material	Excel spreadsheet	OK
	3 Limited quantity classification for a special form material	Excel spreadsheet	OK
	4 Limited quantity classification for a normal form material	Excel spreadsheet	OK
	5 Limited quantity classification for a liquid form material	Excel spreadsheet	OK
	6 Limited quantity classification for tritiated water with a low specific activity (< 0.1 Ci/L)	Excel spreadsheet	OK
	7 Limited quantity classification for tritiated water with an intermediate specific activity (≥ 0.1 Ci/L and ≤ 1.0 Ci/L)	Excel spreadsheet	OK
	8 Limited quantity classification for tritiated water with a high specific activity (> 1.0 Ci/L)	Excel spreadsheet	OK
IIIA	9 Limited quantity classification for tritiated water containing other radionuclides	Excel spreadsheet	OK
	10 Low specific activity classification for a Type A package with low A_2 values (≤ 0.05 Ci)	Excel spreadsheet	OK
	11 Low specific activity classification for a Type B package with intermediate A_2 values (> 0.05 Ci and ≤ 1.0 Ci)	Excel spreadsheet	OK
	12 Low specific activity classification for a Type B package with high A_2 values (> 1.0 Ci)	Excel spreadsheet	OK
	13 Low specific activity classification for a Type A package with mixed A_2 values	Excel spreadsheet	OK
	14 HRCQ classification for a package with a unity fraction $> 3,000$	Excel spreadsheet	OK
	15 HRCQ classification for a package with a total activity $> 30,000$ Ci	Excel spreadsheet	OK

Table 4-1. Radcalc for Windows Validation Cases. (3 sheets total)

Case	Description	Method of validation	Results
16	HRCQ classification for a package with a unity fraction = 3,000 and an activity = 30,000 Ci	Excel spreadsheet	OK
17	Fissile excepted classification	Excel spreadsheet	OK
18	Radioactive material classification	Excel spreadsheet	OK
IV	Other Radcalc features		
A	Unit conversion		
1	Feet/pounds to centimeters/grams	Hand calculations	OK
2	Inches/pounds to centimeters/grams	Hand calculations	OK
3	Meters/kilograms to centimeters/grams	Hand calculations	OK
4	Becquerels to curies	Comparison of Radcalc outputs	OK
5	Container information dialog box unit conversions	Hand calculations	OK
B	Target percent specified		
1	Target percent reached	Comparison of Radcalc outputs	OK
2	Target percent not reached	Comparison of Radcalc outputs	OK
C	Dating routine		
1	Length of month	Hand calculations	OK
2	Leap years	Excel spreadsheet	OK
3	Calculation of end date given start date and time interval	Excel spreadsheet	OK
D	1 Bulk density	Excel spreadsheet	OK
E	1 Heat generation	Excel spreadsheet	OK
F	Pressure		
1	Partial pressure of hydrogen	Excel spreadsheet	OK
2	Total pressure	Excel spreadsheet	OK

HRCQ = Highway route controlled quantity.

5.0 CONFIGURATION CONTROL

Radcalc for Windows, Version 1.0, was developed and is maintained by Packaging Engineering, Transportation and Packaging, WHC, Richland, Washington. Packaging Engineering provides technical support, software maintenance, and software updates for Radcalc for Windows. The Packaging Engineering code custodian is responsible for initiating and completing all changes to Radcalc for Windows. The code custodian is also responsible for

distributing new versions of Radcalc for Windows and for maintaining Radcalc for Windows files and records. Information and support for Radcalc for Windows is available by calling 509-376-0610 or 509-372-0703. Corrections and suggestions for Radcalc for Windows are welcomed.

5.1 CONFIGURATION MANAGEMENT PLAN

The following steps are recommended for software changes or identified problems.

1. Identify the changes that are requested or the problem in the program. Submit the change or problem to the code custodian in Packaging Engineering on the form provided in Appendix F or in writing. The code custodian will keep copies of the submitted requests and a log of the requests which will include the final disposition of the request. The code custodian will also notify the requestor of the final disposition of the request. The code custodian will determine the extent of the change or problem and will obtain approval from the proper line of management to implement the change.
2. Create a temporary version of Radcalc for Windows within a system test area, and alter this program according to the requested change.
3. Once the changes have been made, validate the new program by comparison with the original version and verification test cases.
4. Prepare documentation describing the change, and issue for approval.
5. Upon approval of the documentation, establish the temporary version as the official version by copying the appropriate files to the Radcalc for Windows production area on computer WC50477 in directory wradcalc.
6. Prepare back-ups of the new version of Radcalc for Windows per Section 5.3.

5.2 ARCHIVAL STORAGE AND RECORDS

The source files used in creating Radcalc for Windows are archived in computer WC50477, which is networked to the WHC End System Operating Environment (ESOE). The files are in a read only directory entitled wradcalc in the subdirectory source. Backups of the files also exist on floppy disk and copies are available from the code custodian.

Files needed to create disks with the setup utility are also archived on the same computer in directory wradcalc in subdirectory setup. The subdirectory runrad in the wradcalc directory contains the files necessary for running the programming. These files are:

radcalc.exe	Radcalc.exe is the Windows executable.
radcalc.hlp	Radcalc.hlp is the help file.
data.bin	Data.bin contains the data extracted from FENDL/D-1.0 as well as the transportation value information in binary format.
gdata.bin	Gdata.bin contains all G-value information in binary format.
origen2.dk	Origen2.dk is a binary formatted version of the ORIGEN2 decay database.
verify/test1.rad	Six test cases (test1.rad, test2.rad, etc.) are contained in the verify subdirectory to test the proper functioning of Radcalc for Windows. See section 4.1 for further information.

Copies of the executable files can be obtained from the code custodian in Packaging Engineering, Transportation and Packaging, WHC, by calling 509-376-0610 or 509-372-0703.

Records for Radcalc for Windows will be located in the file cabinets of the code custodian. The exact location of the Radcalc for Windows records can be found by consulting the Records Inventory and Disposition Schedule (RIDS) which is in the first drawer of the custodian's file cabinets.

5.3 BACKUP AND RECOVERY

Upon completion of a version of Radcalc for Windows the code custodian will back up all files for the code. These files are contained in directory wradcalc and subdirectories source, setup, and runrad on computer WC50477. The files will be backed up on floppy disks and kept in a 3.5 in diskette holder marked "Radcalc Backup Files" on the computer workstation of the code custodian. If the computer archiving the files crashes or needs to be replaced the code custodian will replace the files on computer WC50477 with the back-up files.

5.4 DISTRIBUTION

The code custodian will maintain a record of all Radcalc for Windows users which will be filed with Radcalc for Windows documentation and program records. These records can be found by consulting the code custodian's RIDS

form as described in Section 5.2. Upon completion of a new version of Radcalc for Windows all users will be notified of the availability of the new version.

Copies of Radcalc for Windows can be received by calling the Code Custodian or Packaging Engineering Secretary at 509-376-0610 or 509-372-0703.

6.0 REQUIREMENTS SPECIFICATION

Radcalc for Windows is written for applications in transportation and packaging. The requirements listed in this section are selected to provide guidelines appropriate to that environment. The requirements are designed to define the accepted level of performance and confirm that the code operates over the normal range of variables. The requirements are as follows:

1. Hydrogen gas calculation methodologies shall produce results consistent with accepted techniques as shown in Section 2.1 and 2.2.
2. Decay algorithms shall produce results consistent with accepted methodologies as shown in Section 2.5 and Appendix A.
3. Transportation quantity calculations shall produce results consistent with techniques outlined in 49 CFR Subchapter C.
4. Differences of a few percent or more between computed and benchmark results shall be justified.

Documented evidence that these requirements have been met is given in Chapter 4.0. This demonstrates that Radcalc for Windows produces correct results when used to analyze problems within a specific domain of applications. This effort meets the requirements of WHC-CM-4-2.

7.0 SUMMARY

Radcalc for Windows is a user-friendly menu-driven Windows-compatible software with applications in the transportation of radioactive materials. It calculates the radiolytic generation of hydrogen gas in the matrix of low-level and high-level radioactive waste. It also calculates pressure build up due to hydrogen and the decay heat in a package at seal time. It computes the quantity of a radionuclide and its associated products for a given period of time. In addition the code categorizes shipment quantities as radioactive, Type A or Type B, limited quantity, low specific activity, highway route controlled and fissile excepted using DOT definitions and methodologies.

Radcalc for Windows has been extensively tested and validated. It uses NRC-accepted methodology for the calculation of the production of hydrogen gas. The radionuclide database is taken from the well-established FENDL/D 1.0

and ORIGEN2 databases. The transportation database and calculations are based directly on 49 CFR Subchapter C data and methodologies. When used appropriately, Radcalc for Windows can be expected to give accurate and consistent results.

8.0 REFERENCES

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APPENDIX A

**BEST AVAILABLE COPY^A COMPUTER ALGORITHM FOR SOLVING THE
BATEMAN DECAY EQUATIONS**

A Computer Algorithm for Solving the Bateman Decay Equations

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ABSTRACT

Two features are combined to give a new algorithm for solving the Bateman decay equations. First, a hybrid representation for the solution is found that serves as the basis for a fast, general, and numerically stable method. Second, a recursive programming approach yields a convenient way to organize the calculation of complicated decay chains and conserve memory. A FORTRAN code was developed to test the method and illustrates the use of recursive methods in a nonrecursive language.

I. INTRODUCTION

The Bateman decay equations¹ arise in numerous problems in physics, chemistry, and other diverse fields. They represent a well-known example of a set of coupled first-order linear differential equations and have been studied for many years. Despite this intense scrutiny, simple solutions readily amenable to computer algorithms are often restricted to particularly simple classes of problems. This situation arises, in part, because these problems belong to the class of stiff differential equations that are especially susceptible to numerical errors, although closed-form solutions are readily obtainable.

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To be specific, we consider equations of the form

$$= \sum_j a_{-j} n_j \quad (2)$$

where

$$\alpha_{ii} = -\beta_i.$$

For nuclear transmutation and decay problems, n_i represents the amount of the i -th nuclide in a coupled system. The production rate of a daughter nuclide i by a parent j is given by the transfer or rate coefficients α_{ij} , while the destruction by either decay or transmutation is given by the constant β_i . This physical model will be followed for the purpose of discussion, although clearly the same set of equations can represent a wide variety of diverse phenomena.

An inhomogeneous, but constant, production rate is often added as a source term to these equations. However, such a term is readily included in the present set of equations by simply adding a fictitious nuclide with a unit amount, $n_k = 1$, that does not deplete $\beta_k = 0$. Then, a constant source S_i for any nuclide i can be generated by simply choosing a rate constant α_{ik} such that

$$a_{ij}n_j = S_i \quad (3)$$

As one might expect for such a ubiquitous set of equations, extensive literature exists for their solution. Only a few references are noted here, primarily to illustrate some of the possible approaches and their advantages and disadvantages. A typical textbook example with analytical solutions is given

in Reference 2. However, these solutions are susceptible to a loss of numerical precision arising from cancellation of nearly equal terms. This problem is particularly manifest for decay chains with equal destruction constants β_i where terms involving $1/(\beta_i - \beta_j)$ are present.

A completely different approach is to numerically integrate the equations. This is a practical approach³ but, as noted, it requires special numerical techniques appropriate to stiff equations⁴ and may require significant amounts of computer time and memory. Nevertheless, good numerical packages are widely available⁵, and this may be the option of choice in some cases. The difficulty arises in problems with widely varying system time constants. For example, in the nuclear decay problem, nuclear half-lives can easily range from fractions of a second to millions of years.

Another well-known solution is the matrix-exponential result:

$$n = e^{\alpha t} n_0 \quad (4)$$

where α is the transition matrix in Eq.(2), and the exponential propagates the vector of initial concentrations n_0 to a later time t . The matrix exponential form works especially well for smaller times where the power series implied by the exponential in Equation 4 converges rapidly. This method forms the basis of the highly successful ORIGEN⁶ and ORIGEN2⁷ nuclear decay and transmutation codes. However, several special techniques are required to treat cases where convergence is slow. This form is also the basis for matrix-based approaches. One such example is given by Lee⁸ et al. who developed a method using matrix norms to obtain numerically dependable results. The approach taken by Lee is still moderately complicated.

England takes another approach in the CINDER⁹ code by using Laplace transforms to obtain a solution. The CINDER code is well documented and provides a practical solution to a significant class of problems. It is somewhat less general than the ORIGEN algorithm and again requires attention to special cases to control numerical errors.

Other studies include recent work by Raykien and Shlyakhter¹⁰ who focus on the problem of time-dependent rate constants, an aspect not considered here and Miles¹¹ who provides an example of how equal destruction constants can be dealt with. Reference 3, a comprehensive review of nuclear decay heat, also includes a brief survey of calculational methods along with additional references.

Computer memory requirements can also pose problems. As in nuclear transmutation, the fission process can initiate hundreds of coupled chains. Thus, unless special care is taken, or the problem is restricted, memory requirements may become large.

In summary, although many practical numerical solutions are available, they often require restricting the problem to particular classes of problems, or they involve complex numerical methods problems, or they are of questionable precision. In the next section, a general algorithm is developed for solving Eq.(1), and the results are applied to a specific problem in Section III.

II. A GENERAL DECAY ALGORITHM

The algorithm given here is based on standard methods. It is fast, numerically stable, and easily implemented. As a side note, it provides a simple example of the power of recursive programming and its implementation in FORTRAN. The method may be conveniently divided into two parts. In the first part, a standard series development is summarized; it is particularly

appropriate to a recursive programming approach, and it has the additional merit of having a direct physical interpretation. In the second part, the development focuses on the explicit calculation of one single step in the decay chain.

A. Series Development for Nuclide Amounts

In the usual way, we start by multiplying Eq.(2) with the integrating factor $e^{\beta_i t}$ to obtain

$$\frac{dN_i}{dt} = \sum_{j=1}^I \alpha_{ij} e^{\delta_{ij} t} N_j, \quad (5)$$

where

$$\delta_{ij} = \beta_i - \beta_j \quad (6)$$

and

$$N_i = e^{\beta_i t} n_i. \quad (7)$$

(Note: δ_{ij} designates a difference and not the Kronecker delta function).

Integrating Eq.(5) then gives

$$N_i = N_{i0} + \sum_{j=1}^I S_{ij} N_j. \quad (8)$$

where the operator S_{ij} is defined by

$$S_{ij} = \alpha_{ij} e_{ij} \quad (9)$$

with

$$e_{ij}(t) \equiv \int_0^t e^{\delta_{ij} \tau'} d\tau' \quad (10)$$

Eq.(8) may then be iterated to obtain

$$N_i = n_{i0} + \sum_{j=1}^I S_{ij} n_{j0} + \sum_{j=1}^I \sum_{k=1}^I S_{ij} S_{jk} n_{k0} + \dots \quad (11)$$

Convergence of this series is not formally explored here, but based on physical grounds as well as the explicit implementation discussed later, it is not an issue. Clearly, $S_{ij}n_{j0}$ represents the contribution of the transmutation of parent j to daughter i . Repeated applications of the operator S_{ij} give successive daughters in the decay chain. Thus, the terms in Eq.(11) represent one-step decays, two-step decays, and so forth. Convergence is ensured as long as physically reasonable values are chosen for (β_i) and (α_{ij}) . Specifically, these parameters should be positive, and the sum of α_{ij} for a particular parent i should not exceed the destruction, β_i , of the parent, thus ensuring that no net nuclei are generated.

From the physical interpretation as well as from Eq.(10), all terms in Eq.(11) are positive. This ensures that, at least for this step, numerical cancellation of terms is not possible. In contrast, iteration of Eq.(2) after integration would yield negative terms because α_{ij} is negative for $i=j$, unlike the case for $i \neq j$.

The simple physical picture of branching chains of daughter nuclides described by Eq.(11) lends itself readily to a recursive algorithm. One starts with an initial amount n_{j0} of nuclide j . Next, a daughter i is selected, and the amount $S_{ij}n_{j0}$ of daughter i arising from the parent j is calculated.

Successive decays and transmutations are followed for a linear chain until some termination rule is achieved, or the final nuclide is either stable or sufficiently small. A generic implementation is shown here, where a recursive procedure TRANSMUTE is used to calculate the daughter amounts from the parent.

```

Main Program
  Global (Ni)

  Set Ni = 0   (for all i)

  For i := 1 to Nlist
    T := n10
    Call TRANSMUTE(i, T)
  End For-loop

  ni := e-λit Ni   (for all i)
End MAIN

Procedure TRANSMUTE(j, Tj)

  Nj := Nj + Tj

  If Tj > eps Then           (Termination rule)
    For i := 1 to Nlist
      If (αij ≠ 0) Then
        Ti := SijTj
        Call TRANSMUTE(i, Ti)
      EndIf
    End For-loop              (Also terminates with exhausted loop)
  EndIf

Return

```

In this illustration, T_i is the amount of daughter i arising from the amount T_j of a single immediate parent j according to the equation

$$T_i = S_{ij}T_j. \quad (12)$$

The main program first initializes all nuclide amounts to zero. Then for each nuclide in the list of Nlist nuclides, T is set to the initial amount n_{10} , and the TRANSMUTE procedure is called to start the recursive process. The TRANSMUTE procedure first adds the parent amount T_j to the total amount N_j ; then for each daughter i , the daughter amount T_i is calculated according to Eq.(12). Finally TRANSMUTE is recursively called to continue the decay chain calculation.

This algorithm has several advantages. It follows each branch of the decay chain, so that at any given time one is solving a simple linear chain. The use of recursion yields a very simple implementation of what would otherwise be a complicated bookkeeping problem. Moreover, as one proceeds down the various decay chain branches, recursion provides an effective way to maintain only the necessary data in memory. As noted earlier, the terms at this stage are positive, so losing precision from cancelled terms is not a problem. And finally, the process has a clear physical meaning. The problem is now reduced to calculating the amount of daughter i from the parent j .

B. Calculation of a Single Decay Chain Step

This section focuses on a single step in the decay chain calculation. To emphasize this fact, we set the daughter and parent indices, i and j , to specific values, q and p , respectively. Equation (12) then becomes

$$T_q = S_{qp} T_p \quad (12')$$

The daughter concentration T_q may be represented as a power series in time. As noted for the matrix-exponential solution, this works well for small values of τ , but it converges slowly for larger values. An alternative representation for T_q is as a sum over the exponential functions

$(e^{\lambda_j \tau})$ where the sum over j includes all parents j of daughter q as well as q itself. The leading $e^{\lambda_q \tau}$ implicit in $e^{\lambda_j \tau}$ occurs because we are working in the transformed system [Eq.(7)]. The disadvantage in this approach is that it is possible for near-equal terms to cancel, thus leading to large numerical errors. As an alternative approach, we use the form

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$$T_q = \sum_j e^{\delta_{qj} \tau} \sum_{k=0}^{\infty} c_{jk}^{(q)} \tau^k \quad (13)$$

which combines the power series and exponential forms in a non-unique representation. The coefficients $(c_{jk}^{(q)})$ form a two dimensional matrix representing the concentration T_q for the daughter nuclide q . We next show how the non-uniqueness can be used to advantage to provide a numerically accurate solution. Because of the decisive role this form plays in controlling numerical errors, it is henceforth referred to as the standard form or representation. From Eqs. (9,10 and 12,13), we find

$$\begin{aligned} T_q &= \alpha_{qp} \int_0^{\infty} e^{\delta_{qp} \tau'} T_p d\tau' \\ &= \alpha_{qp} \int_0^{\infty} e^{\delta_{qp} \tau'} \left[\sum_k e^{\delta_{pk} \tau'} \sum_{j=0}^{\infty} c_{kj}^{(p)} \tau'^j \right] d\tau' \\ &= \alpha_{qp} \sum_k \sum_{j=0}^{\infty} c_{kj}^{(p)} \int_0^{\infty} e^{\delta_{qk} \tau'} \tau'^j d\tau' \end{aligned} \quad (14)$$

In the Appendix, it is shown that the integral in Eq.(14) is again a series of exponentials multiplied by powers of τ . Two separate forms, designated as Form A and Form B, are given, depending on whether $\delta_{qk} \tau$ is small or large, respectively. Accordingly, the sum over k can be split into two sums one sum consisting of terms where the Form A result is used, and the other sum consisting of terms where the Form B result is used:

$$T_q = T_q^{(A)} + T_q^{(B)} \quad (15)$$

C. Form A Results

For small $\delta_{qk}\tau$, the Form A results give

$$\int_0^\tau e^{\delta_{qk}t'} \tau'^s dt' = e^{\delta_{qk}\tau} \sum_{r=s+1}^{\infty} \frac{s!}{r!} (-\delta_{qk})^{r-s-1} \tau^r. \quad (16)$$

Substituting Eq.(16) into Eq.(14) and interchanging summation limits

$$\sum_{s=0}^{\infty} \sum_{r=s+1}^{\infty} \rightarrow \sum_{r=1}^{\infty} \sum_{s=0}^{r-1}$$

gives

$$\tau_q^{(A)} = \alpha_{qp} \sum_{k \in A} e^{\delta_{qk}\tau} \sum_{r=1}^{\infty} \tau^r \left\{ \sum_{s=0}^{r-1} \left(\frac{s!}{r!} \right) (-\delta_{qk})^{r-s-1} c_{ks}^{(p)} \right\}. \quad (17)$$

Thus, the standard form, Eq.(13), is retained. The coefficients

$(c_{ks}^{(q)})$ representing the daughter concentration T_q are now

obtained from the coefficients $(c_{ks}^{(p)})$ representing the parent

concentration T_p by comparing this result with Eq.(13). The result is

$$a_{ks}^{(q)} = \frac{1}{s!} (\alpha_{qp} \tau) \sum_{r=s}^{\infty} s! (-\delta_{qk} \tau)^{r-s-1} a_{ks}^{(p)} \quad (18)$$

where the dimensionless constants

$$a_{ks}^{(q)} = c_{ks}^{(q)} \tau^s \quad (19)$$

are introduced.

These coefficients may be computed easily and quickly from the starting conditions

$$a_{k0}^{(q)} = 0, \quad a_{k1}^{(q)} = (\alpha_{qp}) a_{k0}^{(p)} \quad (20)$$

and the recursion relation

$$a_{kr}^{(q)} = -\frac{(\delta_{qk})}{r} a_{k,r-1}^{(q)} + \frac{(\alpha_{qp})}{r} a_{k,r-1}^{(p)} \quad (21)$$

($r=2,3, \dots$), $k \in A$.

Note that the recursion relation picks up coefficients from both the parent p and the daughter q . Note also that k is on both sides of Equation (18). In other words, there is no k -mixing for the Form A method; each row k in the daughter matrix ($a_{kr}^{(q)}$) is generated from the same row k in the parent representation ($a_{kr}^{(p)}$). For each row k , Eq.(21) is applied repeatedly, increasing the column index r until the power series in Eq.(17) converges. The number of terms required depends on the row k and the particular daughter q . This largest r -index terminates the series and is denoted by L_k for later reference.

In practice this strongly convergent power series is readily terminated by requiring the ratio of the last term in the series to the series sum to be less than some small number ϵ_r .

D. Form B Results

For $\delta_{qk} \tau > (s+1)/e$, the Form B results from the Appendix are used:

$$\int_0^\infty e^{\delta_{qk} \tau'} \tau'^s d\tau' = \left(\frac{-1}{\delta_{qk}}\right)^{s+1} s! \left[1 - e^{\delta_{qk} \tau} \sum_{r=0}^s \frac{1}{r!} (-\delta_{qk} \tau)^r \right] \quad (22)$$

giving

$$T_q^{(B)} = \alpha_{qp} \sum_{k \in B} \sum_{s=0}^{\infty} c_{ks}^{(p)} \left\{ \left(\frac{-1}{\delta_{qk}}\right)^{s+1} s! \left[e^{\delta_{qk} \tau} - e^{\delta_{qk} \tau} \sum_{r=0}^s \frac{1}{r!} (-\delta_{qk} \tau)^r \right] \right\} \quad (23)$$

where the leading 1 in brackets in Eq.(22) was rewritten as $e^{\delta_{qk} \tau}$

to demonstrate the Standard form is also preserved by Form B.

Now there are two terms that generate daughter coefficients

$c_{k's'}^{(d)}$ from the parent coefficients $c_{ks}^{(p)}$.

(Note the use of the subscripts k' and k to index rows in the daughter and parent matrices respectively.) The second term in brackets in Eq.(23) is the same as before except for the summation limits and sign. Thus, for this term the rows k of the parent again generate the same rows $k'-k$ of the daughter. Specifically, for $k'=k$, interchanging the summation limits in Eq.(23),

$$\sum_{s=0}^{k'} \sum_{r=0}^s \rightarrow \sum_{s=0}^{k'} \sum_{r=k-s}^{k'} \quad \dots$$

and comparing the results with the standard form, we have (in dimensionless form)

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$$a_{k,r}^{(q)} = -\frac{1}{r!} (\alpha_{qp} \tau) \sum_{s=0}^{L_s} s! (-\delta_{qk} \tau)^{r-s-1} a_{k,s}^{(p)} \quad (24)$$

$$(r = 0, 1, \dots, L_s), k \in B$$

where L_s is the upper limit of the s -sum and is established by convergence of the power series in Eq.(17). (See discussion after Eq.(21))

Unlike the Form A case, column 1 ($r=0$) in the $(a_{k,r}^{(q)})$ matrix is now non-zero. Also, the simplest terms in Eq.(24) are for $r=L_s$, and we develop the downward recursion relation

$$a_{k,r}^{(q)} = -\frac{1}{\delta_{qk} \tau} \left[(r+1) a_{k,r+1}^{(q)} - (\alpha_{qp} \tau) a_{k,r}^{(p)} \right] \quad (25)$$

$$(r = L_{s-1}, L_{s-2}, \dots, 0), k \in B$$

with the starting condition

$$a_{k,L_s}^{(q)} = \frac{\alpha_{qp} \tau}{\delta_{qk} \tau} a_{k,L_s}^{(p)} \quad (k \in B) \quad (26)$$

Considering the first term in brackets in Eq.(23) completes the calculation.

Again, comparing this term to the standard form in Eq.(13) yields

$$a_{q,0}^{(q)} = (\alpha_{qp} \tau) \sum_{k \in B} \sum_{s=0}^{L_s} \frac{s!}{(-\delta_{qk} \tau)^{s+1}} a_{k,s}^{(p)} \quad (27)$$

The $k=q$ row and $r=0$ column of the daughter representation thus receives contributions from all of the Form B rows of the parent. This is the only part

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of the calculation that mixes exponentials, (i.e., adds new rows to the daughter matrix). For a particular k , the first term in the sum in Eq.(27) is

$$- [(\alpha_{qp})/(\delta_{qk})] a_{k0}^{(p)}, \text{ and the simple form of the remaining terms again}$$

allows a recursive calculation of the remaining terms in the s -sum.

In summary, the set of recursive relations, Eqs.(20,21 and 25-27) provide a fast and simple algorithm. Convergence is easily controlled, and finally all operations involve only algebraic operations. The latter property both speeds the calculation and reduces the need to control the size of large numbers. The only time an exponential is calculated is at the final step. Since the standard form for T_i contains the factor $e^{t_j^2}$ (see Eq.(13)), then to obtain n_i from N_i , only multiplication by $e^{-t_j^2}$ is needed.

III. FORTRAN IMPLEMENTATION

A FORTRAN code was written to implement and test the algorithm. Most of the code is a straightforward implementation of the above equations. Since FORTRAN is a non-recursive language, a few comments may be required to describe the recursive programming. The method used combined the recursive procedure TRANSMUTE with the calling program so entry and exit from TRANSMUTE could be explicitly programmed. For the purpose of discussion, TRANSMUTE will continue to be referred to as if it were an independent code module. Specifically, the following steps were taken and could be readily applied to other recursive applications:

1. A recursion index, LEVEL, is defined that keeps track of the level of nesting. Starting with one, LEVEL is incremented by one each time TRANSMUTE is "called" and decremented each time TRANSMUTE "returns" to the calling program.
2. Next, each local variable in TRANSMUTE that must retain its value during the recursive calls is stored in an array with the added index LEVEL. A simple variable A would become A(LEVEL), while a dimensioned variable B(I) becomes B(I,LEVEL).
3. In general, to "call" the recursive procedure, one must define a variable representing the return address, say with a computed GOTO statement. Then one "jumps" to the start of the recursive segment with a simple GOTO statement.
4. "Entry" to TRANSMUTE starts by incrementing the level index,
 $LEVEL = LEVEL + 1.$
5. Finally TRANSMUTE is exited by LEVEL-LEVEL-1 followed by a "jump" (i.e., GOTO) to the return address established in step 3 above.

The free use of GOTO statements may be undesirable, but it does allow explicit control of the code flow. Other necessary compromises include the exclusion of IF THEN ELSE statements, where a return simulated by a GOTO statement would otherwise jump into the scope of the IF THEN ELSE structure. On the other hand, the ability to develop the code from a recursive viewpoint can easily offset these disadvantages. In particular, it provides a very convenient and automatic means of allocating and reusing memory locations throughout the recursive tree. Obviously, using the LEVEL index limits the

level of recursion to the value of the LEVEL index; nevertheless, the total number of branches is unlimited.

One final note: in the present case, using a computed GOTO statement and a return address was avoided altogether. Since TRANSMUTE is "called" only from itself and the main calling program, a "return" to the calling program is made only when the LEVEL index decrements to 1; otherwise, TRANSMUTE "returns" to itself.

IV. TESTS AND APPLICATIONS

The decay of ^{238}Pu is an excellent example to illustrate this method. The decay chain includes a long daughter chain of 13 nuclides with half-lives that vary from 200,000 years to less than a millisecond and terminating with the stable nuclide ^{206}Pb . The nuclide chain and decay data are shown in Table I. The decay data are taken from the ORIGEN2⁶ decay libraries. Two of the nuclides shown, ^{218}Ac and ^{216}Tl , are short-side branches that are not part of the main decay chain and for which data are not in the ORIGEN2 library. They were both assumed to be stable for this calculation. Except for these two minor branches, the chain ends with the stable nuclide ^{206}Pb . Table I also includes both the total parent destruction rate (β_j) and the transition rates (α_{ij}). For each nuclide, the sum (usually a single term) of the α_{ij} equals β_j . All values of α_{ij} not explicitly given are zero.

Table II shows the results for a decay time of 1×10^8 seconds starting with an initial amount of one gram-atom of ^{238}Pu . The results are first compared to those from an ORIGEN2 calculation. Although the amounts vary by 27 orders of

magnitude, the two calculations agree within a few percent. For the first four nuclides in the chain, the two calculations agree within the four digits of precision output by the ORIGEN2 code. The first discrepancy (1.4 percent) is for ^{222}Rn , a short-lived nuclide that follows the long-lived ^{226}Ra . The amount of ^{222}Rn calculated by ORIGEN2 can be reproduced by assuming a constant value for the amount of the parent ^{226}Ra . Assuming instead that the amount ^{226}Ra is proportional to t^3 as one would expect for the third member of a long-lived chain, the discrepancy is readily accounted for. The next jump in the percent difference occurs for ^{210}Bi , another short-lived nuclide that follows a long-lived parent.

In order to compare the present method with straightforward numerical integration of the differential equations, a solver for stiff ordinary differential equations, LSODE⁵ was obtained from the National Energy Research Supercomputing Center. Written by A. C. Hindmarsh, LSODE solves a set of differential equations of the form

$$dy/dt = f(t,y). \quad (28)$$

where y is a vector function of t . LSODE allows the user to directly input the Jacobian for these equations which in our case is particularly simple, namely the constant matrix α . Error control for LSODE is provided by two parameters, either of which may be a vector quantity; a relative tolerance RTOL, and an absolute tolerance ATOL. The solver then controls the local errors in y relative to a weighted error based on

$$EWT(i) = RTOL(i) * ABS(Y(i)) + ATOL(i)$$

A method flag was set to MF=21 appropriate for stiff equations with a user-supplied Jacobian.

Because of the wide range in magnitudes for the different nuclides, the absolute tolerance ATOL was set to zero. Since EWT(i) then becomes zero for $Y(i)=0$, this choice required that the initial zero values for $Y(i)$ be reset to some small number. Both this number and a common value for the relative tolerance vector RTOL were selected by trial and error. The choice of a single value for all components RTOL(i) was made to achieve input parameters that did not anticipate the solution.

The results of the LSODE calculations are compared with the previous results in Table II. Most of the calculations were made on a personal computer class machine using 32 bits for single precision real numbers. Various values of RTOL and the small non-zero initial value of $Y(i)$ were tested. Representative results are shown. For the PC-based calculations, the LSODE results are in near perfect agreement with the results of the present method for RTOL = 0.01. (Clearly the precision of the results is much smaller than the tolerance value RTOL.) By the time, RTOL is increased to 1.0, the errors in the LSODE results become excessive. The amount of required cpu time is remarkably insensitive to RTOL, so that there is little reason not to pick a small value. For this case, the current method enjoys a cpu time advantage factor of about 23/0.16-144 over direct integration.

The PC-based LSODE results used a value of 1×10^{-23} for the initial value of $Y(i)$ whenever the true initial value was zero. This value was quite constrained since any value smaller than 1×10^{-26} led to numeric overflows, and a value much larger would be comparable to the magnitude of results for some nuclides. This problem was alleviated by going to a Cray-class machine with 64 bits of precision for real numbers. Several cases were run there as well. Results are shown for the case with RTOL=0.01. It is interesting to note that the deviations in the

results as a function of RTOL were nearly independent of the precision of the computer. The Cray cpu time was a factor of 23/0.12-192 better than the PC-based cpu time. A rough estimate is that about a factor of two of this increased speed arises from vectorization.

Memory utilization is a significant advantage of the present method compared to some other methods. The example given here is too small to make a direct evaluation. Nevertheless, the general behavior is clear. Since the current method always follows one decay chain branch at a time, the data storage requirements become the requirements for a single step in the chain times the maximum length of a chain. Neither the number of chains or nuclides is important. In a method that requires the full transition matrix to be given, the memory size will grow with the problem size, even with the use of sparse matrix techniques.

As noted earlier, a good example of a problem with a large number of nuclides with limited decay chain lengths is for a fissioning nuclide. An initial fission event creates several hundred fission products. Each of these decay in relatively short chains to stable nuclides thus terminating the respective chains.

A final comment in comparing the current algebraic approach with direct numerical integration concerns the generality of the method. The direct integration method undoubtedly solves a wider class of problems; time-dependent rate problems are a good example. However, the scope of the present method can be expanded. For example, it was noted earlier that inhomogenous source terms are already included in the present scheme. And problems with time-dependent rate constants can often be treated by the simple expedient of breaking the

total time interval into smaller subintervals where the rate constants can be approximated by constants.

The algebraic algorithm was found to be very robust. Not only does this ensure good solutions, but it makes it easier to obtain results without the need to iterate or otherwise "fine-tune" the input parameters. The sole parameter affecting the numerical precision of the solution for this example is the convergence parameter ϵ , controlling the convergence of the power series in Eq.(17) and described near the end of Section II.C. A value of $\epsilon = .0001$ used here led to a maximum number 7 of terms in the power series. With the value of ϵ increased to .01, the maximum series length was only reduced by one, and the solution was nearly identical. Likewise, a stronger convergence criterion of 1×10^{-6} increased the series length by only one with a concurrent increase in the cpu time of about 30%.

Examination of intermediate results for this example shows that, as expected, cancellation is also not a problem. For example, the matrix representation for 206pb at the end of the chain is representative of the more complex intermediate terms and consists of several rows of both Form A and Form B calculations. Detailed printouts show that the final result is dominated by a few terms and that it is comparable in size to the largest. That is, no significant cancellation of large terms is noted. Other validity checks include tests with both very small (1 second and zero) and large (1×10^{20} seconds) times. In these cases, one obtains the expected results of either no decay or complete decay to the stable end nuclide respectively. A small amount is diverted to the two offshoot branches.

A more interesting example, in the sense that other methods often do not allow it, is when feedback to a previous parent occurs. A simple case that has an analytical solution is the following set of equations:

$$\begin{aligned}\frac{dn_1}{dt} &= \alpha(n_2 - n_1) \\ \frac{dn_2}{dt} &= \alpha(n_1 - n_2)\end{aligned}\quad (28)$$

which can be readily integrated to give

$$\begin{aligned}n_1 &= \frac{1}{2}n_{10}(1+e^{-2\alpha t}) \\ n_2 &= \frac{1}{2}n_{10}(1-e^{-2\alpha t})\end{aligned}\quad (29)$$

where the initial amounts of n_1 and n_2 are n_{10} and zero, respectively.

A calculation for $\alpha t = 1$ was compared to values obtained from Eq. (29) and gave the following values precise to six decimal places:

$$n_1 = 0.5676677$$

$$n_2 = 0.4323324$$

This result was obtained within 11 (about 5 per nuclide) levels of recursion. For smaller values of αt , the process converges faster. However, for larger values of αt , convergence is slower and can become a practical limitation. This limitation is on the number of recursive levels allowed in examples with feedback loops. It is not associated with the Form A and Form B series convergence discussed in Section II.

V. SUMMARY

A new algorithm for solving the Bateman decay equations was given. Two novel aspects provide a significant alternative to previous methods. First, using simulated recursive FORTRAN programming gives an effective means of following complicated decay branches and provides a nearly automatic method of memory management. Second, the basic decay equation algorithm depends on two

sets of complementary algebraic recursion relations that can be used to span the large time scales that are frequently encountered in nuclear transmutation and other fields. These relations are simple, fast, and avoid the calculation of exponentials that are time-consuming and that complicate the control of large numbers.

Additional features of the new algorithm include the ability to treat weakly coupled feedback and the lack of a multitude of different algorithms to treat special cases. Examples include short-lived nuclides that follow long-lived nuclides, and situations where several nuclides have identical or nearly identical destruction rates. The utility of the method was demonstrated with both practical and analytical examples.

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Table 1. Input data for ^{238}Pu decay chain calculation

nuclide	parent index, j	daughter index, i	half-life	β_j	α_{ij}
^{238}Pu	1	2	87.74y	2.503240E-10	2.503240E-10
^{234}U	2	3	$2.45 \times 10^5 \text{y}$	8.983245E-14	8.983245E-14
^{230}Th	3	4	$7.54 \times 10^4 \text{y}$	2.852458E-13	2.852458E-13
^{226}Ra	4	5	1600y	1.372841E-11	1.372841E-11
^{222}Rn	5	6	3.8235d	2.097903E-06	2.097903E-06
^{218}Po	6	7	3.11m	3.787690E-03	7.574379E-07
	6	8			3.786932E-03
^{218}Ac *	7		$\sim 2.5\text{s}$	0	0
^{214}Pb	8	9	26.8m	4.310617E-04	4.310617E-04
^{214}Bi	9	10	19.8m	5.805253E-04	5.804034E-04
	9	11			1.219103E-07
^{214}Po	10	12	163.7 μs	4.218790E+03	4.218790E+03
^{210}Tl *	11		1.30m	0	0
^{210}Pb	12	13	22.3y	9.850039E-10	9.850039E-10
^{210}Bi	13	14	5.01d	1.600802E-06	1.600802E-06
^{210}Po	14	15	138.38d	5.795545E-08	5.795545E-08
^{206}Pb #	15		stable	0	0

* Not in ORIGEN2 library

Stable

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Table II. Calculated number of gram-atoms in the decay of 1 gram-atom of ^{238}Pu to $t=1 \times 10^6$ seconds. The variation from the present method is given in percent following each case.

Index	Present Method	ORIGEN2 (a)	I.SODE (b) on Personal Computer (RTOL = 0.01)	I.SODE (b) on CRAY (RTOL = 0.01)
1	9.752703E-01	9.753E-01	9.7520E-01	9.7520E-01
2	2.472157E-02	2.472E-02	2.4722E-02	2.4722E-02
3	1.115024E-07	1.115E-07	1.1150E-07	1.1150E-07
4	1.062032E-12	1.060E-12	1.0620E-12	1.0620E-12
5	6.051570E-18	6.950E-18	6.0516E-18	6.0516E-18
6	3.794002E-21	3.049E-21	3.7949E-21	3.7949E-21
7	7.161564E-20	3.302E-20	7.1626E-20	7.1616E-20
8	3.333614E-20	2.511E-20	3.3336E-20	3.3336E-20
9	2.475206E-20	3.455E-27	2.4752E-20	2.4752E-20
10	3.405203E-27	3.550E-16	3.4053E-27	3.4053E-27
11	7.517920E-20	2.190E-19	7.5189E-20	7.5179E-20
12	3.510102E-16	3.402E-10	3.5101E-16	3.5101E-16
13	2.106933E-19	3.591E-18	2.1069E-19	2.1069E-19
14	3.270992E-18	4.97	3.2706E-18	3.2709E-18
15	3.421000E-18	--	3.4209E-18	3.4210E-18
cpu-sec "	0.16	23.10	11.07	0.12

a. Ref. (6)

b. Ref. (5)

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Appendix: Integral Representations

Specific forms of the integral

$$I_n(\tau, a) = \int_0^\tau \tau'^n e^{a\tau'} d\tau' \quad (A.1)$$

are central to the present development and are summarized here. The indefinite integral is readily evaluated and may be represented as an exponential function multiplied by a truncated exponential series giving:

$$I_n(\tau, a) = \frac{(-1)^n n!}{a^{n+1}} \{ e^{a\tau} E_n(-a\tau) - 1 \} \quad (A.2)$$

where

$$E_n(x) = 1 + x + \frac{x^2}{2} + \dots + \frac{x^n}{n!} \quad (A.3)$$

Since

$$e^{a\tau} E_n(-a\tau) = 1 - e^{a\tau} \sum_{k=n+1}^{\infty} \frac{1}{k!} (-a\tau)^k \quad (A.4)$$

then $I_n(\tau, a)$ has two complementary representations:

$$I_n(\tau, a) = \begin{cases} (-\frac{1}{a})^{n+1} n! \sum_{k=n+1}^{\infty} \frac{1}{k!} (-a\tau)^k & \text{Form A} \\ (-\frac{1}{a})^{n+1} n! \left[1 - e^{a\tau} \sum_{k=0}^n \frac{1}{k!} (-a\tau)^k \right] & \text{Form B} \end{cases} \quad (A.5)$$

Form A is suitable when a is small and the series converges rapidly, while Form B is suitable for larger values of a such that the two terms in brackets do not significantly cancel. Note that $(1/a)^{n+1}$ in Form A is canceled by terms in the sum so that this expression is valid for an arbitrarily small a , including zero.

The appropriate range of a for using in Form A or Form B can be made more precise by considering the following form, which is representative of that part of Eq.(A.5) in brackets where cancellation is a concern:

$$\Delta(x) = (-1)^{n+1} \left[1 - e^x \sum_{k=0}^n \frac{1}{k!} (-x)^k \right]. \quad (\text{A.6})$$

By the Taylor remainder theorem, we have

$$\Delta(x) = \frac{1}{(n+1)!} x^{n+1} e^{x^*}, \quad (\text{A.7})$$

where

$$0 \leq x^* \leq x.$$

Then the smallest value of $\Delta(x)$ occurs for $x^* = x$. Thus, we ensure no significant cancellation in Form B as long as

$$\frac{1}{(n+1)!} x^{n+1} > 1. \quad (\text{A.8})$$

On the other hand, since the lhs is the first term in the Form A series, a value less than 1 ensures good convergence of that series. Using Stirling's approximation $n! \approx e^{-n} n^n \sqrt{2\pi n}$ and ignoring the factor

$\sqrt{2\pi n}$, condition (A.8) readily becomes $x > (n+1)/e$. In practical calculations this condition is not critical and $x > n$ was also found to work. The calculations reported here used the $x > (n+1)/e$ criterion.

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APPENDIX B

FENDL/D-1.0

The decay library of the Fusion Energy Nuclear Data Library (FENDL), designated FENDL/D-1.0, was submitted by Westinghouse Hanford Company, United States of America. This file started with the Evaluated Nuclear Data File (ENDF)/B-VI decay data library and was supplemented by experimental data from the Evaluated Nuclear Data Structure File (ENDSF).

The ENDF/B-VI evaluations are full evaluations consisting of both experimental and theoretical data and meet the requirements of the ENDF/B-VI formats manual. Only experimental data are considered for ENSDF. Therefore, these data often lack information for various fields. The translation from ENSDF format into ENDF/B-VI format was accomplished by Brookhaven National Laboratory program RADLIST.

The decay library has data for over 2,800 isotopes. For over 1,200 of these isotopes, rather full data sets exist, including spectra for each radiation type. Only for those isotopes near particle lines of stability does the data set only contain half-life and decay mode information.

For more information, please contact Fred Mann, Westinghouse Hanford Company, 509-376-5728.

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APPENDIX C
RESULTS OF GAMMA ABSORPTION FRACTION ANALYSIS

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LIST OF FIGURES

C-1	Comparison of Original Spreadsheet Fits (QAD-FN) and New Simple Fit (MCNP) for Three Energies	C-1
C-2	Comparison of the Simple and Detailed MCNP 55-Gal Drum Models for Three Energies	C-2
C-3	55-Gal Drum Detailed MCNP Data--Extrapolated Versus MCNP Data Fits for Three Different Energies	C-3
C-4	Comparison of 55-Gal Drum Original Fits (QAD-FN) and Detailed MCNP Fits for Three Energies	C-4
C-5	Absorption Fraction Versus Energy for 55-Gal Drum as a Function of Density	C-5
C-6	Comparison of 4x4 Liner Fits (QAD-FN) and Detailed MCNP Fits for Three Energies	C-6
C-7	Absorption Fraction Versus Energy for 4x4 Liner as a Function of Density	C-7
C-8	Comparison of 5x5 Liner Fits (QAD-FN) and Detailed MCNP Fits for Three Energies	C-8
C-9	Absorption Fraction Versus Energy for 5x5 Liner as a Function of Density	C-9
C-10	Comparison of 6x6 Liner Fits (QAD-FN) and Detailed MCNP Fits for Three Energies	C-10
C-11	Absorption Fraction Versus Energy for 6x6 Liner as a Function of Density	C-11
C-12	Absorption Fraction Versus Energy for 30-Gal Drum as a Function of Density	C-12
C-13	Absorption Fraction Versus Energy for 85-Gal Drum Drum as a Function of Density	C-13
C-14	Absorption Fraction Versus Energy for Doorstop Sample Carrier as a Function of Density	C-14
C-15	Absorption Fraction Versus Energy for Ion Exchange Column as a Function of Density	C-15
C-16	Absorption Fraction Versus Energy for L4-56 Cask as a Function of Density	C-16
C-17	Absorption Fraction Versus Energy for Neutralized Current Acid Waste Cask as a Function of Density	C-17
C-18	Absorption Fraction Versus Energy for Onsite Transfer Cask as a Function of Density	C-18
C-19	Absorption Fraction Versus Energy for PAS-1 Cask as a Function of Density	C-19
C-20	Absorption Fraction Versus Energy for Sample Pig Carrier as a Function of Density	C-20
C-21	Absorption Fraction Versus Energy for Single Pass Fuel Cask as a Function of Density	C-21

LIST OF TABLES

C-1	Coefficients in Fits for the 55-Gal Drum	C-22
C-2	Coefficients in Fits for the 4x4 Liner	C-22
C-3	Coefficients in Fits for the 5x5 Liner	C-23
C-4	Coefficients in Fits for the 6x6 Liner	C-23
C-5	Coefficients in Fits for the 30-Gal Drum	C-24
C-6	Coefficients in Fits for the 85-Gal Drum	C-24
C-7	Coefficients in Fits for the Doorstop Sample Carrier	C-25
C-8	Coefficients in Fits for the Ion Exchange Column	C-25
C-9	Coefficients in Fits for the LR-56 Drum	C-26
C-10	Coefficients in Fits for the Neutralized Current Acid Waste Drum	C-26
C-11	Coefficients in Fits for the Onsite Transfer Cask Drum	C-27
C-12	Coefficients in Fits for the PAS-1 Drum	C-27
C-13	Coefficients in Fits for the Sample Pig Carrier	C-27
C-14	Coefficients in Fits for Single Pass Fuel Cask	C-28

Figure C-1. Comparison of Original Spreadsheet Fits (QAD-FN) and New Simple Fit (MCNP) for Three Energies.

Figure C-2. Comparison of the Simple and Detailed MCNP 55-Gal Drum Models for Three Energies.

Figure C-3. 55-Gal Drum Detailed MCNP Data--Extrapolated Versus MCNP Data Fits for Three Different Energies.

Figure C-4. Comparison of 55-Gal Drum Original Fits (QAD-FN) and Detailed MCNP Fits for Three Energies.

Figure C-5. Absorption Fraction Versus Energy
for 55-Gal Drum as a Function of Density.

Figure C-6. Comparison of 4x4 Liner Fits (QAD-FN) and Detailed MCNP Fits for Three Energies.

Figure C-7. Absorption Fraction Versus Energy
for 4x4 Liner as a Function of Density.

Figure C-8. Comparison of 5x5 Linear Fits (QAD-FN) and Detailed MCNP Fits for Three Energies.

Figure C-9. Absorption Fraction Versus Energy
for 5x5 Liner as a Function of Density.

Figure C-10. Comparison of 6x6 Liner Fits (QAD-FN) and Detailed MCNP Fits for Three Energies.

Figure C-11. Absorption Fraction Versus Energy
for 6x6 Liner as a Function of Density.

Figure C-12. Absorption Fraction Versus Energy
for 30-Gal Drum as a Function of Density.

Figure C-13. Absorption Fraction Versus Energy
for 85-Gal Drum as a Function of Density.

Figure C-14. Absorption Fraction Versus Energy for Doorstop Sample Carrier as a Function of Density.

Figure C-15. Absorption Fraction Versus Energy for Ion Exchange Column as a Function of Density.

Figure C-16. Absorption Fraction Versus Energy
for LR-56 Cask as a Function of Density.

Figure C-17. Absorption Fraction Versus Energy
for Neutralized Current Acid Waste Cask
as a Function of Density.

Figure C-18. Absorption Fraction Versus Energy for Onsite Transfer Cask as a Function of Density.

Figure C-19. Absorption Fraction Versus Energy
for PAS-1 Cask as a Function of Density.

Figure C-20. Absorption Fraction Versus Energy for Sample Pig Carrier as a Function of Density.

Figure C-21. Absorption Fraction Versus Energy for Single Pass Fuel Cask as a Function of Density.

Table C-1. Coefficients in Fits
for the 55-Gal Drum.

	Original spreadsheet fit (0.6 to 2.0 g/cm ³)	Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.388	0.00101	-0.00830
a ₂	-0.579	0.102	0.147
a ₃	-0.871	0.166	-0.0297
a ₄	-0.245	-0.391	-0.435
a ₅	1.354	-0.560	-0.200
a ₆	0.485	-0.153	0.0526
a ₇	0.954	1.53	1.42
a ₈	-0.937	0.317	-0.119
a ₉	3.302E-6	-0.494	-0.289

Table C-2. Coefficients in Fits
for the 4x4 Liner.

	Original spreadsheet fit (0.6 to 2.0 g/cm ³)	Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.0430	-0.2519	0.0467
a ₂	0.1060	0.4805	-0.1013
a ₃	0.1117	0.7487	-0.1710
a ₄	-0.5176	-0.5124	-0.2876
a ₅	-0.1340	-1.3558	0.5118
a ₆	-0.0547	-0.4187	0.1199
a ₇	1.3710	1.6326	0.8330
a ₈	-0.1371	0.6262	-0.5185
a ₉	-9.974E-07	-0.2683	0.2719

Table C-3. Coefficients in Fits
for the 5x5 Liner.

	Original spreadsheet fit (0.6 to 2.0 g/cm ³)	Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.0977	-0.2248	0.0577
a ₂	0.1972	0.3926	-0.1701
a ₃	0.2759	0.6650	-0.1984
a ₄	-0.5433	-0.4363	-0.2054
a ₅	-0.4227	-1.1072	0.6970
a ₆	-0.1576	-0.3517	0.1290
a ₇	1.4278	1.4005	0.5762
a ₈	0.0558	0.4535	-0.6044
a ₉	-1.554E-06	-0.0773	0.4572

Table C-4. Coefficients in Fits
for the 6x6 Liner.

	Original spreadsheet fit (0.6 to 2.0 g/cm ³)	Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.3207	-0.1469	0.0707
a ₂	0.5913	0.2187	-0.2684
a ₃	0.7477	0.4192	-0.2212
a ₄	-0.6337	-0.3129	-0.0598
a ₅	-1.2520	-0.5743	0.9229
a ₆	-0.4018	-0.1635	0.1318
a ₇	1.5491	1.0011	0.1662
a ₈	0.5016	0.0666	-0.6965
a ₉	-2.947E-06	0.2549	0.7427

Table C-5. Coefficients in Fits for the 30-Gal Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0757	-0.0381	a ₆	-0.0337	0.0073
a ₂	-0.0134	0.2453	a ₇	1.3683	1.5199
a ₃	-0.0470	0.0507	a ₈	0.1607	0.0640
a ₄	-0.3161	-0.4544	a ₉	-0.4864	-0.4315
a ₅	-0.2457	-0.4911			

Table C-6. Coefficients in Fits for the 85-Gal Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.0460	0.0029	a ₆	-0.1962	0.0688
a ₂	0.1670	0.1039	a ₇	1.5664	1.3546
a ₃	0.2751	-0.0612	a ₈	0.3380	-0.2045
a ₄	-0.4231	-0.4307	a ₉	-0.4365	-0.1980
a ₅	-0.6844	-0.0605			

Table C-7. Coefficients in Fits for the Doorstop Sample Carrier.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0274	-0.0137	a ₆	0.0153	-0.0185
a ₂	-0.0545	0.0508	a ₇	0.2080	0.4095
a ₃	-0.0649	0.0493	a ₈	-0.0011	0.0983
a ₄	0.0670	0.0002	a ₉	-0.0914	-0.1644
a ₅	0.0498	-0.2542			

Table C-8. Coefficients in Fits for the Ion Exchange Column.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0344	-0.0478	a ₆	-0.0672	-0.0044
a ₂	0.0526	0.2821	a ₇	1.4381	1.6473
a ₃	0.0323	0.0662	a ₈	0.1705	0.0819
a ₄	-0.3668	-0.5279	a ₉	-0.4383	-0.4401
a ₅	-0.3374	-0.5316			

Table C-9. Coefficients in Fits for the LR-56 Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.1318	0.0237	a ₆	-0.2163	0.0828
a ₂	0.2193	-0.0776	a ₇	1.1119	0.5732
a ₃	0.4107	-0.1213	a ₈	0.2043	-0.4850
a ₄	-0.3461	-0.2369	a ₉	0.1441	0.5214
a ₅	-0.6290	0.5039			

Table C-10. Coefficients in Fits for the Neutralized Current Acid Waste Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0418	-0.0051	a ₆	0.0458	-0.0046
a ₂	-0.0859	0.0152	a ₇	0.1171	0.2765
a ₃	-0.1131	0.0231	a ₈	-0.0697	0.0380
a ₄	0.0823	0.0333	a ₉	-0.0423	-0.0936
a ₅	0.1654	-0.1403			

Table C-11. Coefficients in Fits for the Onsite Transfer Cask Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0032	-0.0151	a ₆	0.0030	-0.0203
a ₂	-0.0122	0.0500	a ₇	0.1221	0.2972
a ₃	-0.0273	0.0464	a ₈	0.0091	0.0912
a ₄	0.0538	0.0024	a ₉	-0.0555	-0.1249
a ₅	0.0163	-0.2118			

Table C-12. Coefficients in Fits for the PAS-1 Drum.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0648	-0.0375	a ₆	-0.0284	-0.0206
a ₂	0.0051	0.2097	a ₇	1.1060	1.2686
a ₃	-0.0664	0.0858	a ₈	0.1916	0.1647
a ₄	-0.2162	-0.3014	a ₉	-0.4537	-0.4320
a ₅	-0.2378	-0.5672			

Table C-13. Coefficients in Fits for the Sample Pig Carrier.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	0.0030	-0.0011	a ₆	0.0036	-0.0074
a ₂	-0.0142	-0.0034	a ₇	0.0758	0.1443
a ₃	-0.0194	0.0181	a ₈	0.0069	0.0391
a ₄	0.0574	0.0508	a ₉	-0.0373	-0.0608
a ₅	0.0079	-0.0938			

Table C-14. Coefficients in Fits for Single Pass Fuel Cask.

	Fit for future implementation (0.6 to 3.0 g/cm ³)			Fit for future implementation (0.6 to 3.0 g/cm ³)	
	0.4 to 2.0 MeV	2.0 to 5.0 MeV		0.4 to 2.0 MeV	2.0 to 5.0 MeV
a ₁	-0.0088	0.0415	a ₆	-0.1320	0.1022
a ₂	0.0062	-0.1201	a ₇	1.1491	0.7474
a ₃	0.1559	-0.1408	a ₈	0.0653	-0.5095
a ₄	-0.3120	-0.2337	a ₉	-0.0476	0.2967
a ₅	-0.2010	0.5028			

APPENDIX D

INSTALLATION TEST CASES

Six Radcalc for Windows¹ cases were developed that test proper installation of Radcalc for Windows. Below is a list of the cases and some of the features addressed by each test problem. Radcalc for Windows Input Information and Calculated Results sheets follow. Users should run the six test cases after installation of Radcalc for Windows. The test cases are located in the /verify subdirectory included with the Radcalc for Windows executable files. Identical results indicate proper installation of Radcalc for Windows.

- TEST1.RAD 30-gal drum, liquid waste. Simplest case, tests basic functionality. Decay time before sealing is entered in years and seal time in days.
- TEST2.RAD PAS-1 cask containing "normal" solid waste. Uses the ^{241}Pu decay chain (^{241}Pu , to ^{241}Am to ^{237}Np to ^{233}Pa . . .) for a decay time of 200 years. This decay chain was chosen as a rigorous test of the decay calculations. Tests unit conversions from feet and pounds to centimeters and grams. Waste void volume calculated from difference between bulk density and true density.
- TEST3.RAD Doorstop sample carrier containing "special" solid waste. Uses the ^{241}Pu decay chain for a decay time of two years. Also tests the combination of G-values selected from the on-line database. Tests unit conversions from inches to centimeters. Tests the dating routine.
- TEST4.RAD Sample Pig carrier (smallest container type) containing "special" solid waste. Considers only hydrogen generated from beta radiation. Tests use of "mixed waste." Tests use of becquerels.
- TEST5.RAD Neutralized current acid waste cask containing "special" solid waste. Uses the iteration method for calculating to a specified target percent hydrogen. Uses ^{90}Y shipped as a medical isotope.
- TEST6.RAD LR-56 (largest container type) containing tritiated water. Uses the iteration method for calculating to a specified target percent hydrogen. Tests iteration technique for the case where the target percent is not reached within the maximum iteration time considered (100 years). Tests limited quantity calculation for tritiated water. Tests conversions from meters and kilograms to centimeters and grams. Tests the dating routine, including the final date calculated from the result of the iteration method.

¹ Windows is a trademark of Microsoft Corporation.

Radcalc for Windows 1.0

Date: 09-25-95 15:54

Performed By: _____

Checked By: _____

File: TEST1.RAD

===== Input Information =====

Source from input:
Radionuclide: Cs-137 Curies: 1.00e+001

Waste Form: Normal
Physical Form: Liquid
Container Type: 30 Gallon Drum

Package Void Volume: 7.00e+003 cc
Waste Volume: 1.10e+005 cc
Waste Mass: 1.00e+005 g
Waste True Density: 1.00 g/cc

Days to decay source before seal time: 365.24 days
Days container is sealed: 30.00 days

G Value Material Selection:
Contribution Weight G-Alpha G-Beta G-Gamma Name
100.00% 1 1.6 0.53 0.45 Water (liquid)
(0 indicates the value was calculated from a given value)

G Values calculated from list averaging:
G Alpha G Beta G Gamma
1.6 0.53 0.45

Comments:

===== Calculated Results =====

H2 Percent Concentration: 0.543 %
H2 Volume: 92.7 cc
H2 Generation Rate: 0.129 cc/hour

Heat Generated: 0.0472 Watts
Partial Pressure (H2): 0.553 kPa
Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.97716)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.32572)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
15g Fissile Radionuclides or Less: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.909 g/cc

Source decayed to start of seal time:
Radionuclide: Cs-137 Curies: 9.77e+000
Ba-137m 9.24e+000

Source decayed to end of seal time:
Radionuclide: Cs-137 Curies: 9.75e+000
Ba-137m 9.23e+000

Radcalc for Windows 1.0

Date: 09-25-95 15:55

Performed By: _____

Checked By: _____

File: TEST2.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Pu-241 1.00e+000

Waste Form: Normal
Physical Form: Solid
Container Type: PAS-1 Cask

	Entered Values:	Metric Values:
Package Void Volume:	1.62 ft^3	4.59e+004 cc
Waste Volume:	1.60 ft^3	4.53e+004 cc
Waste Mass:	200. lb	9.07e+004 g
Waste Void Volume:	0.100 ft^3	2.83e+003 cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 73050.00 days

Entered G Values:
G Alpha G Beta G Gamma
1 1 1

Comments:

===== Calculated Results =====

H2 Percent Concentration: 21.9 %
H2 Volume: 1.37e+004 cc
H2 Generation Rate: 0.00779 cc/hour

Heat Generated: 3.18e-005 Watts
Partial Pressure (H2): 28.4 kPa
Total Pressure (H2 and Air): 130. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 10.000)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 2.2046)
HRC Quantity Determination: No
Fissile Quantity: 0.0096736 g
15g Fissile Radionuclides or Less: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 2.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Pu-241 1.00e+000

Source decayed to end of seal time:
Radionuclide: Curies:
Pu-241 6.59e-005
Am-241 2.50e-002
Np-237 1.68e-006
Pa-233 1.68e-006
U-233 6.97e-010
Th-229 4.10e-012
Ra-225 4.10e-012
Ac-225 4.09e-012
Fr-221 4.09e-012
At-217 4.09e-012
Bi-213 4.09e-012
Po-213 4.00e-012
Pb-209 4.09e-012
U-237 1.62e-009

Radcalc for Windows 1.0

Date: 09-25-95 15:56

Performed By: _____

Checked By: _____

File: TEST3.RAD

===== Input Information =====

Source from input:
 Radionuclide: Pu-241 Curies: 1.00e+000

Waste Form: Special
 Physical Form: Solid
 Container Type: Doorstop Sample Carrier

	Entered Values:	Metric Values:
Package Void Volume:	2.40 in ³	39.3 cc
Waste Volume:	87.0 in ³	1.43e+003 cc
Waste Mass:	3.00 lb	1.36e+003 g
Waste Void Volume:	1.00 in ³	16.4 cc

Date to begin source decay: 8:00 Jul. 18, 1993
 Date container sealed: 8:00 Jul. 18, 1993
 Date container received: 8:00 Jul. 18, 1995
 Days to decay source before seal time: 0.00 days
 Days container is sealed: 730.00 days

G Value Material Selection:

Contribution	Weight	G-Alpha	G-Beta	G-Gamma	Name
30.00%	30	0.4*	0.1*	0.1	Dowex 50W
70.00%	70	0.36*	0.09*	0.09	Dowex 1

(* indicates the value was calculated from a given value)

G Values calculated from list averaging:

G Alpha	G Beta	G Gamma
0.372	0.093	0.093

Comments:

===== Calculated Results =====

H2 Percent Concentration: 5.87 %
 H2 Volume: 3.48 cc
 H2 Generation Rate: 0.000198 cc/hour

Heat Generated: 3.18e-005 Watts
 Partial Pressure (H2): 6.32 kPa
 Total Pressure (H2 and Air): 108. kPa

Radioactive: Yes
 Type Determination: A (from unity fraction 0.0010000)
 Limited Quantity: Yes
 LSA Determination: No (from LSA unity fraction 146.97)
 HRC Quantity Determination: No
 Fissile Quantity: 0.0096736 g
 15g Fissile Radionuclides or Less: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.954 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Pu-241	1.00e+000

Source decayed to end of seal time:

Radionuclide:	Curies:
Pu-241	9.08e-001
Am-241	3.05e-003
Np-237	1.02e-009
Pa-233	9.18e-010
U-233	2.59e-015
Th-229	1.14e-019
U-237	2.23e-005

Radcalc for Windows 1.0

Date: 09-25-95 15:56

Performed By: _____

Checked By: _____

File: TEST4.RAD

===== Input Information =====

Source from input:

Radionuclide:	Becquerels:
Sr-90	1.00e+010
M.F.P.	1.00e+010

Waste Form:	Normal
Physical Form:	Solid
Container Type:	Sample Pig Carrier

Package Void Volume:	1.00 cc
Waste Volume:	265. cc
Waste Mass:	264. g
Waste True Density:	1.00 g/cc

Days to decay source before seal time:	30.00 days
Days container is sealed:	7.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0.5	0

Comments:

===== Calculated Results =====

H2 Percent Concentration:	40.5 %
H2 Volume:	1.36 cc
H2 Generation Rate:	0.00811 cc/hour

Heat Generated:	0.00181 Watts
Partial Pressure (H2):	69.0 kPa
Total Pressure (H2 and Air):	170. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 1.3500)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 409.10)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
15g Fissile Radionuclides or Less:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	0.996 g/cc
---------------	------------

Source decayed to start of seal time:

Radionuclide:	Becquerels:
Sr-90	9.98e+009
Y-90	9.98e+009
M.F.P.	1.00e+010

Source decayed to end of seal time:

Radionuclide:	Becquerels:
Sr-90	9.98e+009
Y-90	9.98e+009
M.F.P.	1.00e+010

Radcalc for Windows 1.0

Date: 09-25-95 15:56

Performed By: _____

Checked By: _____

File: TEST5.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Y-90 1.00e+001 Medical Isotope

Waste Form: Normal
Physical Form: Solid
Container Type: NCAW

Package Void Volume: 100. cc
Waste Volume: 5.80e+003 cc
Waste Mass: 5.70e+003 g
Waste Void Volume: 100. cc

Days to decay source before seal time: 0.00 days
Calculate number of days sealed until 5.00% hydrogen is reached.

Entered G Values:
G Alpha G Beta G Gamma
1 1 1

Comments:

===== Calculated Results =====

The sealed container will generate 4.94 % hydrogen in 0.99 days

H2 Volume: 10.4 cc
H2 Generation Rate: 0.438 cc/hour

Heat Generated: 0.0554 Watts
Partial Pressure (H2): 5.27 kPa
Total Pressure (H2 and Air): 107. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 1.0000)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 5.8480)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
15g Fissile Radionuclides or Less: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.983 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Y-90 1.00e+001 Medical Isotope

Source decayed to end of seal time:
Radionuclide: Curies:
Y-90 7.73e+000 Medical Isotope

Radcalc for Windows 1.0

Date: 09-25-95 15:57

Performed By: _____

Checked By: _____

File: TEST6.RAD

===== Input Information =====

Source from input:
 Radionuclide: Curies:
 H-3 1.00e+002

Waste Form: Normal
 Physical Form: Tritiated Water
 Container Type: LR-56

	Entered Values:	Metric Values:
Package Void Volume:	0.700 m ³	7.00e+005 cc
Waste Volume:	4.20 m ³	4.20e+006 cc
Waste Mass:	4.20e+003 kg	4.20e+006 g
Waste Void Volume:	0.100 m ³	1.00e+005 cc

Date to begin source decay: 15:00 Jul. 24, 1995
 Date container sealed: 15:00 Jul. 24, 1995
 Days to decay source before seal time: 0.00 days
 Calculate number of days sealed until 5.00% hydrogen is reached.

G Value Material Selection:

Contribution	Weight	G-Alpha	G-Beta	G-Gamma	Name
100.00%	1	1.6	0.53	0.45	Water (liquid)

(* indicates the value was calculated from a given value)

G Values calculated from list averaging:

G Alpha	G Beta	G Gamma
1.6	0.53	0.45

Comments:

===== Calculated Results =====

The hydrogen concentration of 5.00 % was not calculated in 36500.00 days.
 The hydrogen concentration of 0.311 % is calculated at 36500.00 days.
 This corresponds to date: 15:00 Jun. 29, 2095
 H2 Volume: 2.50e+003 cc
 H2 Generation Rate: 0.00285 cc/hour

Heat Generated: 0.00337 Watts
 Partial Pressure (H2): 0.316 kPa
 Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
 Type Determination: A (from unity fraction 0.10000)
 Limited Quantity: Yes
 LSA Determination: Yes (from LSA unity fraction 0.079365)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 15g Fissile Radionuclides or Less: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
 Radionuclide: Curies:
 H-3 1.00e+002

Source decayed to end of seal time:
 Radionuclide: Curies:
 H-3 3.66e-001

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APPENDIX E
VALIDATION CASES

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CONTENTS

I	HYDROGEN GAS GENERATION	E-1
IA	COMPARISONS TO RADCALC SPREADSHEET	E-1
	Case IA1: 55-Gal Drum--Dewatered Resin	E-1
	Case IA2: 55-Gal Drum--Solidified Concentrates	E-8
	Case IA3: 55-Gal Drum--Cartridge Filter	E-15
	Case IA4: 4X4 Liner--Dewatered Resin	E-22
	Case IA5: 4X4 Liner--Solidified Concentrates	E-29
	Case IA6: 4X4 Liner--Cartridge Filter	E-36
	Case IA7: 5X5 Liner--Dewatered Resin	E-43
	Case IA8: 5X5 Liner--Solidified Concentrates	E-50
	Case IA9: 5X5 Liner--Cartridge Filter	E-57
	Case IA10: 6X6 Liner--Dewatered Resin	E-64
	Case IA11: 6X6 Liner--Solidified Concentrates	E-71
	Case IA12: 6X6 Liner--Cartridge Filter	E-78
IB	GAMMA ABSORPTION FRACTIONS FOR VARIOUS CONTAINER TYPES	E-85
	Case IB1: 30-Gal Drum	E-85
	Case IB2: Single Pass Fuel Cask	E-87
	Case IB3: Sample Pig Carrier	E-89
	Case IB4: LR-56 Container	E-91
IC	USE OF G VALUES	E-93
	Case IC1: G Values Selected from Radcalc's Database, Using a Single Absorbing Material and a Beta/Gamma Source	E-93
	Case IC2: G Values Selected from Radcalc's Database, Using Two Absorbing Materials and an Alpha Source	E-95
	Case IC3: G Values Entered Directly, With All G Values Equal	E-97
	Case IC4: G Values Entered Directly, Using Only a G-Beta Value	E-99
	Case IC5: G Values Entered Directly, Using Only G-Beta and G-Gamma Values	E-101
ID	PERCENT HYDROGEN	E-103
	Case ID1: Percent Hydrogen Using Direct Entry of Interstitial Void Volume	E-103
	Case ID2: Percent Hydrogen Using a Calculation of Interstitial Void Volume	E-103
CASE IE:	HYDROGEN GENERATION RATE	E-103
II	DECAY ALGORITHMS	E-104
IIA	ACTIVITY AS A FUNCTION OF TIME	E-104
	Case IIA1: Simple Decay	E-104
	Case IIA2: Parent-Daughter Decay	E-104
	Case IIA3: Complex Decay Chain	E-105
IIB	INTEGRATED DISINTEGRATIONS OVER TIME	E-105
	Case IIB1: Simple Decay	E-106
	Case IIB2: Parent-Daughter Decay	E-106
	Case IIB3: Complex Decay Chain	E-107

CONTENTS (cont)

IIIA	TRANSPORTATION CALCULATIONS	E-107
Case IIIA1:	Type Classification for a Normal Form Material	E-108
Case IIIA2:	Type Classification for a Special Form Material	E-111
Case IIIA3:	Limited Quantity Classification for a Special Form Material	E-113
Case IIIA4:	Limited Quantity Classification for a Normal Form Material	E-116
Case IIIA5:	Limited Quantity Classification for a Liquid Form Material	E-118
Case IIIA6:	Limited Quantity Classification for Tritiated Water With a Low Specific Activity (< 0.1 Ci/L)	E-120
Case IIIA7:	Limited Quantity Classification for Tritiated Water With an Intermediate Specific Activity (≥ 0.1 Ci/L and ≤ 1.0 Ci/L)	E-123
Case IIIA8:	Limited Quantity Classification for Tritiated Water With a High Specific Activity (> 1.0 Ci/L)	E-125
Case IIIA9:	Limited Quantity Classification for Tritiated Water Containing Other Radionuclides	E-127
Case IIIA10:	Low Specific Activity Classification for a Type A Package With Low A_2 Values (≤ 0.05 Ci)	E-129
Case IIIA11:	Low Specific Activity Classification for a Type B Package With Intermediate A_2 Values (> 0.05 Ci and ≤ 1.0 Ci)	E-134
Case IIIA12:	Low Specific Activity Classification for a Type B Package With High A_2 Values (> 1.0 Ci)	E-137
Case IIIA13:	Low Specific Activity Classification for a Type A Package With Mixed A_2 Values	E-139
Case IIIA14:	Highway Route Controlled Quantity Classification for a Package With a Unity Fraction $> 3,000$	E-141
Case IIIA15:	Highway Route Controlled Quantity Classification for a Package With a Total Activity $> 30,000$ Ci	E-144
Case IIIA16:	Highway Route Controlled Quantity Classification for a Package With a Unity Fraction = 3,000 and an Activity = 30,000 Ci	E-146
Case IIIA17:	Fissile Excepted Classification	E-148
Case IIIA18:	Radioactive Material Classification	E-151

CONTENTS (cont)

IV	OTHER RADCALC FEATURES	E-154
IVA	UNIT CONVERSION	E-154
	Case IVA1: Feet/Pounds to Centimeters/Grams	E-154
	Case IVA2: Inches/Pounds to Centimeters/Grams	E-154
	Case IVA3: Meters/Kilograms to Centimeters/Grams	E-154
	Case IVA4: Becquerels to Curies	E-155
	Case IVA5: Container Information Dialog Box	
	Unit Conversions	E-158
IVB	TARGET PERCENT SPECIFIED	E-159
	Case IVB1: Target Percent Reached	E-159
	Case IVB2: Target Percent Not Reached	E-161
IVC	DATING ROUTINE	E-161
	Case IVC1: Length of Month	E-161
	Case IVC2: Leap Years	E-163
	Case IVC3: Calculation of End Date Given Start Date and Time Interval	E-163
CASE IVD:	BULK DENSITY	E-163
CASE IVE:	HEAT GENERATION	E-164
IVF	PRESSURE	E-164
	Case IVF1: Partial Pressure of Hydrogen	E-164
	Case IVF2: Total Pressure	E-164

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APPENDIX E

VALIDATION CASES

I HYDROGEN GAS GENERATION

IA COMPARISONS TO RADCALC SPREADSHEET

Cases IA1 - IA12 compare Radcalc for Windows¹ with the Excel version of the Radcalc spreadsheet (which is based on the original Electric Power Research Institute [EPRI] spreadsheet) for the four geometries that the two codes have in common (55-gal drum, 4x4 liner, 5x5 liner, 6x6 liner). Three of the cases are also documented in the Analytical Resources (1994) manual for the U.S. Department of Energy (DOE) hydrogen gas training workshop. The workshop manual presents results from the original EPRI spreadsheet.

Case IA1: 55-Gal Drum--Dewatered Resin

Discussion and Conclusion

Information for dewatered ion exchange resins contained in a 55-gal drum was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ⁹⁰Sr, ¹³⁷Cs, and ¹⁴⁴Ce; however, in Radcalc for Windows the daughter products were added to the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows gives 0.860% H₂ concentration and the spreadsheet 0.820%. The difference of 0.040 reflects a 4.65% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

¹Windows is a trademark of Microsoft Corporation.

Radcalc for Windows 1.0

Date: 09-23-95 12:36

Performed By: J Green

Checked By: _____

File: IA1.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
Physical Form: Liquid
Container Type: 55 Gallon Drum

	Entered Values:	Metric Values:
Package Void Volume:	10.0 ft ³	2.83e+005 cc
Waste Volume:	110. ft ³	3.12e+006 cc
Waste Mass:	4.70e+003 lb	2.13e+006 g
Waste True Density:	65.0 lb/ft ³	1.04 g/cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.5	0.5	0.5

Comments:

Case IA1
Dewatered Resin
55 Gallon Drum

===== Calculated Results =====

H2 Percent Concentration: 0.860 %
H2 Volume: 1.17e+004 cc
H2 Generation Rate: 0.668 cc/hour

Heat Generated: 0.329 Watts
Partial Pressure (H2): 0.879 kPa
Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 27.700)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.98268)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.684 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA1.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattage..		CHECKED:	
RP Genoni/JG Field, Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description	>	Dewatered Resin	
"	>	55 Gallon Drum	
"	>		
Enter waste form ("Special" or "Normal")	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")	>	Liquid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner	>	1	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations	>	06/26/90	
Enter date last sealed*	>	06/26/90	>>
Enter date to be shipped	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt	>	06/26/92	
CALCULATED Decay before sealing (years)	=	0.00	Days= 0
CALCULATED Decay before shipment (years)	=	0.00	Days= 0
CALCULATED Duration package is sealed (years)	=	2.00	Days= 731
Enter package interior volume	>	120.0	ft ³
Enter waste volume	>	110.0	ft ³
CALCULATED Container void volume:		10.0	ft ³
Enter estimated waste void volume	>		ft ³
** OR **			
Enter waste true density (vendor data)	>	65.0	Lbs/ft ³
CALCULATED Waste void fraction	=	0.342	
CALCULATED Waste void volume	=	37.66	ft ³
CALCULATED Package interior volume	=	3.398E+06	cc
CALCULATED Waste volume	=	3.115E+06	cc
CALCULATED Total void volume	=	1.350E+06	cc
Enter waste weight	>	4700	Lbs
CALCULATED Weight	=	2.134E+06	gms
CALCULATED Waste bulk density	=	0.6850	gms/cc
Enter G-H2 (molecules/100 ev)	>	0.50	
OR			
Enter volume cation resin (cu ft)	>		
Enter volume anion resin (cu ft)	>		

Enter volume mix bed resin (cu ft)-----	>			
Enter volume other resin (cu ft)-----	>			
Enter G-H2 of other resin-----	>			
CALCULATED G-H2 for waste =	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =	=	4.490E+05	Rads	
H2 Volume =	=	1.116E+04	cm3	
H2 Concentration =	=	0.820	%	
H2 Generation Rate =	=	6.361E-01	cc/hr	
Pressure Buildup Rate =	=	1.664E-04	psi/day	
Pressure (seal to ship) =	=	0.00	psi	
Enter Measured H2 Concentration (if known)-----	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =	=	0.00		
Activity Summary @ Shipment:				
Total Activity* =	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =	=	0.013	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years -----	-----	1.018E+01	µCi/cc	
T 1/2 > 5 Years -----	-----	8.026E+00	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) -----	-----	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A) -----	-----	0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) -----	-----	0.000	gms	
Other DOE Accountable Material (DOE 5633.3) -----	-----	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics -----	-----	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes -----	-----	0.000	A	Class B
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Sr-90
Table 2 Isotopes -----	-----	81.884	A	
(Short Lived)		0.058	B	Miscellaneous
		0.001	C	
Transportation Classification:				
LSA Determination -----	-----	9.865E-01	LSA	
Type Determination -----	-----	2.785E+01	LSA, > Type 'A'	

INPUT: LISTED ISOTOPES (**** = Daughter Product)					Curies when Sealed	Curies when Shipped
Total Curies	Curies	or	%			
(ONLY if entering %) =					xxxxx	xxxxx
H-3					0.000E+00	0.000E+00
C-14					0.000E+00	0.000E+00
Na-22					0.000E+00	0.000E+00
Cr-51					0.000E+00	0.000E+00
Mn-54	2.000E+00				2.000E+00	2.000E+00
Fe-55					0.000E+00	0.000E+00
Co-57					0.000E+00	0.000E+00
Co-58	1.000E+01				9.996E+00	9.996E+00
Fe-59					0.000E+00	0.000E+00
Ni-59					0.000E+00	0.000E+00
Co-60	1.000E+01				1.000E+01	1.000E+01
Ni-63					0.000E+00	0.000E+00
Zn-65					0.000E+00	0.000E+00
Se-79					0.000E+00	0.000E+00
Kr-85					0.000E+00	0.000E+00
Sr-89					0.000E+00	0.000E+00
Sr-90	1.000E+01				1.000E+01	1.000E+01
Y-90	****		****		1.000E+01	1.000E+01
Y-91					0.000E+00	0.000E+00
Zr-93					0.000E+00	0.000E+00
Nb-93m					0.000E+00	0.000E+00
Nb-94					0.000E+00	0.000E+00
Zr-95	3.000E+00				2.999E+00	2.999E+00
Nb-95					0.000E+00	0.000E+00
Nb-95m					0.000E+00	0.000E+00
Tc-99					0.000E+00	0.000E+00
Ru-103					0.000E+00	0.000E+00
Rh-103m	****		****		0.000E+00	0.000E+00
Ru-106					0.000E+00	0.000E+00
Rh-106	****		****		0.000E+00	0.000E+00
Pd-107					0.000E+00	0.000E+00
Cd-109					0.000E+00	0.000E+00
Ag-110m					0.000E+00	0.000E+00
Ag-110	****		****		0.000E+00	0.000E+00
Sn-113					0.000E+00	0.000E+00
In-113m	****		****		0.000E+00	0.000E+00
Cd-113m					0.000E+00	0.000E+00
Cd-115m					0.000E+00	0.000E+00
Sn-119m					0.000E+00	0.000E+00
Sn-121m					0.000E+00	0.000E+00
Sn-123					0.000E+00	0.000E+00
Tc-123m					0.000E+00	0.000E+00
Sb-124					0.000E+00	0.000E+00
Sb-125					0.000E+00	0.000E+00
Tc-125m					0.000E+00	0.000E+00
Sn-126					0.000E+00	0.000E+00
Sb-126m	****		****		0.000E+00	0.000E+00
Sb-126					0.000E+00	0.000E+00
Tc-127m					0.000E+00	0.000E+00
Tc-127	****		****		0.000E+00	0.000E+00

E-7

Case IA2: 55-Gal Drum--Solidified Concentrates**Discussion and Conclusion**

Information for solidified concentrates contained in a 55-gal drum was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were added to the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 4.70% and the spreadsheet a concentration of 4.47%. The difference of 0.23 reflects a 4.98% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:37

Performed By: J Green

Checked By: _____

File: IA2.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Solid
 Container Type: 55 Gallon Drum

	Entered Values:	Metric Values:
Package Void Volume:	5.00 ft ³	1.42e+005 cc
Waste Volume:	45.0 ft ³	1.27e+006 cc
Waste Mass:	4.20e+003 lb	1.91e+006 g
Waste Void Volume:	0.000 ft ³	0.000 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.24	0.24	0.24

Comments:

Case IA2
 Solidified Concentrates
 55 Gallon Drum

===== Calculated Results =====

H2 Percent Concentration: 4.70 %
 H2 Volume: 6.98e+003 cc
 H2 Generation Rate: 0.398 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 4.99 kPa
 Total Pressure (H2 and Air): 106. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 1.0997)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 1.49 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA2.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wottage..		CHECKED:	
RP Genoni/JG Field, Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description-----	>		Solidified Concentrates
"-----	>		55 Gallon Drum
"-----	>		
Enter waste form ("Special" or "Normal")-----	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")-----	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")-----	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1-55 gal. drum, 2-4x4 liner-----	>	1	>> Req'd input for H2 calculations
3-5x5 liner, 4-6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")-----	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations-----	>	06/26/90	
Enter date last sealed*-----	>	06/26/90	>>
Enter date to be shipped-----	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt-----	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume-----	>	50.0	ft ³
Enter waste volume-----	>	45.0	ft ³
CALCULATED Container void volume:		5.0	ft ³
Enter estimated waste void volume-----	>	0.0	ft ³
** OR **			
Enter waste true density (vendor data)-----	>		Lbs/ft ³
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	ft ³
CALCULATED Package interior volume =		1.416E+06	cc
CALCULATED Waste volume =		1.274E+06	cc
CALCULATED Total void volume =		1.416E+05	cc
Enter waste weight-----	>	4200	Lbs
CALCULATED Weight =		1.907E+06	gms
CALCULATED Waste bulk density =		1.4964	gms/cc
Enter G-H2 (molecules/100 ev)-----	>	0.24	
OR			
Enter volume cation resin (cu ft)-----	>		
Enter volume anion resin (cu ft)-----	>		

Enter volume mix bed resin (cu ft) _____	>			
Enter volume other resin (cu ft) _____	>			
Enter G-H2 of other resin _____	>			
CALCULATED G-H2 for waste	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose	=	6.211E+05	Rads	
H2 Volume	=	6.623E+03	cm3	
H2 Concentration	=	4.47	%	
H2 Generation Rate	=	3.775E-01	cc/hr	
Pressure Buildup Rate	=	9.412E-04	psi/day	
Pressure (seal to ship)	=	0.00	psi	
Enter Measured H2 Concentration (if known) _____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations	=	0.00		
Activity Summary @ Shipment:				
Total Activity*	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total*	=	0.033	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years	=	2.489E+01	μCi/cc	
T 1/2 > 5 Years	=	1.962E+01	μCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment	=	0.344	Watts	
or	=	1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71)	=	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)	=	0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM)	=	0.000	gms	
Other DOE Accountable Material (DOE 5633.3)	=	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics	=	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes	=	0.000	A	Class B
(Long Lived)	=	N/A	B	
	=	0.000	C	Limiting Isotope
				Sr-90
Table 2 Isotopes	=	200.162	A	
(Short Lived)	=	0.141	B	Miscellaneous
	=	0.002	C	
Transportation Classification:				
LSA Determination	=	1.104E+00	> LSA	
Type Determination	=	2.785E+01	Type 'B'	

INPUT: LISTED ISOTOPES						
(**** = Daughter Product)						
Total Curies	Curies	or	%	Curies when Sealed	Curies when Shipped	
(ONLY if entering %) =				xxxxx	xxxxx	
H-3→				0.000E+00	0.000E+00	
C-14→				0.000E+00	0.000E+00	
Na-22→				0.000E+00	0.000E+00	
Cr-51→				0.000E+00	0.000E+00	
Mn-54→	2.000E+00			2.000E+00	2.000E+00	
Fe-55→				0.000E+00	0.000E+00	
Co-57→				0.000E+00	0.000E+00	
Co-58→	1.000E+01			9.996E+00	9.996E+00	
Fe-59→				0.000E+00	0.000E+00	
Ni-59→				0.000E+00	0.000E+00	
Co-60→	1.000E+01			1.000E+01	1.000E+01	
Ni-63→				0.000E+00	0.000E+00	
Zn-65→				0.000E+00	0.000E+00	
Se-79→				0.000E+00	0.000E+00	
Kr-85→				0.000E+00	0.000E+00	
Sr-89→				0.000E+00	0.000E+00	
Sr-90→	1.000E+01			1.000E+01	1.000E+01	
Y-90→	****		****	1.000E+01	1.000E+01	
Y-91→				0.000E+00	0.000E+00	
Zr-93→				0.000E+00	0.000E+00	
Nb-93m→				0.000E+00	0.000E+00	
Nb-94→				0.000E+00	0.000E+00	
Zr-95→	3.000E+00			2.999E+00	2.999E+00	
Nb-95→				0.000E+00	0.000E+00	
Nb-95m→				0.000E+00	0.000E+00	
Tc-99→				0.000E+00	0.000E+00	
Ru-103→				0.000E+00	0.000E+00	
Rh-103m→	****		****	0.000E+00	0.000E+00	
Ru-106→				0.000E+00	0.000E+00	
Rh-106→	****		****	0.000E+00	0.000E+00	
Pd-107→				0.000E+00	0.000E+00	
Cd-109→				0.000E+00	0.000E+00	
Ag-110m→				0.000E+00	0.000E+00	
Ag-110→	****		****	0.000E+00	0.000E+00	
Sn-113→				0.000E+00	0.000E+00	
In-113m→	****		****	0.000E+00	0.000E+00	
Cd-113m→				0.000E+00	0.000E+00	
Cd-115m→				0.000E+00	0.000E+00	
Sn-119m→				0.000E+00	0.000E+00	
Sn-121m→				0.000E+00	0.000E+00	
Sn-123→				0.000E+00	0.000E+00	
Te-123m→				0.000E+00	0.000E+00	
Sb-124→				0.000E+00	0.000E+00	
Sb-125→				0.000E+00	0.000E+00	
Te-125m→				0.000E+00	0.000E+00	
Sn-126→				0.000E+00	0.000E+00	
Sb-126m→	****		****	0.000E+00	0.000E+00	
Sb-126→				0.000E+00	0.000E+00	
Te-127m→				0.000E+00	0.000E+00	
Te-127→	****		****	0.000E+00	0.000E+00	

Case IA3: 55-Gal Drum--Cartridge Filter**Discussion and Conclusion**

Information for a cartridge filter contained in a 55-gal drum was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The input values for this case were taken from the DOE hydrogen gas generation workshop manual (Analytical Resources 1994). The manual case was run on the original EPRI spreadsheet on which the Excel version of the Radcalc spreadsheet is based. The inventory consists of eight radionuclides. The Radcalc spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 1.18% and the Excel spreadsheet a concentration of 1.13%, which agrees with the DOE manual output value. The difference of 0.05 reflects a 4.24% difference between the code and the spreadsheets. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:37

Performed By: J. Green

Checked By: _____

File: IA3.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Solid
 Container Type: 55 Gallon Drum

	Entered Values:	Metric Values:
Package Void Volume:	6.38 ft ³	1.81e+005 cc
Waste Volume:	0.825 ft ³	2.34e+004 cc
Waste Mass:	47.0 lb	2.13e+004 g
Waste Void Volume:	0.410 ft ³	1.16e+004 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.09	0.09	0.09

Comments:

Case IA3
 Cartridge Filter
 55 Gallon Drum

===== Calculated Results =====

H2 Percent Concentration: 1.18 %
 H2 Volume: 2.30e+003 cc
 H2 Generation Rate: 0.131 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 1.21 kPa
 Total Pressure (H2 and Air): 103. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 98.268)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.912 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA3.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Delete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattage..		CHECKED:	
RP Genoni/JG Field..Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description-----	>	Cartridge Filter	
"-----	>	55 Gallon Drum	
"-----	>		
Enter waste form ("Special" or "Normal")-----	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")-----	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")-----	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner-----	>	1	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")-----	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations-----	>	06/26/90	
Enter date last sealed-----	>	06/26/90	>>
Enter date to be shipped-----	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt-----	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume-----	>	7.2	ft ³
Enter waste volume-----	>	0.8	ft ³
CALCULATED Container void volume:		6.4	ft ³
Enter estimated waste void volume-----	>	0.4	ft ³
** OR **			
Enter waste true density (vendor data)-----	>	0.0	Lbs/ft ³
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	ft ³
CALCULATED Package interior volume =		2.039E+05	cc
CALCULATED Waste volume =		2.336E+04	cc
CALCULATED Total void volume =		1.921E+05	cc
Enter waste weight-----	>	47	Lbs
CALCULATED Weight =		2.134E+04	gms
CALCULATED Waste bulk density =		0.9134	gms/cc
Enter G-H2 (molecules/100 ev)-----	>	0.09	
OR			
Enter volume cation resin (cu ft)-----	>		
Enter volume anion resin (cu ft)-----	>		

Enter volume mix bed resin (cu ft)_____	>			
Enter volume other resin (cu ft)_____	>			
Enter G-H2 of other resin_____	>			
CALCULATED G-H2 for waste =		0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =		4.904E+07	Rads	
H2 Volume =		2.194E+03	cm3	
H2 Concentration =		1.13	%	
H2 Generation Rate =		1.251E-01	cc/hr	
Pressure Buildup Rate =		2.298E-04	psi/day	
Pressure (seal to ship) =		0.00	psi	
Enter Measured H2 Concentration (if known)_____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =		0.00		
Activity Summary @ Shipment:				
Total Activity* =		4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =		1.776	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years =		1.358E+03	µCi/cc	
T 1/2 > 5 Years =		1.070E+03	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =		0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) =		0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) =		0.000	gms	
Other DOE Accountable Material (DOE 5633.3) =		0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics =		0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes =	Unity Fraction			Classification
(Long Lived)	0.000	A		Class C
	N/A	B		
	0.000	C		Limiting Isotope
				Cs-137
Table 2 Isotopes =	10917.908	A		
(Short Lived)	7.718	B		Miscellaneous
	0.108	C		
Transportation Classification:				
LSA Determination =	Unity Fraction			
Type Determination =	9.865E+01	> LSA		
	2.785E+01	Type B'		

INPUT: LISTED ISOTOPES					
(* * * * = Daughter Product)					
Total Curies	Curies	or	%	Curies when Sealed	Curies when Shipped
(ONLY if entering %) =				xxxxx	xxxxx
H-3-->				0.000E+00	0.000E+00
C-14-->				0.000E+00	0.000E+00
Na-22-->				0.000E+00	0.000E+00
Cr-51-->				0.000E+00	0.000E+00
Mn-54-->	2.000E+00			2.000E+00	2.000E+00
Fe-55-->				0.000E+00	0.000E+00
Co-57-->				0.000E+00	0.000E+00
Co-58-->	1.000E+01			9.996E+00	9.996E+00
Fe-59-->				0.000E+00	0.000E+00
Ni-59-->				0.000E+00	0.000E+00
Co-60-->	1.000E+01			1.000E+01	1.000E+01
Ni-63-->				0.000E+00	0.000E+00
Zn-65-->				0.000E+00	0.000E+00
Se-79-->				0.000E+00	0.000E+00
Kr-85-->				0.000E+00	0.000E+00
Sr-89-->				0.000E+00	0.000E+00
Sr-90-->	1.000E+01			1.000E+01	1.000E+01
Y-90-->	****		****	1.000E+01	1.000E+01
Y-91-->				0.000E+00	0.000E+00
Zr-93-->				0.000E+00	0.000E+00
Nb-93m-->				0.000E+00	0.000E+00
Nb-94-->				0.000E+00	0.000E+00
Zr-95-->	3.000E+00			2.999E+00	2.999E+00
Nb-95-->				0.000E+00	0.000E+00
Nb-95m-->				0.000E+00	0.000E+00
Tc-99-->				0.000E+00	0.000E+00
Ru-103-->				0.000E+00	0.000E+00
Rh-103m-->	****		****	0.000E+00	0.000E+00
Ru-106-->				0.000E+00	0.000E+00
Rh-106-->	****		****	0.000E+00	0.000E+00
Pd-107-->				0.000E+00	0.000E+00
Cd-109-->				0.000E+00	0.000E+00
Ag-110m-->				0.000E+00	0.000E+00
Ag-110-->	****		****	0.000E+00	0.000E+00
Sn-113-->				0.000E+00	0.000E+00
In-113m-->	****		****	0.000E+00	0.000E+00
Cd-113m-->				0.000E+00	0.000E+00
Cd-115m-->				0.000E+00	0.000E+00
Sn-119m-->				0.000E+00	0.000E+00
Sn-121m-->				0.000E+00	0.000E+00
Sn-123-->				0.000E+00	0.000E+00
Te-123m-->				0.000E+00	0.000E+00
Sb-124-->				0.000E+00	0.000E+00
Sb-125-->				0.000E+00	0.000E+00
Te-125m-->				0.000E+00	0.000E+00
Sn-126-->				0.000E+00	0.000E+00
Sb-126m-->	****		****	0.000E+00	0.000E+00
Sb-126-->				0.000E+00	0.000E+00
Te-127m-->				0.000E+00	0.000E+00
Te-127-->	****		****	0.000E+00	0.000E+00

E-21

Case IA4: 4X4 Liner--Dewatered Resin**Discussion and Conclusion**

Information for dewatered ion exchange resins contained in a 4x4 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows gives 1.03% H_2 concentration and the spreadsheet 0.976%. The difference of 0.054 reflects a 5.24% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:38

Performed By: J. Grew

Checked By: _____

File: 1A4.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Liquid
 Container Type: 4 x 4 Liner

	Entered Values:	Metric Values:
Package Void Volume:	10.0 ft ³	2.83e+005 cc
Waste Volume:	110. ft ³	3.12e+006 cc
Waste Mass:	4.70e+003 lb	2.13e+006 g
Waste True Density:	65.0 lb/ft ³	1.04 g/cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.5	0.5	0.5

Comments:

Case 1A4
 Dewatered Resin
 4X4 Liner

===== Calculated Results =====

H2 Percent Concentration: 1.03 %
 H2 Volume: 1.41e+004 cc
 H2 Generation Rate: 0.803 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 1.06 kPa
 Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: Yes (from LSA unity fraction 0.98268)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.684 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA4.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wastage..		CHECKED:	
RP Genoni/JG Field.. Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description_____	>		Dewatered Resin
"_____	>		4x4 Liner
"_____	>		
Enter waste form ("Special" or "Normal")_____	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")_____	>	Liquid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")_____	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner_____	>	2	>> Req'd input for H2 calculations
3=5x3 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")_____	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations _____	>	06/26/90	
Enter date last sealed*_____	>	06/26/90	>>
Enter date to be shipped_____	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt_____	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume_____	>	120.0	Ft3
Enter waste volume_____	>	110.0	Ft3
CALCULATED Container void volume:		10.0	Ft3
Enter estimated waste void volume_____	>		Ft3
** OR **			
Enter waste true density (vendor data)_____	>	65.0	Lbm/Ft3
CALCULATED Waste void fraction =		0.342	
CALCULATED Waste void volume =		37.66	Ft3
CALCULATED Package interior volume =		3.398E+06	cc
CALCULATED Waste volume =		3.115E+06	cc
CALCULATED Total void volume =		1.350E+06	cc
Enter waste weight_____	>	4700	Lbm
CALCULATED Weight =		2.134E+06	gms
CALCULATED Waste bulk density =		0.6850	gms/cc
Enter G-H2 (molecules/100 ev)_____	>	0.50	
OR			
Enter volume cation resin (cu ft)_____	>		
Enter volume anion resin (cu ft)_____	>		

Enter volume mix bed resin (cu ft)_____	>			
Enter volume other resin (cu ft)_____	>			
Enter G-H2 of other resin_____	>			
CALCULATED G-H2 for waste =		0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =		5.353E+05	Rads	
H2 Volume ~		1.331E+04	cm3	
H2 Concentration =		0.976	%	
H2 Generation Rate =		7.584E-01	cc/hr	
Pressure Buildup Rate =		1.984E-04	psi/day	
Pressure (seal to ship) =		0.00	psi	
Enter Measured H2 Concentration (if known)_____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =		0.00		
Activity Summary @ Shipment:				
Total Activity* =		4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =		0.013	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years =		1.018E+01	µCi/cc	
T 1/2 > 5 Years =		8.026E+00	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =		0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) =		0.000	gms	
Other DOE Fissile Material (DOE 5480.1A) =		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) =		0.000	gms	
Other DOE Accountable Material (DOE 5633.3) =		0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics =		0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes =	Unity Fraction			Classification
(Long Lived)	0.000	A		Class B
	N/A	B		
	0.000	C		Limiting Isotope
				Sr-90
Table 2 Isotopes =	81.884	A		
(Short Lived)	0.058	B		Miscellaneous
	0.001	C		
Transportation Classification:				
LSA Determination =	9.865E-01	LSA		
Type Determination =	2.785E+01	LSA, > Type 'A'		

INPUT: LISTED ISOTOPES						
(**** = Daughter Product)					Curies when	Curies when
	Total Curies	Curies	or	%	Sealed	Shipped
(ONLY if entering %) =					XXXXX	XXXXX
	H-3-->				0.000E+00	0.000E+00
	C-14-->				0.000E+00	0.000E+00
	Na-22-->				0.000E+00	0.000E+00
	Cr-51-->				0.000E+00	0.000E+00
	Mn-54-->	2.000E+00			2.000E+00	2.000E+00
	Fe-55-->				0.000E+00	0.000E+00
	Co-57-->				0.000E+00	0.000E+00
	Co-58-->	1.000E+01			9.996E+00	9.996E+00
	Fe-59-->				0.000E+00	0.000E+00
	Ni-59-->				0.000E+00	0.000E+00
	Co-60-->	1.000E+01			1.000E+01	1.000E+01
	Ni-63-->				0.000E+00	0.000E+00
	Zn-65-->				0.000E+00	0.000E+00
	Se-79-->				0.000E+00	0.000E+00
	Kr-85-->				0.000E+00	0.000E+00
	Sr-89-->				0.000E+00	0.000E+00
	Sr-90-->	1.000E+01			1.000E+01	1.000E+01
	Y-90-->	****		****	1.000E+01	1.000E+01
	Y-91-->				0.000E+00	0.000E+00
	Zr-93-->				0.000E+00	0.000E+00
	Nb-93m-->				0.000E+00	0.000E+00
	Nb-94-->				0.000E+00	0.000E+00
	Zr-95-->	3.000E+00			2.999E+00	2.999E+00
	Nb-95-->				0.000E+00	0.000E+00
	Nb-95m-->				0.000E+00	0.000E+00
	Tc-99-->				0.000E+00	0.000E+00
	Ru-103-->				0.000E+00	0.000E+00
	Rh-103m-->	****		****	0.000E+00	0.000E+00
	Ru-106-->				0.000E+00	0.000E+00
	Rh-106-->	****		****	0.000E+00	0.000E+00
	Pd-107-->				0.000E+00	0.000E+00
	Cd-109-->				0.000E+00	0.000E+00
	Ag-110m-->				0.000E+00	0.000E+00
	Ag-110-->	****		****	0.000E+00	0.000E+00
	Sn-113-->				0.000E+00	0.000E+00
	In-113m-->	****		****	0.000E+00	0.000E+00
	Cd-113m-->				0.000E+00	0.000E+00
	Cd-115m-->				0.000E+00	0.000E+00
	Sn-119m-->				0.000E+00	0.000E+00
	Sn-121m-->				0.000E+00	0.000E+00
	Sn-123-->				0.000E+00	0.000E+00
	Te-123m-->				0.000E+00	0.000E+00
	Sb-124-->				0.000E+00	0.000E+00
	Sb-125-->				0.000E+00	0.000E+00
	Te-125m-->				0.000E+00	0.000E+00
	Sn-126-->				0.000E+00	0.000E+00
	Sb-126m-->	****		****	0.000E+00	0.000E+00
	Sb-126-->				0.000E+00	0.000E+00
	Te-127m-->				0.000E+00	0.000E+00
	Te-127-->	****		****	0.000E+00	0.000E+00

Case IA5: 4X4 Liner--Solidified Concentrates**Discussion and Conclusion**

Information for solidified concentrates contained in a 4x4 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. Input values for this case were taken from the DOE hydrogen gas generation workshop manual (Analytical Resources 1994). The manual case was run on the original EPRI spreadsheet on which the Excel version of the Radcalc spreadsheet is based. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were added to the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 5.27% and the spreadsheet a concentration of 4.95%, which agrees with the manual value. The difference of 0.32 reflects a 6.07% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:38

Performed By: J. Green

Checked By: _____

File: IAS.RAD

***** Input Information *****

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Solid
 Container Type: 4 x 4 Liner

	Entered Values:	Metric Values:
Package Void Volume:	5.00 ft^3	1.42e+005 cc
Waste Volume:	45.0 ft^3	1.27e+006 cc
Waste Mass:	4.20e+003 lb	1.91e+006 g
Waste Void Volume:	0.000 ft^3	0.000 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.24	0.24	0.24

Comments:

Case IAS
 Solidified Concentrates
 4X4 Liner

***** Calculated Results *****

H2 Percent Concentration: 5.27 %
 H2 Volume: 7.88e+003 cc
 H2 Generation Rate: 0.449 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 5.64 kPa
 Total Pressure (H2 and Air): 107. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 1.0997)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 1.49 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA5.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattage..		CHECKED:	
RP Genoni/JG Field..Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description_____	>		Solidified Concentrates
"_____	>		4x4 Liner
"_____	>		
Enter waste form ("Special" or "Normal")_____	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")_____	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")_____	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner_____	>	2	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")_____	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations_____	>	06/26/90	
Enter date last sealed_____	>	06/26/90	>>
Enter date to be shipped_____	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt_____	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume_____	>	50.0	ft3
Enter waste volume_____	>	45.0	ft3
CALCULATED Container void volume:		5.0	ft3
Enter estimated waste void volume_____	>	0.0	ft3
** OR **			
Enter waste true density (vendor data)_____	>		Lbs/ft3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	ft3
CALCULATED Package interior volume =		1.416E+06	cc
CALCULATED Waste volume =		1.274E+06	cc
CALCULATED Total void volume =		1.416E+05	cc
Enter waste weight_____	>	4200	Lbs
CALCULATED Weight =		1.907E+06	gms
CALCULATED Waste bulk density =		1.4964	gms/cc
Enter G-H2 (molecules/100 ev)_____	>	0.24	
OR			
Enter volume cation resin (cu ft)_____	>		
Enter volume anion resin (cu ft)_____	>		

Enter volume mix bed resin (cu ft)_____	>			
Enter volume other resin (cu ft)_____	>			
Enter G-H2 of other resin_____	>			
CALCULATED G-H2 for waste =		0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =		6.920E+05	Rads	
H2 Volume =		7.379E+03	cm3	
H2 Concentration =		4.95	%	
H2 Generation Rate =		4.206E-01	cc/hr	
Pressure Buildup Rate =		1.049E-03	psi/day	
Pressure (seal to ship) =		0.00	psi	
Enter Measured H2 Concentration (if known)_____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =		0.00		
Activity Summary @ Shipment:				
Total Activity* =		4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =		0.033	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years =		2.489E+01	µCi/cc	
T 1/2 > 5 Years =		1.962E+01	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =		0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) =		0.000	gms	
Other DOE Fissile Material (DOE 5480.1A) =		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) =		0.000	gms	
Other DOE Accountable Material (DOE 5633.3) =		0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics =		0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes =	Unity Fraction			Classification
(Long Lived)	0.000	A		Class B
	N/A	B		
	0.000	C		Limiting Isotope
Table 2 Isotopes =	200.162	A		Sr-90
(Short Lived)	0.141	B		Miscellaneous
	0.002	C		
Transportation Classification:				
LSA Determination =	Unity Fraction			
Type Determination =	1.104E+00	> LSA		
	2.785E+01	Type 'B'		

INPUT: LISTED ISOTOPES							
(**** = Daughter Product)							
		Curies	or	%	Curies when Sealed	Curies when Shipped	
	Total Curies	(ONLY if entering %) =				xxxxx	xxxxx
	H-3→				0.000E+00	0.000E+00	
	C-14→				0.000E+00	0.000E+00	
	Na-22→				0.000E+00	0.000E+00	
	Cr-51→				0.000E+00	0.000E+00	
	Mn-54→	2.000E+00			2.000E+00	2.000E+00	
	Fe-55→				0.000E+00	0.000E+00	
	Co-57→				0.000E+00	0.000E+00	
	Co-58→	1.000E+01			9.996E+00	9.996E+00	
	Fe-59→				0.000E+00	0.000E+00	
	Ni-59→				0.000E+00	0.000E+00	
	Co-60→	1.000E+01			1.000E+01	1.000E+01	
	Ni-63→				0.000E+00	0.000E+00	
	Zn-65→				0.000E+00	0.000E+00	
	Se-79→				0.000E+00	0.000E+00	
	Kr-85→				0.000E+00	0.000E+00	
	Sr-89→				0.000E+00	0.000E+00	
	Sr-90→	1.000E+01			1.000E+01	1.000E+01	
	Y-90→	****		****	1.000E+01	1.000E+01	
	Y-91→				0.000E+00	0.000E+00	
	Zr-93→				0.000E+00	0.000E+00	
	Nb-93m→				0.000E+00	0.000E+00	
	Nb-94→				0.000E+00	0.000E+00	
	Zr-95→	3.000E+00			2.999E+00	2.999E+00	
	Nb-95→				0.000E+00	0.000E+00	
	Nb-95m→				0.000E+00	0.000E+00	
	Tc-99→				0.000E+00	0.000E+00	
	Ru-103→				0.000E+00	0.000E+00	
	Rh-103m→	****		****	0.000E+00	0.000E+00	
	Ru-106→				0.000E+00	0.000E+00	
	Rh-106→	****		****	0.000E+00	0.000E+00	
	Pd-107→				0.000E+00	0.000E+00	
	Cd-109→				0.000E+00	0.000E+00	
	Ag-110m→				0.000E+00	0.000E+00	
	Ag-110→	****		****	0.000E+00	0.000E+00	
	Sn-113→				0.000E+00	0.000E+00	
	In-113m→	****		****	0.000E+00	0.000E+00	
	Cd-113m→				0.000E+00	0.000E+00	
	Cd-115m→				0.000E+00	0.000E+00	
	Sn-119m→				0.000E+00	0.000E+00	
	Sn-121m→				0.000E+00	0.000E+00	
	Sn-123→				0.000E+00	0.000E+00	
	Te-123m→				0.000E+00	0.000E+00	
	Sb-124→				0.000E+00	0.000E+00	
	Sb-125→				0.000E+00	0.000E+00	
	Te-125m→				0.000E+00	0.000E+00	
	Sn-126→				0.000E+00	0.000E+00	
	Sb-126m→	****		****	0.000E+00	0.000E+00	
	Sb-126→				0.000E+00	0.000E+00	
	Te-127m→				0.000E+00	0.000E+00	
	Te-127→	****		****	0.000E+00	0.000E+00	

Case IA6: 4X4 Liner--Cartridge Filter**Discussion and Conclusion**

Information for a cartridge filter contained in a 4x4 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 1.58% and the Excel spreadsheet a concentration of 1.31%. The difference of 0.07 reflects a 5.07% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:39

Performed By: J. Green

Checked By: _____

File: IA6.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

	Entered Values:	Metric Values:
Package Void Volume:	6.38 ft ³	1.81e+005 cc
Waste Volume:	0.825 ft ³	2.34e+004 cc
Waste Mass:	47.0 lb	2.13e+004 g
Waste Void Volume:	0.410 ft ³	1.16e+004 cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.09	0.09	0.09

Comments:

Case IA6
Cartridge Filter
4X4 Liner

===== Calculated Results =====

H2 Percent Concentration: 1.38 %
H2 Volume: 2.69e+003 cc
H2 Generation Rate: 0.154 cc/hour

Heat Generated: 0.329 Watts
Partial Pressure (H2): 1.42 kPa
Total Pressure (H2 and Air): 103. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 27.700)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 98.268)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.912 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA6.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Delta... Analytical Resources, Inc., 2/85 & 6/90		BY:	I. Green
(Modified for DOE Radionuclides and Thermal Wastage..		CHECKED:	
RP Gencon/JG Field.. Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description_____	>	Cartridge Filter	
"_____	>	4x4 Liner	
"_____	>		
Enter waste form ("Special" or "Normal")_____	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")_____	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")_____	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner_____	>	2	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")_____	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations_____	>	06/26/90	
Enter date last sealed*_____	>	06/26/90	>>
Enter date to be shipped_____	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt_____	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume_____	>	7.2	Ft3
Enter waste volume_____	>	0.8	Ft3
CALCULATED Container void volume:		6.4	Ft3
Enter estimated waste void volume_____	>	0.4	Ft3
** OR **			
Enter waste true density (vendor data)_____	>	0.0	Lbs/Ft3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	Ft3
CALCULATED Package interior volume =		2.039E+05	cc
CALCULATED Waste volume =		2.336E+04	cc
CALCULATED Total void volume =		1.921E+05	cc
Enter waste weight_____	>	47	Lbs
CALCULATED Weight =		2.134E+04	gms
CALCULATED Waste bulk density =		0.9134	gms/cc
Enter G-H2 (molecules/100 ev)_____	>	0.09	
OR			
Enter volume cation resin (cu ft)_____	>		
Enter volume anion resin (cu ft)_____	>		

Enter volume mix bed resin (cu ft)_____	>			
Enter volume other resin (cu ft)_____	>			
Enter G-H2 of other resin_____	>			
CALCULATED G-H2 for waste	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose	=	5.699E+07	Rads	
H2 Volume	=	2.550E+03	cm3	
H2 Concentration	=	1.31	%	
H2 Generation Rate	=	1.453E-01	cc/hr	
Pressure Buildup Rate	=	2.670E-04	psi/day	
Pressure (seal to ship)	=	0.00	psi	
Enter Measured H2 Concentration (if known)_____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations	=	0.00		
Activity Summary @ Shipment:				
Total Activity*	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total*	=	1.776	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years	----	1.358E+03	µCi/cc	
T 1/2 > 5 Years	----	1.070E+03	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71)	----	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)	----	0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM)	----	0.000	gms	
Other DOE Accountable Material (DOE 5633.3)	----	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics	----	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes	----	0.000	A	Class C
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Cs-137
Table 2 Isotopes	----	10917.908	A	
(Short Lived)		7.718	B	Miscellaneous
		0.108	C	
Transportation Classification:				
LSA Determination	----	9.865E+01	> LSA	
Type Determination	----	2.785E+01	Type 'B'	

INPUT: LISTED ISOTOPES						
(**** = Daughter Product)					Curies when	Curies when
Total Curies	Curies	or	%		Sealed	Shipped
(ONLY if entering %) =					xxxxx	xxxxx
H-3→					0.000E+00	0.000E+00
C-14→					0.000E+00	0.000E+00
Na-22→					0.000E+00	0.000E+00
Cr-51→					0.000E+00	0.000E+00
Mn-54→	2.000E+00				2.000E+00	2.000E+00
Fe-55→					0.000E+00	0.000E+00
Co-57→					0.000E+00	0.000E+00
Co-58→	1.000E+01				9.996E+00	9.996E+00
Fe-59→					0.000E+00	0.000E+00
Ni-59→					0.000E+00	0.000E+00
Co-60→	1.000E+01				1.000E+01	1.000E+01
Ni-63→					0.000E+00	0.000E+00
Zn-65→					0.000E+00	0.000E+00
Se-79→					0.000E+00	0.000E+00
Kr-85→					0.000E+00	0.000E+00
Sr-89→					0.000E+00	0.000E+00
Sr-90→	1.000E+01				1.000E+01	1.000E+01
Y-90→	****		****		1.000E+01	1.000E+01
Y-91→					0.000E+00	0.000E+00
Zr-93→					0.000E+00	0.000E+00
Nb-93m→					0.000E+00	0.000E+00
Nb-94→					0.000E+00	0.000E+00
Zr-95→	3.000E+00				2.999E+00	2.999E+00
Nb-95→					0.000E+00	0.000E+00
Nb-95m→					0.000E+00	0.000E+00
Tc-99→					0.000E+00	0.000E+00
Ru-103→					0.000E+00	0.000E+00
Rh-103m→	****		****		0.000E+00	0.000E+00
Ru-106→					0.000E+00	0.000E+00
Rh-106→	****		****		0.000E+00	0.000E+00
Pd-107→					0.000E+00	0.000E+00
Cd-109→					0.000E+00	0.000E+00
Ag-110m→					0.000E+00	0.000E+00
Ag-110→	****		****		0.000E+00	0.000E+00
Sn-113→					0.000E+00	0.000E+00
In-113m→	****		****		0.000E+00	0.000E+00
Cd-113m→					0.000E+00	0.000E+00
Cd-115m→					0.000E+00	0.000E+00
Sn-119m→					0.000E+00	0.000E+00
Sn-121m→					0.000E+00	0.000E+00
Sn-123→					0.000E+00	0.000E+00
Te-123m→					0.000E+00	0.000E+00
Sb-124→					0.000E+00	0.000E+00
Sb-125→					0.000E+00	0.000E+00
Te-125m→					0.000E+00	0.000E+00
Sn-126→					0.000E+00	0.000E+00
Sb-126m→	****		****		0.000E+00	0.000E+00
Sb-126→					0.000E+00	0.000E+00
Te-127m→					0.000E+00	0.000E+00
Te-127→	****		****		0.000E+00	0.000E+00

[illegible]

Case IA7: 5X5 Liner--Dewatered Resin**Discussion and Conclusion**

Information for dewatered ion exchange resins contained in a 5x5 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. Input values for this case were taken from the DOE hydrogen gas generation workshop manual (Analytical Resources 1994). The manual case was run on the original EPRI spreadsheet on which the Excel version of the Radcalc spreadsheet is based. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows gives 1.07% H_2 concentration and the spreadsheet 1.01%, which agrees with the manual value. The difference of 0.06 reflects a 5.61% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:39

Performed By: J. Green

Checked By: _____

File: IA7.RAD

***** Input Information *****

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
Physical Form: Liquid
Container Type: 5 x 5 Liner

	Entered Values:	Metric Values:
Package Void Volume:	10.0 ft ³	2.83e+005 cc
Waste Volume:	110. ft ³	3.12e+006 cc
Waste Mass:	4.70e+003 lb	2.13e+006 g
Waste True Density:	65.0 lb/ft ³	1.04 g/cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.5	0.5	0.5

Comments:

Case IA7
Dewatered Resin
5x5 Liner

***** Calculated Results *****

H2 Percent Concentration: 1.07 %
H2 Volume: 1.46e+004 cc
H2 Generation Rate: 0.833 cc/hour

Heat Generated: 0.329 Watts
Partial Pressure (H2): 1.10 kPa
Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 27.700)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.98268)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.684 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA7.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltete...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattage..		CHECKED:	
RP Genoni/JG Field, Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description-----	>	Dewatered Resin	
"-----	>	5x5 Liner	
"-----	>		
Enter waste form ("Special" or "Normal")-----	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")-----	>	Liquid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")-----	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner-----	>	3	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")-----	>	No	"Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations-----	>	06/26/90	
Enter date last sealed*-----	>	06/26/90	>>
Enter date to be shipped-----	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt-----	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume-----	>	120.0	Fi3
Enter waste volume-----	>	110.0	Fi3
CALCULATED Container void volume:		10.0	Fi3
Enter estimated waste void volume-----	>		Fi3
** OR **			
Enter waste true density (vendor data)-----	>	65.0	Lbs/Fi3
CALCULATED Waste void fraction =		0.342	
CALCULATED Waste void volume =		37.66	Fi3
CALCULATED Package interior volume =		3.398E+06	cc
CALCULATED Waste volume =		3.115E+06	cc
CALCULATED Total void volume =		1.350E+06	cc
Enter waste weight-----	>	4700	Lbs
CALCULATED Weight =		2.134E+06	gms
CALCULATED Waste bulk density =		0.6850	gms/cc
Enter G-H2 (molecules/100 ev)-----	>	0.50	
OR			
Enter volume cation resin (cu ft)-----	>		
Enter volume anion resin (cu ft)-----	>		

Enter volume mix bed resin (cu ft)-----	>			
Enter volume other resin (cu ft)-----	>			
Enter G-H2 of other resin-----	>			
CALCULATED G-H2 for waste	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose	=	5.561E+05	Rads	
H2 Volume	=	1.382E+04	cm3	
H2 Concentration	=	1.01	%	
H2 Generation Rate	=	7.879E-01	cc/hr	
Pressure Buildup Rate	=	2.061E-04	psi/day	
Pressure (seal to ship)	=	0.00	psi	
Enter Measured H2 Concentration (if known)-----	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations	=	0.00		
Activity Summary @ Shipment:				
Total Activity*	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total*	=	0.013	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years	=====	1.018E+01	µCi/cc	
T 1/2 > 5 Years	=====	8.026E+00	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71)	=====	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM)	=====	0.000	gms	
Other DOE Accountable Material (DOE 5633.3)	=====	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics	=====	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes	=====	0.000	A	Class B
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Sr-90
Table 2 Isotopes	=====	81.884	A	
(Short Lived)		0.058	B	Miscellaneous
		0.001	C	
Transportation Classification:				
LSA Determination	=====	9.865E-01	LSA	
Type Determination	=====	2.785E+01	LSA, > Type 'A'	

INPUT: LISTED ISOTOPES (**** = Daughter Product)						
		Curies	or	%	Curies when Sealed	Curies when Shipped
	Total Curies					
	(ONLY if entering %) =				XXXXX	XXXXX
	H-3-->				0.000E+00	0.000E+00
	C-14-->				0.000E+00	0.000E+00
	Na-22-->				0.000E+00	0.000E+00
	Cr-51-->				0.000E+00	0.000E+00
	Mn-54-->	2.000E+00			2.000E+00	2.000E+00
	Fe-55-->				0.000E+00	0.000E+00
	Co-57-->				0.000E+00	0.000E+00
	Co-58-->	1.000E+01			9.996E+00	9.996E+00
	Fe-59-->				0.000E+00	0.000E+00
	Ni-59-->				0.000E+00	0.000E+00
	Co-60-->	1.000E+01			1.000E+01	1.000E+01
	Ni-63-->				0.000E+00	0.000E+00
	Zn-65-->				0.000E+00	0.000E+00
	Se-79-->				0.000E+00	0.000E+00
	Kr-85-->				0.000E+00	0.000E+00
	Sr-89-->				0.000E+00	0.000E+00
	Sr-90-->	1.000E+01			1.000E+01	1.000E+01
	Y-90-->	****		****	1.000E+01	1.000E+01
	Y-91-->				0.000E+00	0.000E+00
	Zr-93-->				0.000E+00	0.000E+00
	Nb-93m-->				0.000E+00	0.000E+00
	Nb-94-->				0.000E+00	0.000E+00
	Zr-95-->	3.000E+00			2.999E+00	2.999E+00
	Nb-95-->				0.000E+00	0.000E+00
	Nb-95m-->				0.000E+00	0.000E+00
	Tc-99-->				0.000E+00	0.000E+00
	Ru-103-->				0.000E+00	0.000E+00
	Rh-103m-->	****		****	0.000E+00	0.000E+00
	Ru-106-->				0.000E+00	0.000E+00
	Rh-106-->	****		****	0.000E+00	0.000E+00
	Pd-107-->				0.000E+00	0.000E+00
	Cd-109-->				0.000E+00	0.000E+00
	Ag-110m-->				0.000E+00	0.000E+00
	Ag-110-->	****		****	0.000E+00	0.000E+00
	Sn-113-->				0.000E+00	0.000E+00
	In-113m-->	****		****	0.000E+00	0.000E+00
	Cd-113m-->				0.000E+00	0.000E+00
	Cd-115m-->				0.000E+00	0.000E+00
	Sn-119m-->				0.000E+00	0.000E+00
	Sn-121m-->				0.000E+00	0.000E+00
	Sn-123-->				0.000E+00	0.000E+00
	Te-123m-->				0.000E+00	0.000E+00
	Sb-124-->				0.000E+00	0.000E+00
	Sb-125-->				0.000E+00	0.000E+00
	Te-125m-->				0.000E+00	0.000E+00
	Sn-126-->				0.000E+00	0.000E+00
	Sb-126m-->	****		****	0.000E+00	0.000E+00
	Sb-126-->				0.000E+00	0.000E+00
	Te-127m-->				0.000E+00	0.000E+00
	Te-127-->	****		****	0.000E+00	0.000E+00

E-49

Case IA8: 5X5 Liner--Solidified Concentrates**Discussion and Conclusion**

Information for solidified concentrates contained in a 5x5 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 5.38% and the spreadsheet a concentration of 5.05%. The difference of 0.33 reflects a 6.13% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:40

Performed By: J. Green

Checked By: _____

File: IAS.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Solid
 Container Type: 5 x 5 Liner

	Entered Values:	Metric Values:
Package Void Volume:	5.00 ft ³	1.42e+005 cc
Waste Volume:	45.0 ft ³	1.27e+006 cc
Waste Mass:	4.20e+003 lb	1.91e+006 g
Waste Void Volume:	0.000 ft ³	0.000 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.24	0.24	0.24

Comments:
 Case IAS
 Solidified Concentrates
 5x5 Liner

===== Calculated Results =====

H2 Percent Concentration: 5.38 %
 H2 Volume: 8.05e+003 cc
 H2 Generation Rate: 0.459 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 5.76 kPa
 Total Pressure (H2 and Air): 107. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 1.0997)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 1.49 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA8.ds
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Delta...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattle..		CHECKED:	
RP Genoni/JG Field, Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description-----	>		Solidified Concentrates
"-----	>		5x5 Liner
"-----	>		
Enter waste form ("Special" or "Normal")-----	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")-----	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")-----	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1-55 gal. drum, 2-4x4 liner-----	>	3	>> Req'd input for H2 calculations
3-5x5 liner, 4-6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")-----	>	No	*Note: For a vented HIC, assume
			"Date sealed" is date shipped in Cask
Enter date of curie calculations -----	>	06/26/90	
Enter date last sealed*-----	>	06/26/90	>>
Enter date to be shipped-----	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt-----	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume-----	>	50.0	ft3
Enter waste volume-----	>	45.0	ft3
CALCULATED Container void volume:		5.0	ft3
Enter estimated waste void volume-----	>	0.0	ft3
** OR **			
Enter waste true density (vendor data)-----	>		Lbs/ft3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	ft3
CALCULATED Package interior volume =		1.416E+06	cc
CALCULATED Waste volume =		1.274E+06	cc
CALCULATED Total void volume =		1.416E+05	cc
Enter waste weight-----	>	4200	Lbs
CALCULATED Weight =		1.907E+06	gms
CALCULATED Waste bulk density =		1.4964	gms/cc
Enter G-H2 (molecules/100 ev)-----	>	0.24	
OR			
Enter volume cation resin (cu ft)-----	>		
Enter volume anion resin (cu ft)-----	>		

*** CALCULATED RESULTS ***					
H2 Generation Summary:					
=	Total Integrated Dose	7.057E+05	Rads		
=	H2 Volume	7.524E+03	cm3		
=	H2 Concentration	5.05	% >> Verify H2 Limit		
=	H2 Generation Rate	4.289E-01	cc/hr		
=	Pressure Buildup Rate	1.069E-03	psi/day		
=	Pressure (seal to ship)	0.00	psi		
<	Ratio Measured H2 Concentration (if known)	0.00	%		
=	Ratio Measured to Calculated H2 Concentrations	0.00			
Activity Summary @ Shipment:					
=	Total Activity*	4.149E+01	Ci	(Excludes Daughters	
=	Specific Activity, Total*	0.033	mCi/cc	with T 1/2 < 10 days)	
=	Specific Activity*, T 1/2 < 5 Years	2.489E+01	µCi/cc		
=	T 1/2 > 5 Years	1.962E+01	µCi/cc >> Verify Disposal License		
Decay Heat @ Shipment:					
-	Decay Heat @ Shipment	0.344	Watts		
or		1.173	BTU/hr		
Fissile Material:					
=	Fissile Material (49 CFR 173 & 10 CFR 71)	0.000	grams		
=	Other DOE Fissile Material (DOE 5480.1A)	0.000	grams >> Isotope list is incomplete		
Special Nuclear Material:					
=	Special Nuclear Material (SNM)	0.000	grams		
=	Other DOE Accountable Material (DOE 5633.3)	0.000	grams >> Isotope list is incomplete		
Transuramics:					
=	Specific Activity, Transuramics	0.000	nCi/gms		
10 CFR 61.55 Classification:					
=	Table 1 Isotopes	0.000	A	Class B	
=	(Long Lived)	N/A	B		
=	Table 2 Isotopes	0.000	C	Limiting Isotope	Sr-90
=	(Short Lived)	0.141	B	Miscellaneous	
=	Unity Fraction	0.002	C		
Transportation Classification:					
=	LSA Determination	1.104E+00	> LSA	Type B	
=	Type Determination	2.785E+01			

INPUT: LISTED ISOTOPES					
(**** = Daughter Product)				Curies when	Curies when
	Curies	or	%	Sealed	Shipped
Total Curies					
(ONLY if entering %) =				xxxxx	xxxxx
H-3				0.000E+00	0.000E+00
C-14				0.000E+00	0.000E+00
Na-22				0.000E+00	0.000E+00
Cr-51				0.000E+00	0.000E+00
Mn-54	2.000E+00			2.000E+00	2.000E+00
Fe-55				0.000E+00	0.000E+00
Co-57				0.000E+00	0.000E+00
Co-58	1.000E+01			9.996E+00	9.996E+00
Fe-59				0.000E+00	0.000E+00
Ni-59				0.000E+00	0.000E+00
Co-60	1.000E+01			1.000E+01	1.000E+01
Ni-63				0.000E+00	0.000E+00
Zn-65				0.000E+00	0.000E+00
Se-79				0.000E+00	0.000E+00
Kr-85				0.000E+00	0.000E+00
Sr-89				0.000E+00	0.000E+00
Sr-90	1.000E+01			1.000E+01	1.000E+01
Y-90	****		****	1.000E+01	1.000E+01
Y-91				0.000E+00	0.000E+00
Zr-93				0.000E+00	0.000E+00
Nb-93m				0.000E+00	0.000E+00
Nb-94				0.000E+00	0.000E+00
Zr-95	3.000E+00			2.999E+00	2.999E+00
Nb-95				0.000E+00	0.000E+00
Nb-95m				0.000E+00	0.000E+00
To-99				0.000E+00	0.000E+00
Ru-103				0.000E+00	0.000E+00
Rh-103m	****		****	0.000E+00	0.000E+00
Ru-106				0.000E+00	0.000E+00
Rh-106	****		****	0.000E+00	0.000E+00
Pd-107				0.000E+00	0.000E+00
Cd-109				0.000E+00	0.000E+00
Ag-110m				0.000E+00	0.000E+00
Ag-110	****		****	0.000E+00	0.000E+00
Sn-113				0.000E+00	0.000E+00
In-113m	****		****	0.000E+00	0.000E+00
Cd-113m				0.000E+00	0.000E+00
Cd-115m				0.000E+00	0.000E+00
Sn-119m				0.000E+00	0.000E+00
Sn-121m				0.000E+00	0.000E+00
Sn-123				0.000E+00	0.000E+00
Te-123m				0.000E+00	0.000E+00
Sb-124				0.000E+00	0.000E+00
Sb-125				0.000E+00	0.000E+00
Te-125m				0.000E+00	0.000E+00
Sn-126				0.000E+00	0.000E+00
Sb-126m	****		****	0.000E+00	0.000E+00
Sb-126				0.000E+00	0.000E+00
Te-127m				0.000E+00	0.000E+00
Te-127	****		****	0.000E+00	0.000E+00

Case IA9: 5X5 Liner--Cartridge Filter**Discussion and Conclusion**

Information for a cartridge filter contained in a 5x5 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 1.42% and the Excel spreadsheet a concentration of 1.35%. The difference of 0.07 reflects a 4.93% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:40

Performed By: J. Green

Checked By: _____

File: IA9.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Solid
 Container Type: 5 x 5 Liner

	Entered Values:	Metric Values:
Package Void Volume:	6.38 ft ³	1.81e+005 cc
Waste Volume:	0.825 ft ³	2.34e+004 cc
Waste Mass:	47.0 lb	2.13e+004 g
Waste Void Volume:	0.410 ft ³	1.16e+004 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.09	0.09	0.09

Comments:

Case IA9
 Cartridge Filter
 5x5 Liner

===== Calculated Results =====

H2 Percent Concentration: 1.42 %
 H2 Volume: 2.78e+003 cc
 H2 Generation Rate: 0.158 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 1.46 kPa
 Total Pressure (H2 and Air): 103. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 98.268)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.912 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE			
CONTAINERS for TRANSPORTATION and DISPOSAL		FILE REF:	IA9.xls
CP Deltete... Analytical Resources, Inc., 2/85 & 6/90			
(Modified for DOE Radionuclides and Thermal Wattage..		DATE:	9/4/95
RP Genoni/JG Field.. Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research		BY:	J. Green
Institute in NP-4938 and NP-4757		CHECKED:	
*** WASTE GENERAL INFORMATION ***			
Enter waste description_____	>		Cartridge Filter
"_____	>		5x5 Liner
"_____	>		
Enter waste form ("Special" or "Normal")_____	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")_____	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")_____	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner_____	>	3	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")_____	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations _____	>	06/26/90	
Enter date last sealed*_____	>	06/26/90	>>
Enter date to be shipped_____	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt_____	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume_____	>	7.2	Fi3
Enter waste volume_____	>	0.8	Fi3
CALCULATED Container void volume:		6.4	Fi3
Enter estimated waste void volume_____	>	0.4	Fi3
** OR **			
Enter waste true density (vendor data)_____	>	0.0	Lbs/Fi3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	Fi3
CALCULATED Package interior volume =		2.039E+05	cc
CALCULATED Waste volume =		2.336E+04	cc
CALCULATED Total void volume =		1.921E+05	cc
Enter waste weight_____	>	47	Lbs
CALCULATED Weight =		2.134E+04	gms
CALCULATED Waste bulk density =		0.9134	gms/cc
Enter G-H2 (molecules/100 ev)_____	>	0.09	
OR			
Enter volume cation resin (cu ft)_____	>		
Enter volume anion resin (cu ft)_____	>		

Enter volume mix bed resin (cu ft) _____	>			
Enter volume other resin (cu ft) _____	>			
Enter G-H2 of other resin _____	>			
CALCULATED G-H2 for waste	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose	=	5.878E+07	Rads	
H2 Volume	=	2.630E+03	cm3	
H2 Concentration	=	1.35	%	
H2 Generation Rate	=	1.499E-01	cc/hr	
Pressure Buildup Rate	=	2.754E-04	psi/day	
Pressure (seal to ship)	=	0.00	psi	
Enter Measured H2 Concentration (if known) _____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations	=	0.00		
Activity Summary @ Shipment:				
Total Activity*	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total*	=	1.776	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years	---	1.358E+03	µCi/cc	
T 1/2 > 5 Years	---	1.070E+03	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71)	---	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)	---	0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM)	---	0.000	gms	
Other DOE Accountable Material (DOE 5633.3)	---	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics	---	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes	---	0.000	A	Class C
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Cs-137
Table 2 Isotopes	---	10917.908	A	
(Short Lived)		7.718	B	Miscellaneous
		0.108	C	
Transportation Classification:				
LSA Determination	---	9.865E+01	> LSA	
Type Determination	---	2.785E+01	Type B'	

INPUT: LISTED ISOTOPES						
(**** = Daughter Product)						
		Curies	or	%	Curies when Sealed	Curies when Shipped
Total Curies						
(ONLY if entering %) =					xxxxx	xxxxx
H-3	→				0.000E+00	0.000E+00
C-14	→				0.000E+00	0.000E+00
Na-22	→				0.000E+00	0.000E+00
Cr-51	→				0.000E+00	0.000E+00
Mn-54	→	2.000E+00			2.000E+00	2.000E+00
Fe-55	→				0.000E+00	0.000E+00
Co-57	→				0.000E+00	0.000E+00
Co-58	→	1.000E+01			9.996E+00	9.996E+00
Fe-59	→				0.000E+00	0.000E+00
Ni-59	→				0.000E+00	0.000E+00
Co-60	→	1.000E+01			1.000E+01	1.000E+01
Ni-63	→				0.000E+00	0.000E+00
Zn-65	→				0.000E+00	0.000E+00
Se-79	→				0.000E+00	0.000E+00
Kr-85	→				0.000E+00	0.000E+00
Sr-89	→				0.000E+00	0.000E+00
Sr-90	→	1.000E+01			1.000E+01	1.000E+01
Y-90	→	****		****	1.000E+01	1.000E+01
Y-91	→				0.000E+00	0.000E+00
Zr-93	→				0.000E+00	0.000E+00
Nb-93m	→				0.000E+00	0.000E+00
Nb-94	→				0.000E+00	0.000E+00
Zr-95	→	3.000E+00			2.999E+00	2.999E+00
Nb-95	→				0.000E+00	0.000E+00
Nb-95m	→				0.000E+00	0.000E+00
Tc-99	→				0.000E+00	0.000E+00
Ru-103	→				0.000E+00	0.000E+00
Rh-103m	→	****		****	0.000E+00	0.000E+00
Ru-106	→				0.000E+00	0.000E+00
Rh-106	→	****		****	0.000E+00	0.000E+00
Pd-107	→				0.000E+00	0.000E+00
Cd-109	→				0.000E+00	0.000E+00
Ag-110m	→				0.000E+00	0.000E+00
Ag-110	→	****		****	0.000E+00	0.000E+00
Sn-113	→				0.000E+00	0.000E+00
In-113m	→	****		****	0.000E+00	0.000E+00
Cd-113m	→				0.000E+00	0.000E+00
Cd-115m	→				0.000E+00	0.000E+00
Sn-119m	→				0.000E+00	0.000E+00
Sn-121m	→				0.000E+00	0.000E+00
Sn-123	→				0.000E+00	0.000E+00
Te-123m	→				0.000E+00	0.000E+00
Sb-124	→				0.000E+00	0.000E+00
Sb-125	→				0.000E+00	0.000E+00
Te-125m	→				0.000E+00	0.000E+00
Sn-126	→				0.000E+00	0.000E+00
Sb-126m	→	****		****	0.000E+00	0.000E+00
Sb-126	→				0.000E+00	0.000E+00
Te-127m	→				0.000E+00	0.000E+00
Te-127	→	****		****	0.000E+00	0.000E+00

Case IA10: 6X6 Liner--Dewatered Resin**Discussion and Conclusion**

Information for dewatered ion exchange resins contained in a 6x6 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were included in the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows gives 1.13% H_2 concentration and the spreadsheet 1.07%. The difference of 0.06 reflects a 5.31% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:40

Performed By: J. Green

Checked By: _____

File: IA10.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
 Physical Form: Liquid
 Container Type: 6 x 6 Liner

	Entered Values:	Metric Values:
Package Void Volume:	10.0 ft ³	2.83e+005 cc
Waste Volume:	110. ft ³	3.12e+006 cc
Waste Mass:	4.70e+003 lb	2.13e+006 g
Waste True Density:	65.0 lb/ft ³	1.04 g/cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.5	0.5	0.5

Comments:

Case IA10
 Dewatered Resin
 6x6 Liner

===== Calculated Results =====

H2 Percent Concentration: 1.13 %
 H2 Volume: 1.54e+004 cc
 H2 Generation Rate: 0.878 cc/hour

Heat Generated: 0.329 Watts
 Partial Pressure (H2): 1.16 kPa
 Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 27.700)
 Limited Quantity: No
 LSA Determination: Yes (from LSA unity fraction 0.98268)
 HRC Quantity Determination: No
 Fissile Quantity: 0.00000 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.684 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA10.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltate...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattle..		CHECKED:	
RP Genoni/JG Field.. Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description-----	>		Dewatered Resin
"-----	>		6x6 Liner
"-----	>		
Enter waste form ("Special" or "Normal")-----	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")-----	>	Liquid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")-----	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner-----	>	4	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")-----	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations-----	>	06/26/90	
Enter date last sealed*-----	>	06/26/90	>>
Enter date to be shipped-----	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt-----	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume-----	>	120.0	ft ³
Enter waste volume-----	>	110.0	ft ³
CALCULATED Container void volume:		10.0	ft ³
Enter estimated waste void volume-----	>		ft ³
** OR **			
Enter waste true density (vendor data)-----	>	65.0	Lbs/ft ³
CALCULATED Waste void fraction =		0.342	
CALCULATED Waste void volume =		37.66	ft ³
CALCULATED Package interior volume =		3.398E+06	cc
CALCULATED Waste volume =		3.115E+06	cc
CALCULATED Total void volume =		1.350E+06	cc
Enter waste weight-----	>	4700	Lbs
CALCULATED Weight =		2.134E+06	gms
CALCULATED Waste bulk density =		0.6850	gms/cc
Enter G-H2 (molecules/100 ev)-----	>	0.50	
OR			
Enter volume cation resin (cu ft)-----	>		
Enter volume anion resin (cu ft)-----	>		

Enter volume mix bed resin (cu ft)_____	>			
Enter volume other resin (cu ft)_____	>			
Enter G-H2 of other resin_____	>			
CALCULATED G-H2 for waste =	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =	=	5.870E+05	Rads	
H2 Volume =	=	1.459E+04	cm3	
H2 Concentration =	=	1.07	%	
H2 Generation Rate =	=	8.317E-01	cc/hr	
Pressure Buildup Rate =	=	2.175E-04	psi/day	
Pressure (seal to ship) =	=	0.00	psi	
Enter Measured H2 Concentration (if known)_____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =	=	0.00		
Activity Summary @ Shipment:				
Total Activity* =	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =	=	0.013	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years =	=	1.018E+01	µCi/cc	
T 1/2 > 5 Years =	=	8.026E+00	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) =	=	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A) =	=	0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) =	=	0.000	gms	
Other DOE Accountable Material (DOE 5633.3) =	=	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics =	=	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes =	=	0.000	A	Class B
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Sr-90
Table 2 Isotopes =	=	81.884	A	
(Short Lived)		0.058	B	Miscellaneous
		0.001	C	
Transportation Classification:				
LSA Determination =	=	9.865E-01	LSA	
Type Determination =	=	2.785E+01	LSA, > Type 'A'	

INPUT: LISTED ISOTOPES (**** = Daughter Product)					Curies when	Curies when
Total Curies	Curies	or	%		Sealed	Shipped
(ONLY if entering %) =					xxxxx	xxxxx
H-3					0.000E+00	0.000E+00
C-14					0.000E+00	0.000E+00
Na-22					0.000E+00	0.000E+00
Cr-51					0.000E+00	0.000E+00
Mn-54	2.000E+00				2.000E+00	2.000E+00
Fe-55					0.000E+00	0.000E+00
Co-57					0.000E+00	0.000E+00
Co-58	1.000E+01				9.996E+00	9.996E+00
Fe-59					0.000E+00	0.000E+00
Ni-59					0.000E+00	0.000E+00
Co-60	1.000E+01				1.000E+01	1.000E+01
Ni-63					0.000E+00	0.000E+00
Zn-65					0.000E+00	0.000E+00
Se-79					0.000E+00	0.000E+00
Kr-85					0.000E+00	0.000E+00
Sr-89					0.000E+00	0.000E+00
Sr-90	1.000E+01				1.000E+01	1.000E+01
Y-90	****		****		1.000E+01	1.000E+01
Y-91					0.000E+00	0.000E+00
Zr-93					0.000E+00	0.000E+00
Nb-93m					0.000E+00	0.000E+00
Nb-94					0.000E+00	0.000E+00
Zr-95	3.000E+00				2.999E+00	2.999E+00
Nb-95					0.000E+00	0.000E+00
Nb-95m					0.000E+00	0.000E+00
To-99					0.000E+00	0.000E+00
Ru-103					0.000E+00	0.000E+00
Rh-103m	****		****		0.000E+00	0.000E+00
Ru-106					0.000E+00	0.000E+00
Rh-106	****		****		0.000E+00	0.000E+00
Pd-107					0.000E+00	0.000E+00
Cd-109					0.000E+00	0.000E+00
Ag-110m					0.000E+00	0.000E+00
Ag-110	****		****		0.000E+00	0.000E+00
Sn-113					0.000E+00	0.000E+00
In-113m	****		****		0.000E+00	0.000E+00
Cd-113m					0.000E+00	0.000E+00
Cd-115m					0.000E+00	0.000E+00
Sn-119m					0.000E+00	0.000E+00
Sn-121m					0.000E+00	0.000E+00
Sn-123					0.000E+00	0.000E+00
Te-123m					0.000E+00	0.000E+00
Sb-124					0.000E+00	0.000E+00
Sb-125					0.000E+00	0.000E+00
Te-125m					0.000E+00	0.000E+00
Sn-126					0.000E+00	0.000E+00
Sb-126m	****		****		0.000E+00	0.000E+00
Sb-126					0.000E+00	0.000E+00
Te-127m					0.000E+00	0.000E+00
Te-127	****		****		0.000E+00	0.000E+00

Case IA11: 6X6 Liner--Solidified Concentrates**Discussion and Conclusion**

Information for solidified concentrates contained in a 6x6 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were added to the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 5.53% and the spreadsheet a concentration of 5.18%. The difference of 0.35 reflects a 6.33% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:41

Performed By: J. Bacon

Checked By: _____

File: IA11.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
Physical Form: Solid
Container Type: 6 x 6 Liner

	Entered Values:	Metric Values:
Package Void Volume:	5.00 ft^3	1.42e+005 cc
Waste Volume:	45.0 ft^3	1.27e+006 cc
Waste Mass:	4.20e+003 lb	1.91e+006 g
Waste Void Volume:	0.000 ft^3	0.000 cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.24	0.24	0.24

Comments:

Case IA11
Solidified Concentrates
6x6 Liner

===== Calculated Results =====

H2 Percent Concentration: 5.53 %
H2 Volume: 8.28e+003 cc
H2 Generation Rate: 0.472 cc/hour

Heat Generated: 0.329 Watts
Partial Pressure (H2): 5.93 kPa
Total Pressure (H2 and Air): 107. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 27.700)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 1.0997)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.49 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA11.xls
CONTAINERS for TRANSPORTATION and DISPOSAL		DATE:	9/4/95
CP Deltate...Analytical Resources, Inc., 2/85 & 6/90		BY:	J. Green
(Modified for DOE Radionuclides and Thermal Wattage..		CHECKED:	
RP Genoni/JG Field. Westinghouse-Hanford Co....6/88)			
Originally Published by the Electric Power Research			
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description:_____	>		Solidified Concentrates
"_____	>		6x6 Liner
"_____	>		
Enter waste form ("Special" or "Normal")_____	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas")_____	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No")_____	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner_____	>	4	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No")_____	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations _____	>	06/26/90	
Enter date last sealed*_____	>	06/26/90	>>
Enter date to be shipped_____	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt_____	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume_____	>	50.0	Fi3
Enter waste volume_____	>	45.0	Fi3
CALCULATED Container void volume:		5.0	Fi3
Enter estimated waste void volume_____	>	0.0	Fi3
** OR **			
Enter waste true density (vendor data)_____	>		Lbs/Fi3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	Fi3
CALCULATED Package interior volume =		1.416E+06	cc
CALCULATED Waste volume =		1.274E+06	cc
CALCULATED Total void volume =		1.416E+05	cc
Enter waste weight_____	>	4200	Lbs
CALCULATED Weight =		1.907E+06	gms
CALCULATED Waste bulk density =		1.4964	gms/cc
Enter G-H2 (molecules/100 ev)_____	>	0.24	
OR			
Enter volume cation resin (cu ft)_____	>		
Enter volume anion resin (cu ft)_____	>		

Enter volume mix bed resin (cu ft) _____	>			
Enter volume other resin (cu ft) _____	>			
Enter G-H2 of other resin _____	>			
CALCULATED G-H2 for waste	=	0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose	=	7.249E+05	Rads	
H2 Volume	=	7.730E+03	cm3	
H2 Concentration	=	5.18	%	>> Verify H2 Limit
H2 Generation Rate	=	4.406E-01	cc/hr	
Pressure Buildup Rate	=	1.098E-03	psi/day	
Pressure (seal to ship)	=	0.00	psi	
Enter Measured H2 Concentration (if known) _____	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations	=	0.00		
Activity Summary @ Shipment:				
Total Activity*	=	4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total*	=	0.033	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years	=====	2.489E+01	µCi/cc	
T 1/2 > 5 Years	=====	1.962E+01	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment	=	0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71)	=====	0.000	gms	
Other DOE Fissile Material (DOE 5480.1A)		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM)	=====	0.000	gms	
Other DOE Accountable Material (DOE 5633.3)	=====	0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics	=====	0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes	=====	0.000	A	Class B
(Long Lived)		N/A	B	
		0.000	C	Limiting Isotope
				Sr-90
Table 2 Isotopes	=====	200.162	A	
(Short Lived)		0.141	B	Miscellaneous
		0.002	C	
Transportation Classification:				
LSA Determination	=====	1.104E+00	> LSA	
Type Determination	=====	2.785E+01	Type 'B'	

INPUT: LISTED ISOTOPES						
(**** = Daughter Product)						
	Total Curies	Curies	or	%	Curies when Sealed	Curies when Shipped
	(ONLY if entering %) =				xxxxx	xxxxx
H-3					0.000E+00	0.000E+00
C-14					0.000E+00	0.000E+00
Na-22					0.000E+00	0.000E+00
Cr-51					0.000E+00	0.000E+00
Mn-54		2.000E+00			2.000E+00	2.000E+00
Fe-55					0.000E+00	0.000E+00
Co-57					0.000E+00	0.000E+00
Co-58		1.000E+01			9.996E+00	9.996E+00
Fe-59					0.000E+00	0.000E+00
Ni-59					0.000E+00	0.000E+00
Co-60		1.000E+01			1.000E+01	1.000E+01
Ni-63					0.000E+00	0.000E+00
Zn-65					0.000E+00	0.000E+00
Se-79					0.000E+00	0.000E+00
Kr-85					0.000E+00	0.000E+00
Sr-89					0.000E+00	0.000E+00
Sr-90		1.000E+01			1.000E+01	1.000E+01
Y-90		****		****	1.000E+01	1.000E+01
Y-91					0.000E+00	0.000E+00
Zr-93					0.000E+00	0.000E+00
Nb-93m					0.000E+00	0.000E+00
Nb-94					0.000E+00	0.000E+00
Zr-95		3.000E+00			2.999E+00	2.999E+00
Nb-95					0.000E+00	0.000E+00
Nb-95m					0.000E+00	0.000E+00
Tc-99					0.000E+00	0.000E+00
Ru-103					0.000E+00	0.000E+00
Rh-103m		****		****	0.000E+00	0.000E+00
Ru-106					0.000E+00	0.000E+00
Rh-106		****		****	0.000E+00	0.000E+00
Pd-107					0.000E+00	0.000E+00
Cd-109					0.000E+00	0.000E+00
Ag-110m					0.000E+00	0.000E+00
Ag-110		****		****	0.000E+00	0.000E+00
Sn-113					0.000E+00	0.000E+00
In-113m		****		****	0.000E+00	0.000E+00
Cd-113m					0.000E+00	0.000E+00
Cd-115m					0.000E+00	0.000E+00
Sn-119m					0.000E+00	0.000E+00
Sn-121m					0.000E+00	0.000E+00
Sn-123					0.000E+00	0.000E+00
Te-123m					0.000E+00	0.000E+00
Sb-124					0.000E+00	0.000E+00
Sb-125					0.000E+00	0.000E+00
Te-125m					0.000E+00	0.000E+00
Sn-126					0.000E+00	0.000E+00
Sb-126m		****		****	0.000E+00	0.000E+00
Sb-126					0.000E+00	0.000E+00
Te-127m					0.000E+00	0.000E+00
Te-127		****		****	0.000E+00	0.000E+00

Case IA12: 6X6 Liner--Cartridge Filter**Discussion and Conclusion**

Information for a cartridge filter contained in a 6x6 liner was run on the Excel version of the Radcalc spreadsheet and on Radcalc for Windows. The inventory consists of eight radionuclides. The spreadsheet automatically includes the equilibrium daughter products of ^{90}Sr , ^{137}Cs , and ^{144}Ce ; however, in Radcalc for Windows the daughter products were added to the source term. All other input values for the spreadsheet and Radcalc for Windows are the same.

A printout of the Radcalc for Windows Input and Calculated Results sheet is followed by a copy of the Radcalc spreadsheet. Radcalc for Windows yields an H_2 concentration of 1.49% and the Excel spreadsheet a concentration of 1.41%. The difference of 0.08 reflects a 5.37% difference between the code and the spreadsheet. This spread can be accounted for by the variation in the radionuclide libraries (half-lives, energy values, etc.), gamma absorption fractions, and rounding.

Radcalc for Windows 1.0

Date: 09-23-95 12:41

Performed By: J. Green

Checked By: _____

File: IA12.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000
Ce-144	5.00e-001
Pr-144	5.00e-001

Waste Form: Normal
Physical Form: Solid
Container Type: 6 x 6 Liner

	Entered Values:	Metric Values:
Package Void Volume:	6.38 ft^3	1.81e+005 cc
Waste Volume:	0.825 ft^3	2.34e+004 cc
Waste Mass:	47.0 lb	2.13e+004 g
Waste Void Volume:	0.410 ft^3	1.16e+004 cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 731.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0.09	0.09	0.09

Comments:

Case IA12
Cartridge Filter
6x6 Liner

===== Calculated Results =====

H2 Percent Concentration: 1.49 %
H2 Volume: 2.90e+003 cc
H2 Generation Rate: 0.165 cc/hour

Heat Generated: 0.329 Watts
Partial Pressure (H2): 1.53 kPa
Total Pressure (H2 and Air): 103. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 27.700)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 98.268)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.912 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Mn-54	2.00e+000
Co-58	1.00e+001
Co-60	1.00e+001
Sr-90	1.00e+001
Y-90	1.00e+001
Cs-134	1.00e+000
Cs-137	5.00e+000
Ba-137m	4.73e+000

Ce-144	5.00e-001
Pr-144	5.00e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Mn-54	3.95e-001
Co-58	7.78e-003
Co-60	7.69e+000
Sr-90	9.53e+000
Y-90	9.54e+000
Cs-134	5.10e-001
Cs-137	4.77e+000
Ba-137m	4.52e+000
Ce-144	8.41e-002
Pr-144	8.41e-002
Pr-144m	1.01e-003

PROGRAM to CLASSIFY RADIOACTIVE WASTE		FILE REF:	IA12.xls
CONTAINERS for TRANSPORTATION and DISPOSAL			
CP Deltate...Analytical Resources, Inc., 2/85 & 6/90		DATE:	9/4/95
(Modified for DOE Radionuclides and Thermal Wattage..			
RP Genoni/JG Field..Westinghouse-Hanford Co....6/88)		BY:	J. Green
Originally Published by the Electric Power Research		CHECKED:	
Institute in NP-4938 and NP-4757			
*** WASTE GENERAL INFORMATION ***			
Enter waste description.....	>		Cartridge Filter
"	>		6x6 Liner
"	>		
Enter waste form ("Special" or "Normal").....	>	Normal	>> Req'd input for DOT calculations
Enter physical form ("Solid", "Liquid" or "Gas").....	>	Solid	>> Req'd input for DOT calculations
Is waste Activated Metal ? ("Yes", or "No").....	>	No	>> Req'd input for 10CFR61 calculations
Enter container type (1=55 gal. drum, 2=4x4 liner	>	4	>> Req'd input for H2 calculations
3=5x5 liner, 4=6x6 liner)			
Is container a vented HIC ? ("Yes", or "No").....	>	No	*Note: For a vented HIC, assume "Date sealed" is date shipped in Cask
Enter date of curie calculations	>	06/26/90	
Enter date last sealed*.....	>	06/26/90	>>
Enter date to be shipped.....	>	06/26/90	>> Must be later than Ci calcs
Enter date of shipment receipt.....	>	06/26/92	
CALCULATED Decay before sealing (years) =		0.00	Days= 0
CALCULATED Decay before shipment (years) =		0.00	Days= 0
CALCULATED Duration package is sealed (years) =		2.00	Days= 731
Enter package interior volume.....	>	7.2	ft3
Enter waste volume.....	>	0.8	ft3
CALCULATED Container void volume:		6.4	ft3
Enter estimated waste void volume.....	>	0.4	ft3
** OR **			
Enter waste true density (vendor data).....	>	0.0	Lbs/ft3
CALCULATED Waste void fraction =		0.000	
CALCULATED Waste void volume =		0.00	ft3
CALCULATED Package interior volume =		2.039E+05	cc
CALCULATED Waste volume =		2.336E+04	cc
CALCULATED Total void volume =		1.921E+05	cc
Enter waste weight.....	>	47	Lbs
CALCULATED Weight =		2.134E+04	gms
CALCULATED Waste bulk density =		0.9134	gms/cc
Enter G-H2 (molecules/100 ev).....	>	0.09	
OR			
Enter volume cation resin (cu ft).....	>		
Enter volume anion resin (cu ft).....	>		

Enter volume mix bed resin (cu ft)-----	>			
Enter volume other resin (cu ft)-----	>			
Enter G-H2 of other resin-----	>			
CALCULATED G-H2 for waste =		0.00		
*** CALCULATED RESULTS ***				
H2 Generation Summary:				
Total Integrated Dose =		6.130E+07	Rads	
H2 Volume =		2.743E+03	cm3	
H2 Concentration =		1.41	%	
H2 Generation Rate =		1.563E-01	cc/hr	
Pressure Buildup Rate =		2.872E-04	psi/day	
Pressure (seal to ship) =		0.00	psi	
Enter Measured H2 Concentration (if known)-----	>	0.00	%	
Ratio Measured to Calculated H2 Concentrations =		0.00		
Activity Summary @ Shipment:				
Total Activity* =		4.149E+01	Ci	(*Excludes Daughters
Specific Activity, Total* =		1.776	mCi/cc	with T 1/2 < 10 days)
Specific Activity*, T 1/2 < 5 Years =		1.358E+03	µCi/cc	
T 1/2 > 5 Years =		1.070E+03	µCi/cc	>> Verify Disposal License
Decay Heat @ Shipment:				
Decay Heat @ Shipment =		0.344	Watts	
or		1.173	BTU/hr	
Fissile Material:				
Fissile Material (49 CFR 173 & 10 CFR 71) =		0.000	gms	
Other DOE Fissile Material (DOE 5480.1A) =		0.000	gms	>> Isotope list is incomplete
Special Nuclear Material:				
Special Nuclear Material (SNM) =		0.000	gms	
Other DOE Accountable Material (DOE 5633.3) =		0.000	gms	>> Isotope list is incomplete
Transuranics:				
Specific Activity, Transuranics =		0.000	nCi/gms	
10 CFR 61.55 Classification:				
Table 1 Isotopes -----	Unity Fraction			Classification
(Long Lived)	0.000	A		Class C
	N/A	B		
	0.000	C		Limiting Isotope
				Cs-137
Table 2 Isotopes -----	10917.908	A		
(Short Lived)	7.718	B		Miscellaneous
	0.108	C		
Transportation Classification:				
LSA Determination =	9.865E+01	> LSA		
Type Determination =	2.785E+01	Type 'B'		

INPUT: LISTED ISOTOPES					
(**** = Daughter Product)				Curies when	Curies when
Total Curies	Curies	or	%	Sealed	Shipped
(ONLY if entering %) =				xxxxx	xxxxx
H-3→				0.000E+00	0.000E+00
C-14→				0.000E+00	0.000E+00
Na-22→				0.000E+00	0.000E+00
Cr-51→				0.000E+00	0.000E+00
Mn-54→	2.000E+00			2.000E+00	2.000E+00
Fe-55→				0.000E+00	0.000E+00
Co-57→				0.000E+00	0.000E+00
Co-58→	1.000E+01			9.996E+00	9.996E+00
Fe-59→				0.000E+00	0.000E+00
Ni-59→				0.000E+00	0.000E+00
Co-60→	1.000E+01			1.000E+01	1.000E+01
Ni-63→				0.000E+00	0.000E+00
Zn-65→				0.000E+00	0.000E+00
Se-79→				0.000E+00	0.000E+00
Kr-85→				0.000E+00	0.000E+00
Sr-89→				0.000E+00	0.000E+00
Sr-90→	1.000E+01			1.000E+01	1.000E+01
Y-90→	****		****	1.000E+01	1.000E+01
Y-91→				0.000E+00	0.000E+00
Zr-93→				0.000E+00	0.000E+00
Nb-93m→				0.000E+00	0.000E+00
Nb-94→				0.000E+00	0.000E+00
Zr-95→	3.000E+00			2.999E+00	2.999E+00
Nb-95→				0.000E+00	0.000E+00
Nb-95m→				0.000E+00	0.000E+00
To-99→				0.000E+00	0.000E+00
Ru-103→				0.000E+00	0.000E+00
Rh-103m→	****		****	0.000E+00	0.000E+00
Ru-106→				0.000E+00	0.000E+00
Rh-106→	****		****	0.000E+00	0.000E+00
Pd-107→				0.000E+00	0.000E+00
Cd-109→				0.000E+00	0.000E+00
Ag-110m→				0.000E+00	0.000E+00
Ag-110→	****		****	0.000E+00	0.000E+00
Sn-113→				0.000E+00	0.000E+00
In-113m→	****		****	0.000E+00	0.000E+00
Cd-113m→				0.000E+00	0.000E+00
Cd-115m→				0.000E+00	0.000E+00
Sn-119m→				0.000E+00	0.000E+00
Sn-121m→				0.000E+00	0.000E+00
Sn-123→				0.000E+00	0.000E+00
Te-123m→				0.000E+00	0.000E+00
Sb-124→				0.000E+00	0.000E+00
Sb-125→				0.000E+00	0.000E+00
Te-125m→				0.000E+00	0.000E+00
Sn-126→				0.000E+00	0.000E+00
Sb-126m→	****		****	0.000E+00	0.000E+00
Sb-126→				0.000E+00	0.000E+00
Te-127m→				0.000E+00	0.000E+00
Te-127→	****		****	0.000E+00	0.000E+00

IB GAMMA ABSORPTION FRACTIONS FOR VARIOUS CONTAINER TYPES

Cases IB1 - IB4 test dependence of hydrogen generation on container type, with a focus on the influence of the gamma absorption fraction. As mentioned in Chapter 3.0, the gamma absorption fraction used in the hydrogen generation calculation depends on container geometry. There are two curve fits used for calculation of the gamma absorption fraction for each container type: a curve fit for gamma energies between 0.4 MeV and 2.0 MeV and a second curve fit for gamma energies between 2.0 MeV and 5.0 MeV. Hydrogen volume calculated by Radcalc for Windows is compared with results of Excel Version 4.0 spreadsheet calculations.

The Excel spreadsheets calculate the volume of hydrogen gas generated using the Radcalc for Windows methodology and decay energy data from the Fusion Energy Nuclear Data Library (FENDL)/D-1.0² database, as outlined in Chapter 2.0. The spreadsheets calculate the gamma absorption fraction using Radcalc for Windows curve fits, as outlined in Chapter 3.0. The density used in the gamma absorption fraction is calculated from the waste mass divided by waste volume as in Radcalc for Windows. Time integrated disintegrations were calculated using standard analytical solutions (see discussion under following Section IIB). Half-lives and branching ratios for the calculation of time integrated disintegrations were taken from the Oak Ridge Isotope Generation and Depletion Code (ORIGEN)²³ decay database used by Radcalc for Windows. Agreement between the values for the volume of hydrogen gas generated by the two methods (Radcalc and Excel spreadsheet) is interpreted as validating Radcalc's gamma absorption fraction calculational methodology, as well as the corresponding container database.

Case IB1: 30-Gal Drum

Discussion and Conclusion

The 30-gal drum is the first container in the array of curve fit coefficients used in the gamma absorption fraction calculation. The ¹³⁷Cs source emits a 0.662 MeV gamma. A density of 1.5 g/cm³ was used. The Excel spreadsheet and Radcalc for Windows give identical results for hydrogen gas generated within the three significant figures reported by Radcalc for Windows. The Radcalc for Windows Input and Calculated Results sheet for this case, designated IB1, follows.

² FENDL/D is a decay data library for fusion (and other) applications, Version 1 of January 1992. Prepared for use with the neutron activation data library FENDL/A. Summary documentation by A. B. Pashchenko. Index No. IAEA-NDS-167 in Index to the IAEA-NDS-Documentation Series.

³ Croff, A. G., 1980, A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code, ORNL-5621, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Radcalc for Windows 1.0

Date: 09-23-95 13:05

Performed By: TS Hall

Checked By: _____

File: IB1.RAD

===== Input Information =====

Source from input:
Radionuclide: Cs-137 Curies: 1.00e+001

Waste Form: Normal
Physical Form: Liquid
Container Type: 30 Gallon Drum

Package Void Volume: 7.00e+003 cc
Waste Volume: 1.10e+005 cc
Waste Mass: 1.00e+005 g
Waste True Density: 1.00 g/cc

Days to decay source before seal time: 365.24 days
Days container is sealed: 30.00 days

G Value Material Selection:
Contribution Weight G-Alpha G-Beta G-Gamma Name
100.00% 1 1.6 0.53 0.45 Water (liquid)
(^ indicates the value was calculated from a given value)

G Values calculated from list averaging:

G Alpha	G Beta	G Gamma
1.6	0.53	0.45

Comments:

Test Case of Gamma Absorption Fractions for the 30 Gallon
Drum (IB1)

===== Calculated Results =====

H2 Percent Concentration: 0.543 %
H2 Volume: 92.7 cc
H2 Generation Rate: 0.129 cc/hour

Heat Generated: 0.0472 Watts
Partial Pressure (H2): 0.553 kPa
Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.97716)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.32572)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density: 0.909 g/cc

Source decayed to start of seal time:
Radionuclide: Cs-137 Curies: 9.77e+000
Ba-137m 9.24e+000

Source decayed to end of seal time:
Radionuclide: Cs-137 Curies: 9.75e+000
Ba-137m 9.23e+000

Case IB2: Single Pass Fuel Cask

Discussion and Conclusion

The Single Pass Fuel Cask is the last container in the array of curve fit coefficients used in the gamma absorption fraction calculation. This case has a source input of 1.0 Ci of ^{241}Pu . ^{241}Pu decays to ^{241}Am , which in turn decays to ^{237}Np and so on. In the Excel spreadsheet, only ^{241}Pu , ^{241}Am , and ^{237}Np are considered, with the remaining daughter radionuclides considered negligible in terms of hydrogen production. Because the object of this test case is to determine the proper functioning of Radcalc's use of gamma absorption fractions, the G values for alpha and beta radiation are set to zero. If the alpha and beta G values were included, the hydrogen gas generation would be dominated by alphas and betas, rendering comparison with the spreadsheet results impossible. It should be noted that there are a large number of low-energy gammas from these three radionuclides (over 200). A density of 2.0 g/cm^3 is used. The Excel spreadsheet and Radcalc for Windows give identical results for the amount of hydrogen gas volume generated within the three significant figures reported by Radcalc for Windows. The Radcalc for Windows Input and Calculated Results sheet for this case, designated IB2, follows.

Radcalc for Windows 1.0

Date: 09-23-95 13:06

Performed By: K. Hillel

Checked By: _____

File: IB2.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Pu-241	1.00e+000

Waste Form:	Normal
Physical Form:	Solid
Container Type:	Single Pass Fuel Cask

	Entered Values:	Metric Values:
Package Void Volume:	1.62 ft^3	4.59e+004 cc
Waste Volume:	1.60 ft^3	4.53e+004 cc
Waste Mass:	200. lb	9.07e+004 g
Waste Void Volume:	0.100 ft^3	2.83e+003 cc

Days to decay source before seal time:	0.00 days
Days container is sealed:	73050.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	1

Comments:

Test Case of Gamma Absorption Fractions for the Single Pass
Fuel Cask (IB2)

===== Calculated Results =====

H2 Percent Concentration:	0.147 %
H2 Volume:	71.8 cc
H2 Generation Rate:	4.10e-005 cc/hour

Heat Generated:	3.18e-005 Watts
Partial Pressure (H2):	0.149 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 10.000)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 2.2046)
HRC Quantity Determination:	No
Fissile Quantity:	0.0096736 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	2.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
Pu-241	1.00e+000

Source decayed to end of seal time:

Radionuclide:	Curies:
Pu-241	6.59e-005
Am-241	2.50e-002
Np-237	1.68e-006
Pa-233	1.68e-006
U-233	6.97e-010
Th-229	4.10e-012
Ra-225	4.10e-012
Ac-225	4.09e-012
Fr-221	4.09e-012
At-217	4.09e-012
Bi-213	4.09e-012
Po-213	4.00e-012
Pb-209	4.09e-012
U-237	1.62e-009

Case IB3: Sample Pig Carrier**Discussion and Conclusion**

The Sample Pig Carrier, with a maximum internal volume of 266 cm³, is the smallest container type available in Radcalc for Windows. ²⁴Na was chosen for the source because of its prominent 1.3686 MeV and 2.754 MeV gammas, which will exercise both the 0.4 to 2.0 MeV and the 2.0 MeV to 5.0 MeV curve fits for the Sample Pig Carrier. The Excel spreadsheet and Radcalc for Windows give identical results for the amount of hydrogen gas generated within the three significant figures reported by Radcalc for Windows. The Radcalc for Windows Input and Calculated Results sheet for this case, designated IB3, follows.

Radcalc for Windows 1.0

Date: 09-23-95 13:06

Performed By: K. Hillel

Checked By: _____

File: IB3.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Na-24	1.00e+001

Waste Form:	Normal
Physical Form:	Solid
Container Type:	Sample Pig Carrier

Package Void Volume:	1.00 cc
Waste Volume:	265. cc
Waste Mass:	265. g
Waste Void Volume:	1.00 cc

Days to decay source before seal time:	0.00 days
Days container is sealed:	1.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	1

Comments:

Test Case of Gamma Absorption Fractions for the Sample Pig Carrier (IB3)

===== Calculated Results =====

H2 Percent Concentration:	52.4 %
H2 Volume:	2.20 cc
H2 Generation Rate:	0.0918 cc/hour

Heat Generated:	0.277 Watts
Partial Pressure (H2):	112. kPa
Total Pressure (H2 and Air):	213. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 2.0000)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 125.79)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:	
Radionuclide:	Curies:
Na-24	1.00e+001

Source decayed to end of seal time:	
Radionuclide:	Curies:
Na-24	3.30e+000

Case IB4: LR-56 Container**Discussion and Conclusion**

The LR-56, with a maximum internal volume of $4.93\text{E}6\text{ cm}^3$, is the largest container type available in Radcalc for Windows. ^{24}Na was chosen for the source because of its prominent 1.3686 MeV and 2.754 MeV gammas, which will exercise both the 0.4 to 2.0 MeV and the 2.0 MeV to 5.0 MeV curve fits for the LR-56. The Excel spreadsheet and Radcalc for Windows give identical results for the amount of hydrogen gas generated within the three significant figures reported by Radcalc for Windows. The Radcalc for Windows Input and Calculated Results sheet for this case, designated IB4, follows.

Radcalc for Windows 1.0

Date: 09-23-95 13:07

Performed By: X. Hillel

Checked By: _____

File: IB4.RAD

===== Input Information =====

Source from input:
Radionuclide: Na-24 Curies: 1.00e+001

Waste Form: Normal
Physical Form: Solid
Container Type: LR-56

	Entered Values:	Metric Values:
Package Void Volume:	0.700 m ³	7.00e+005 cc
Waste Volume:	4.20 m ³	4.20e+006 cc
Waste Mass:	4.20e+003 kg	4.20e+006 g
Waste Void Volume:	0.100 m ³	1.00e+005 cc

Days to decay source before seal time: 0.00 days
Days container is sealed: 1.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 1

Comments:
Test Case of Gamma Absorption Fractions for the LR-56
Container (IB4)

===== Calculated Results =====

H2 Percent Concentration: 0.00291 %
H2 Volume: 23.3 cc
H2 Generation Rate: 0.969 cc/hour

Heat Generated: 0.277 Watts
Partial Pressure (H2): 0.00295 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 2.0000)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.0079365)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Na-24 Curies: 1.00e+001

Source decayed to end of seal time:
Radionuclide: Na-24 Curies: 3.30e+000

IC USE OF G VALUES

Cases IC1 - IC5 address the use of G values by Radcalc for Windows. The amount of hydrogen generated by each radiation type is proportional to the corresponding G value of the waste matrix. Hydrogen volume calculated by Radcalc for Windows is compared with results of Excel spreadsheet calculations. The spreadsheets are set up to use Radcalc for Windows methodology and decay energy data, as was done for the cases listed under Section IB. Agreement between the values for the volume of hydrogen gas generated by the two methods (Radcalc and Excel spreadsheet) is interpreted as validating Radcalc's use of G values.

Case IC1: G Values Selected from Radcalc's Database, Using a Single Absorbing Material and a Beta/Gamma Source

Discussion and Conclusion

In case IC1, the G values used are selected from Radcalc for Windows' on-line database, assuming the only absorbing material present is water. The ^{137}Cs source used (in secular equilibrium with $^{137\text{m}}\text{Ba}$) provides a means of testing a set of G-beta and G-gamma values from Radcalc's on-line database, as well as its calculational methodology. As shown by the printout of case IC1, the hydrogen volumes calculated by the Excel spreadsheet and by Radcalc for Windows agree within the three significant figures reported by Radcalc for Windows.

Radcalc for Windows 1.0

Date: 09-23-95 13:07

Performed By: K. Hildner

Checked By: _____

File: IC1.RAD

===== Input Information =====

Source from input:
Radionuclide: Cs-137 Curies: 1.00e+001

Waste Form: Normal
Physical Form: Liquid
Container Type: 30 Gallon Drum

Package Void Volume: 7.00e+003 cc
Waste Volume: 1.10e+005 cc
Waste Mass: 1.00e+005 g
Waste True Density: 1.00 g/cc

Days to decay source before seal time: 365.24 days
Days container is sealed: 30.00 days

G Value Material Selection:
Contribution Weight G-Alpha G-Beta G-Gamma Name
100.00% 1 1.6 0.53 0.45 Water (liquid)
(* indicates the value was calculated from a given value)

G Values calculated from list averaging:
G Alpha G Beta G Gamma
1.6 0.53 0.45

Comments:

===== Calculated Results =====

H2 Percent Concentration: 0.543 %
H2 Volume: 92.7 cc
H2 Generation Rate: 0.129 cc/hour

Heat Generated: 0.0472 Watts
Partial Pressure (H2): 0.553 kPa
Total Pressure (H2 and Air): 102. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.97716)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.32572)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.909 g/cc

Source decayed to start of seal time:
Radionuclide: Cs-137 Curies: 9.77e+000
Ba-137m 9.24e+000

Source decayed to end of seal time:
Radionuclide: Cs-137 Curies: 9.75e+000
Ba-137m 9.23e+000

**Case IC2: G Values Selected from Radcalc's Database, Using
Two Absorbing Materials and an Alpha Source**

Discussion and Conclusion

In case IC2, the G values used are once again selected from Radcalc for Windows' on-line database. In this case, a cation/anion ion exchange mixture consisting of two different absorbing materials is used, forcing Radcalc to calculate a weighted average G value. The value found by Radcalc agrees with a separate hand calculation of the weighted average G value. The ^{241}Pu source used generates ^{241}Am , a heavy alpha emitter, providing a means of testing a set of G-alpha values from Radcalc's on-line database, as well as its calculational methodology. As shown by the printout of case IC2, which follows, the hydrogen volumes calculated by the Excel spreadsheet and by Radcalc for Windows agree within the three significant figures reported by Radcalc for Windows.

Radcalc for Windows 1.0

Date: 09-23-95 13:08

Performed By: K. Helled

Checked By: _____

File: IC2.RAD

===== Input Information =====

Source from input:
 Radionuclide: Pu-241 Curies: 1.00e+000

Waste Form: Special
 Physical Form: Solid
 Container Type: Doorstop Sample Carrier

	Entered Values:	Metric Values:
Package Void Volume:	2.40 in ³	39.3 cc
Waste Volume:	87.0 in ³	1.43e+003 cc
Waste Mass:	3.00 lb	1.36e+003 g
Waste Void Volume:	1.00 in ³	16.4 cc

Date to begin source decay: 8:00 Jul. 18, 1993
 Date container sealed: 8:00 Jul. 18, 1993
 Date container received: 8:00 Jul. 18, 1995
 Days to decay source before seal time: 0.00 days
 Days container is sealed: 730.00 days

G Value Material Selection:

Contribution	Weight	G-Alpha	G-Beta	G-Gamma	Name
30.00%	30	0.4*	0.1*	0.1	Dowex 50W
70.00%	70	0.36*	0.09*	0.09	Dowex 1

(* indicates the value was calculated from a given value)

G Values calculated from list averaging:

G Alpha	G Beta	G Gamma
0.372	0.093	0.093

Comments:

Test Case for G Values Selected from Radcalc's Database,
 Using Two Absorbing Materials and an Alpha Source (IC2)

===== Calculated Results =====

H2 Percent Concentration: 5.87 %
 H2 Volume: 3.48 cc
 H2 Generation Rate: 0.000198 cc/hour

Heat Generated: 3.18e-005 Watts
 Partial Pressure (H2): 6.32 kPa
 Total Pressure (H2 and Air): 108. kPa

Radioactive: Yes
 Type Determination: A (from unity fraction 0.0010000)
 Limited Quantity: Yes
 LSA Determination: No (from LSA unity fraction 146.97)
 HRC Quantity Determination: No
 Fissile Quantity: 0.0096736 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 0.954 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
Pu-241	1.00e+000

Source decayed to end of seal time:

Radionuclide:	Curies:
Pu-241	9.08e-001
Am-241	3.05e-003
Np-237	1.02e-009
Pa-233	9.18e-010
U-233	2.59e-015
Th-229	1.14e-019
U-237	2.23e-005

Case IC3: G Values Entered Directly, With All G Values Equal**Discussion and Conclusion**

In case IC3, all three G values are entered directly and set equal to 1.0. The ^{241}Pu source used generates ^{241}Am , a heavy alpha emitter, so it is mainly Radcalc's use of the given G-alpha value and calculational methodology that is being tested. As shown by the printout of case IC3, which follows, the hydrogen volumes calculated by the Excel spreadsheet and by Radcalc for Windows agree within the three significant figures reported by Radcalc for Windows.

Radcalc for Windows 1.0

Date: 09-23-95 13:08

Performed By: K. Hillen

Checked By: _____

File: IC3.RAD

===== Input Information =====

Source from input:
 Radionuclide: Pu-241 Curies: 1.00e+000

Waste Form: Normal
 Physical Form: Solid
 Container Type: PAS-1 Cask

	Entered Values:	Metric Values:
Package Void Volume:	1.62 ft ³	4.59e+004 cc
Waste Volume:	1.60 ft ³	4.53e+004 cc
Waste Mass:	200. lb	9.07e+004 g
Waste Void Volume:	0.100 ft ³	2.83e+003 cc

Days to decay source before seal time: 0.00 days
 Days container is sealed: 73050.00 days

Entered G Values:
 G Alpha G Beta G Gamma
 1 1 1

Comments:

Test Case for G Values Entered Directly, With All G Values
 Equal (IC3)

===== Calculated Results =====

H2 Percent Concentration: 21.9 %
 H2 Volume: 1.37e+004 cc
 H2 Generation Rate: 0.00779 cc/hour

Heat Generated: 3.18e-005 Watts
 Partial Pressure (H2): 28.4 kPa
 Total Pressure (H2 and Air): 130. kPa

Radioactive: Yes
 Type Determination: B (from unity fraction 10.000)
 Limited Quantity: No
 LSA Determination: No (from LSA unity fraction 2.2046)
 HRC Quantity Determination: No
 Fissile Quantity: 0.0096736 g
 Less than 15g Fissile Radionuclides: Yes
 (Fissile Excepted per 49CFR173.453(a))
 Note: Transportation classifications assume three significant figures.

Bulk Density: 2.00 g/cc

Source decayed to start of seal time:
 Radionuclide: Pu-241 Curies: 1.00e+000

Source decayed to end of seal time:
 Radionuclide: Curies:
 Pu-241 6.59e-005
 Am-241 2.50e-002
 Np-237 1.68e-006
 Pa-233 1.68e-006
 U-233 6.97e-010
 Th-229 4.10e-012
 Ra-225 4.10e-012
 Ac-225 4.09e-012
 Fr-221 4.09e-012
 At-217 4.09e-012
 Bi-213 4.09e-012
 Po-213 4.00e-012
 Pb-209 4.09e-012
 U-237 1.62e-009

Case IC4: G Values Entered Directly, Using Only a G-Beta Value**Discussion and Conclusion**

Case IC4 singles out hydrogen generation due to beta radiation alone by setting the G values for the alpha and gamma radiation types to zero. A ^{90}Sr beta source (in secular equilibrium with ^{90}Y) is used. As shown by the printout of case IC4, which follows, the hydrogen volumes calculated by the Excel spreadsheet and by Radcalc for Windows agree within the three significant figures reported by Radcalc for Windows.

Radcalc for Windows 1.0

Date: 09-23-95 13:09

Performed By: K. Hille

Checked By: _____

File: IC4.RAD

===== Input Information =====

Source from input:
Radionuclide: Becquerels:
Sr-90 1.00e+010
M.F.P. 1.00e+010

Waste Form: Normal
Physical Form: Solid
Container Type: Sample Pig Carrier

Package Void Volume: 1.00 cc
Waste Volume: 265. cc
Waste Mass: 264. g
Waste True Density: 1.00 g/cc

Days to decay source before seal time: 30.00 days
Days container is sealed: 7.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0.5 0

Comments:

Test Case for G Values Entered Directly, Using Only a
G-Beta Value (IC4)

===== Calculated Results =====

H2 Percent Concentration: 40.5 %
H2 Volume: 1.36 cc
H2 Generation Rate: 0.00811 cc/hour

Heat Generated: 0.00181 Watts
Partial Pressure (H2): 69.0 kPa
Total Pressure (H2 and Air): 170. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 1.3500)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 409.10)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.996 g/cc

Source decayed to start of seal time:
Radionuclide: Becquerels:
Sr-90 9.98e+009
Y-90 9.98e+009
M.F.P. 1.00e+010

Source decayed to end of seal time:
Radionuclide: Becquerels:
Sr-90 9.98e+009
Y-90 9.98e+009
M.F.P. 1.00e+010

**Case IC5: G Values Entered Directly, Using Only
G-Beta and G-Gamma Values**

Discussion and Conclusion

Case IC5 uses a source exhibiting both beta and gamma radiation (^{24}Na), for which the G values have been set equal to 1.0 and 0.5 molecules/100 eV, respectively. This combination provides a means of singling out hydrogen generation due to beta and gamma radiation. As shown by the printout of case IC5, which follows, the hydrogen volumes calculated by the Excel spreadsheet and by Radcalc for Windows agree within the three significant figures reported by Radcalc for Windows.

Radcalc for Windows 1.0

Date: 09-23-95 13:09

Performed By: X. Giller

Checked By: _____

File: IC5.RAD

===== Input Information =====

Source from input:
Radionuclide: Na-24 Curies: 5.00e+003

Waste Form: Normal
Physical Form: Solid
Container Type: Single Pass Fuel Cask

Package Void Volume: 5.00e+005 cc
Waste Volume: 5.00e+005 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 1.00e+004 cc

Date to begin source decay: 0:00 Feb. 28, 2000
Date container sealed: 0:00 Feb. 28, 2000
Days to decay source before seal time: 0.00 days
Calculate number of days sealed until 3.00% hydrogen is reached.

Entered G Values:
G Alpha G Beta G Gamma
2 1 0.5

Comments:
Test Case for G Values Entered Directly, Using Only G-Beta
and G-Gamma Values (IC5)

===== Calculated Results =====

The hydrogen concentration of 3.00 % was not calculated in 36500.00 days.
The hydrogen concentration of 2.41 % is calculated at 36500.00 days.
This corresponds to date: 0:00 Feb. 3, 2100
H2 Volume: 1.26e+004 cc
H2 Generation Rate: 0.0144 cc/hour

Heat Generated: 139. Watts
Partial Pressure (H2): 2.50 kPa
Total Pressure (H2 and Air): 104. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 1000.0)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 16.667)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 2.00 g/cc

Source decayed to start of seal time:
Radionuclide: Na-24 Curies: 5.00e+003

Source decayed to end of seal time:
Radionuclide: Na-24 Curies: 0.00e+000

ID PERCENT HYDROGEN

Percent hydrogen concentration is calculated from the hydrogen volume and total void volume. The total void volume is the sum of the package void volume and the interstitial void volume in the waste. Radcalc for Windows results are compared against Excel spreadsheet calculations. The spreadsheets are set up to use Radcalc for Windows methodology and decay energy data in the calculation of hydrogen volume, as was done for the cases listed under Section IB. The percent hydrogen concentration is calculated by the Excel spreadsheets from the package volume, interstitial void volume, and hydrogen volume using the Radcalc for Windows methodology outlined in Chapter 2.0.

Case ID1: Percent Hydrogen Using Direct Entry of Interstitial Void Volume

Discussion and Conclusion

Cases IB2, IB3, IB4, IC2, IC3, and IC5 presented previously use a directly entered interstitial void volume in conjunction with the package void volume and hydrogen volume to calculate the percent hydrogen. The Radcalc for Windows and spreadsheet calculations give identical results for percent hydrogen concentrations within the three significant figures reported by Radcalc for Windows in all cases.

Case ID2: Percent Hydrogen Using a Calculation of Interstitial Void Volume

Discussion and Conclusion

Cases IB1 and IC4 calculate the interstitial void volume from the waste mass, waste volume, and waste true density entered by the user. The spreadsheets calculate interstitial void volume from these quantities using the Radcalc for Windows methodology outlined in Chapter 2.0. The Radcalc for Windows and spreadsheet calculations give identical results for percent hydrogen concentrations within the three significant figures reported by Radcalc for Windows in both cases.

CASE IE: HYDROGEN GENERATION RATE

Discussion and Conclusion

Hydrogen generation rates calculated by Radcalc for Windows are compared against Excel spreadsheet calculations. The hydrogen generation rate is found by dividing the hydrogen volume by the seal time in both Radcalc for Windows and the spreadsheet calculations. The spreadsheets are set up to use Radcalc for Windows methodology and decay energy data in the calculation of hydrogen volume, as was done for cases listed under Section IB. The Radcalc for Windows and spreadsheet calculations give identical results for the hydrogen generation rates within the three significant figures reported by Radcalc for Windows in cases IB1, IB2, IB3, IB4, IC2, IC3, IC4, and IC5 presented previously.

II DECAY ALGORITHMS

IIA ACTIVITY AS A FUNCTION OF TIME

The decay algorithm used by Radcalc for Windows was tested against calculations using standard analytical solutions to the decay equation. John M. West (Etherington 1958) gives analytical solutions for decay chains of up to four generations. Half-lives and branching ratios in all calculations came from the ORIGEN2 database used by Radcalc for Windows.

Case IIA1: Simple Decay

Discussion and Results

Radcalc for Windows was compared to Excel spreadsheet calculations for cases involving radionuclides that decay directly to stable isotopes (one generation). The spreadsheet calculations use the standard analytical solution to the decay equation for one generation of decay. One curie each of ^{60}Co (5.27-year half-life), ^{90}Y (64-hour half-life), and ^{14}C (5,730-year half-life) were decayed for 1, 100, and 100,000 days. In all cases, Radcalc for Windows gave results identical to the spreadsheet calculations within the three significant figures reported by Radcalc for Windows. The results of these calculations are given below. Note that after decaying one curie of ^{90}Y for 100,000 days, the result is smaller than can be represented by Radcalc for Windows or the spreadsheet and is therefore given as zero.

	1 day	100 days	100,000 days
^{14}C	1.00E+00 Ci	1.00E+00 Ci	9.67E-01 Ci
^{60}Co	1.00E+00	9.65E-01	2.29E-16
^{90}Y	7.71E-01	5.14E-12	0.00E+00

Case IIA2: Parent-Daughter Decay

Discussion and Results

Radcalc for Windows was compared to Excel spreadsheet calculations for cases involving radionuclides that decay from parent to daughter and then to a stable isotope (two generations). The spreadsheet calculations use the standard analytical solution to the decay equation for two generations of decay. One curie each of ^{137}Cs and ^{90}Sr were decayed for 1, 100, and 100,000 days. ^{137}Cs decays to $^{137\text{m}}\text{Ba}$. ^{90}Sr decays to ^{90}Y . In all cases Radcalc for Windows gave results identical to the spreadsheet calculations within the three significant figures reported by Radcalc for Windows. The results of these calculations are given below.

	1 day	100 days	100,000 days
^{90}Sr	1.00E+00 Ci	9.94E-01 Ci	1.48E-03 Ci
^{90}Y	2.29E-01	9.94E-01	1.48E-03
^{137}Cs	1.00E+00	9.94E-01	1.79E-03
$^{137\text{m}}\text{Ba}$	9.46E-01	9.40E-01	1.69E-03

Case IIA3: Complex Decay Chain**Discussion and Conclusion**

Radcalc for Windows was compared to simple FORTRAN code calculations for the decay of ^{241}Pu . The FORTRAN code calculations are based on the analytical solution to the decay equation for three generations. Due to the complexity of the analytical solution, only three generations are considered. The decay of ^{241}Pu represents a complex decay chain calculation. ^{241}Pu (14.4-year half-life) decays to ^{241}Am (432.2-year half-life), which in turn decays to ^{237}Np (2.14-million-year half-life). The ^{241}Pu decay chain was chosen because of its progression of half-lives from short to long. Calculations were done for 730.5 days, 7305 days, 73,050 days, and 730,500 days. Radcalc for Windows results are given below under the heading RADCALC. The results for ^{237}Np from the FORTRAN code are given under the heading FORTRAN.

	730.5 days	7,305 days	73,050 days	730,500 days
RADCALC				
^{241}Pu	9.08E-01 Ci	3.82E-01 Ci	6.59E-05 Ci	0.00E+00 Ci
^{241}Am	3.05E-03	2.02E-02	2.50E-02	1.39E-03
^{237}Np	1.02E-09	7.65E-08	1.68E-06	6.44E-06
FORTRAN				
^{237}Np	1.01E-09	7.64E-08	1.68E-06	6.44E-06

Except for ^{237}Np , Radcalc for Windows and the FORTRAN calculations give identical results within the three significant figures reported by Radcalc for Windows. The discrepancy in the value for ^{237}Np is attributed to loss of precision in the use of the analytical solution by the FORTRAN code; i.e., the near cancellation of two terms by subtraction.

IIB INTEGRATED DISINTEGRATIONS OVER TIME

Time integrated disintegrations are used in the hydrogen generation calculations. The algorithm used by Radcalc for Windows for calculating time integrated disintegrations was tested against calculations based on the standard analytical solutions to the decay equation. John M. West (Etherington 1958) gives analytical solutions for decay chains of up to four generations. These equations are integrated with respect to time to obtain analytical expressions for total disintegrations of a radionuclide over a given time interval. Half-lives and branching ratios used for all calculations came from the ORIGEN2 database used by Radcalc for Windows.

The official release version of Radcalc for Windows does not print out time integrated disintegrations. A test version of Radcalc for Windows was therefore created to print out the time integrated disintegrations used internally by Radcalc for Windows to six significant figures. This special test version uses the same source code as the release version, but uses "debug" compiler and linker options to allow for the use of "debug prints." All output by the test version is identical to that given by the release version. Through use of the test version, time integrated disintegrations calculated by Radcalc for Windows can be compared directly to calculations based on analytical solutions to the decay equations, as described above.

Because time integrated disintegrations are used in the hydrogen gas generation calculations, cases listed under Sections IB and IC are also relevant to the validation of time integrated disintegration calculations. The same method for calculating time integrated disintegrations from analytical decay equation solutions used here was also used for the spreadsheet calculations mentioned in Sections IB and IC. Specific cases from Sections IB and IC are given below.

Case IIB1: Simple Decay

Discussion and Results

Time integrated disintegrations given by the test version of Radcalc for Windows described previously were compared to Excel spreadsheet calculations for cases involving radionuclides that decay directly to stable isotopes (one generation). The spreadsheet calculations are based on the standard analytical solution to the decay equation for one generation of decay. One curie each of ^{60}Co (5.27-year half-life), ^{90}Y (64-hour half-life), and ^{14}C (5,730-year half-life) were decayed for 1, 100, and 100,000 days. In all cases, Radcalc for Windows gave results identical to the spreadsheet calculations. Time integrated disintegrations are given below.

	1 day	100 days	100,000 days
^{14}C	3.19680E+15 Ci	3.19675E+17 Ci	3.14443E+20 Ci
^{60}Co	3.19622E+15	3.13992E+17	8.87705E+18
^{90}Y	2.81510E+15	1.22987E+16	1.22987E+16

Additional support for the correctness of Radcalc's methodology comes from cases IB3, IB4, and IC5 presented previously, which also gave correct results based on time integrated disintegrations calculated for one generation of decay.

Case IIB2: Parent-Daughter Decay

Discussion and Results

Time integrated disintegrations given by the test version of Radcalc for Windows described previously were compared to Excel spreadsheet calculations for cases involving radionuclides that decay from parent to daughter and then to a stable isotope (two generations). The spreadsheet calculations are based on the standard analytical solution to the decay equation for two generations of decay. One curie each of ^{137}Cs and ^{90}Sr were decayed for 1, 100, and 100,000 days. ^{137}Cs decays to $^{137\text{m}}\text{Ba}$. ^{90}Sr decays to ^{90}Y . In all cases, Radcalc for Windows gave results identical to the spreadsheet calculations. Time integrated disintegrations are given below.

	1 day	100 days	100,000 days
^{90}Sr	3.19670E+15 Ci	3.18641E+17 Ci	4.89834E+19 Ci
^{90}Y	3.81689E+14	3.06419E+17	4.89834E+19
^{137}Cs	3.19670E+15	3.18671E+17	5.04442E+19
$^{137\text{m}}\text{Ba}$	3.01635E+15	3.01455E+17	4.77202E+19

Additional support for the correctness of Radcalc's methodology comes from cases IB1 and IC4 presented previously, which also gave correct results based on time integrated disintegrations calculated for two generations of decay.

Case IIB3: Complex Decay Chain

Discussion and Results

Time integrated disintegrations given by the test version of Radcalc for Windows described previously were compared to simple FORTRAN code calculations in the decay of ^{241}Pu . The FORTRAN code calculations are based on the analytical solution to the decay equation for three generations. The decay of ^{241}Pu represents a complex decay chain calculation. Due to the complexity of the analytical solution, only three generations are considered. ^{241}Pu (14.4-year half-life) decays to ^{241}Am (432.2-year half-life), which in turn decays to ^{237}Np (2.14-million-year half-life). The ^{241}Pu decay chain was chosen because of its progression of half-lives from short to long. Calculations were done for 730.5 days, 7,305 days, 73,050 days, and 730,500 days. The Radcalc for Windows and FORTRAN code results are given below. The FORTRAN program has precision to no more than four significant figures.

		730.5 days	7,305 days	73,050 days	730,500 days
RADCALC	^{241}Pu	2.226E+18 Ci	1.499E+19 Ci	2.425E+19 Ci	2.426E+19 Ci
FORTTRAN	^{241}Pu	2.226E+18	1.500E+19	2.425E+19	2.426E+19
RADCALC	^{241}Am	3.624E+15	2.753E+17	6.049E+18	2.324E+19
FORTTRAN	^{241}Am	3.624E+15	2.753E+17	6.050E+18	2.324E+19
RADCALC	^{237}Np	8.064E+08	6.422E+11	1.864E+14	1.085E+16
FORTTRAN	^{237}Np	7.890E+08	6.409E+11	1.864E+14	1.084E+16

The largest discrepancies are for ^{237}Np at 730.5 and 7,305 days. As in IIA3, the discrepancies in the values for ^{237}Np are attributed to loss of numerical precision in the use of the analytical solution by the FORTRAN code; i.e., the near cancellation of two terms by subtraction.

Additional support for the correctness of Radcalc's methodology comes from cases IB2, IC2, and IC3 presented previously, which also gave correct results based on time integrated disintegrations calculated for the ^{241}Pu decay chain.

IIIA TRANSPORTATION CALCULATIONS

Cases IIIA1 - IIIA17 compare Radcalc for Windows with calculations performed using an Excel Version 5.0 spreadsheet created specifically to evaluate transportation classifications. Cases 1 and 2 verify type classifications for both normal and special forms. Cases 3 - 9 verify limited quantity classifications. Cases 10 - 13 verify low specific activity

classifications. Cases 14 - 16 verify highway route controlled quantity classifications. Case 17 verifies fissile excepted classifications.

A common methodology was employed to test most of the classification algorithms. First, a group of either three or four radionuclides was selected at random, and the activities of the radionuclides were chosen so that the group's combined unity fraction was exactly equal to the limiting value associated with the classification of interest. Radcalc was then run with these values to confirm that the "borderline" case was correctly categorized. Next, one of the activities was increased slightly, so as to make the combined unity fraction exceed the limiting value by 1%. Radcalc was then run using this new set of values in order to confirm that the package was once again correctly classified. Printouts of both the original "borderline" Radcalc output and the final "1% over limit" output will be given for the first example in each major classification category, but not for subsequent examples.

Case IIIA1: Type Classification for a Normal Form Material

Discussion and Conclusion

Information for a normal form solid containing four radionuclides was run on Radcalc for Windows. The activities of the four radionuclides were chosen to be exactly one quarter of their associated A_2 values, so that the combined unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA1a) shows that the package was correctly identified as Type A.

The printout that follows (designated IIIA1b) shows the effect of slightly increasing one of the four activities used previously. With a combined unity fraction of 1.01, the package was correctly identified as Type B.

Radcalc for Windows 1.0

Date: 09-22-95 13:50

Performed By: H. Harris

Checked By: _____

File: IIIA1A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Co-60 1.75e+000
Tc-99 6.25e+000
I-131 2.50e+000
Am-241 2.00e-003

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Type A Normal Form Material (IIIA1a)
Combined Unity Fraction = 1.0 Using A2 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.0387 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 1.0000)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.055000)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Co-60 1.75e+000
Tc-99 6.25e+000
I-131 2.50e+000
Am-241 2.00e-003

Source decayed to end of seal time:
Radionuclide: Curies:
Co-60 1.73e+000
Tc-99 6.25e+000
I-131 1.88e-001
Am-241 2.00e-003
Np-237 5.32e-011
Pa-233 1.61e-011
U-233 2.05e-018

Radcalc for Windows 1.0

Date: 09-22-95 13:51

Performed By: A. Harris

Checked By: _____

File: IIIA1B.RAD

===== Input Information =====

Source from input:	
Radionuclide:	Curies:
Co-60	1.75e+000
Tc-99	6.25e+000
I-131	2.50e+000
Am-241	2.08e-003

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:		
G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Type B Normal Form Material (IIIA1b)
Combined Unity Fraction = 1.01 Using A2 Values

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	0.0387 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 1.0100)
Limited Quantity:	No
LSA Determination:	Yes (from LSA unity fraction 0.055800)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:	
Radionuclide:	Curies:
Co-60	1.75e+000
Tc-99	6.25e+000
I-131	2.50e+000
Am-241	2.08e-003

Source decayed to end of seal time:	
Radionuclide:	Curies:
Co-60	1.73e+000
Tc-99	6.25e+000
I-131	1.88e-001
Am-241	2.08e-003
Np-237	5.53e-011
Pa-233	1.67e-011
U-233	2.13e-018

Case IIIA2: Type Classification for a Special Form Material**Discussion and Conclusion**

Information for a special form material containing four radionuclides was run on Radcalc for Windows. The activities of the four radionuclides were chosen to be exactly one quarter of their associated A_1 values, so that the combined unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA2a) shows that the package was correctly identified as Type A. When one of the activities was increased slightly, raising the combined unity fraction to 1.01, Radcalc correctly identified the package as Type B.

Radcalc for Windows 1.0

Date: 09-22-95 13:52

Performed By: H. Harris

Checked By: _____

File: IIIA2A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Co-60 1.75e+000
Tc-99 2.50e+002
I-131 1.00e+001
Am-241 2.00e+000

Waste Form: Special
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:
Test Case for a Type A Special Form Material (IIIA2a)
Combined Unity Fraction = 1.0 Using A1 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.253 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 1.0000)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 20.873)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Co-60 1.75e+000
Tc-99 2.50e+002
I-131 1.00e+001
Am-241 2.00e+000

Source decayed to end of seal time:
Radionuclide: Curies:
Co-60 1.73e+000
Tc-99 2.50e+002
I-131 7.53e-001
Am-241 2.00e+000
Np-237 5.32e-008
Pa-233 1.61e-008
U-233 2.05e-015

**Case IIIA3: Limited Quantity Classification for a
Special Form Material**

Discussion and Conclusion

Information for a special form material containing four radionuclides was run on Radcalc for Windows. The activities of the four radionuclides were chosen to be exactly $2.5\text{E-}4$ of their associated A_1 values, so that the combined unity fraction was exactly $1.0\text{E-}3$. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA3a) shows that the package was correctly identified as limited quantity.

The printout that follows (designated IIIA3b) shows the effect of slightly increasing one of the four activities used previously. With a combined unity fraction of $1.01\text{E-}3$, the package was correctly identified as having exceeded the limited quantity standard.

Radcalc for Windows 1.0

Date: 09-22-95 13:54

Performed By: A. Harris

Checked By: _____

File: IIIA3A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Na-24 1.25e-003
P-32 7.50e-003
Ru-103 7.50e-003
Ir-192 5.00e-003

Waste Form: Special
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Limited Quantity of a Special Form Material
(IIIA3a)

Combined Unity Fraction = 0.001 Using A1 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.000121 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.0010000)
Limited Quantity: Yes
LSA Determination: Yes (from LSA unity fraction 7.0833e-005)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Na-24 1.25e-003
P-32 7.50e-003
Ru-103 7.50e-003
Ir-192 5.00e-003

Source decayed to end of seal time:
Radionuclide: Curies:
Na-24 4.44e-018
P-32 1.75e-003
Ru-103 4.42e-003
Rh-103m 3.98e-003
Ir-192 3.78e-003

Radcalc for Windows 1.0

Date: 09-22-95 13:54

Performed By: H. Harris

Checked By: _____

File: IIIA3B.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Na-24 1.30e-003
P-32 7.50e-003
Ru-103 7.50e-003
Ir-192 5.00e-003

Waste Form: Special
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Limited Quantity of a Special Form Material
(IIIA3b)

Combined Unity Fraction > 0.001 Using A1 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.000122 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.0010100)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 7.1000e-005)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Na-24 1.30e-003
P-32 7.50e-003
Ru-103 7.50e-003
Ir-192 5.00e-003

Source decayed to end of seal time:
Radionuclide: Curies:
Na-24 4.62e-018
P-32 1.75e-003
Ru-103 4.42e-003
Rh-103m 3.98e-003
Ir-192 3.78e-003

**Case IIIA4: Limited Quantity Classification for a
Normal Form Material**

Discussion and Conclusion

Information for a normal form solid containing three radionuclides was run on Radcalc for Windows. The activities of the three radionuclides were chosen to be exactly $3.33\text{E-}4$ of their associated A_2 values, so that the combined unity fraction was exactly $1.0\text{E-}3$. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA4a) shows that the package was correctly identified as limited quantity. When one of the activities was increased slightly, raising the combined unity fraction to $1.01\text{E-}3$, Radcalc correctly identified the package as having exceeded the limited quantity limit.

Radcalc for Windows 1.0

Date: 09-22-95 13:55

Performed By: H. Harris

Checked By: _____

File: IIIA4A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
C-14	2.00e-002
Sn-113	2.00e-002
Pu-238	1.00e-006

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Limited Quantity of a Normal Form Solid
(IIIA4a)
Combined Unity Fraction = 0.001 Using A2 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 9.22e-006 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.0010000)
Limited Quantity: Yes
LSA Determination: Yes (from LSA unity fraction 0.00014333)
HRC Quantity Determination: No
Fissile Quantity: 5.8384e-008 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
C-14	2.00e-002
Sn-113	2.00e-002
Pu-238	1.00e-006

Source decayed to end of seal time:

Radionuclide:	Curies:
C-14	2.00e-002
Sn-113	1.39e-002
In-113m	6.98e-003
Pu-238	9.99e-007
U-234	2.33e-013
Th-230	8.61e-020

Case IIIA5: Limited Quantity Classification for
a Liquid Form Material

Discussion and Conclusion

Information for a normal form liquid containing four radionuclides was run on Radcalc for Windows. The activities of the four radionuclides were chosen to be exactly $2.5\text{E-}5$ of their associated A_2 values, so that the combined unity fraction was exactly $1.0\text{E-}4$. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA5a) shows that the package was correctly identified as limited quantity. When one of the activities was increased slightly, raising the combined unity fraction to $1.01\text{E-}4$, Radcalc correctly identified the package as having exceeded the limited quantity limit.

Radcalc for Windows 1.0

Date: 09-25-95 09:25

Performed By: A. Harris

Checked By: _____

File: IIIA5A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Na-22 2.00e-004
Mn-54 5.00e-004
Eu-154 1.25e-004
Pu-239 5.00e-008

Waste Form: Normal
Physical Form: Liquid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Limited Quantity of a Normal Form Liquid
(IIIA5a)

Combined Unity Fraction = 0.0001 Using A2 Values

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 6.46e-006 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: No
Type Determination: A (from unity fraction 0.00010000)
Limited Quantity: Yes
LSA Determination: Yes (from LSA unity fraction 3.2500e-006)
HRC Quantity Determination: No
Fissile Quantity: 8.0591e-007 g

Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:

Radionuclide: Curies:
Na-22 2.00e-004
Mn-54 5.00e-004
Eu-154 1.25e-004
Pu-239 5.00e-008

Source decayed to end of seal time:

Radionuclide: Curies:
Na-22 1.96e-004
Mn-54 4.68e-004
Eu-154 1.24e-004
Pu-239 5.00e-008
U-235 4.04e-018

**Case IIIA6: Limited Quantity Classification for Tritiated
Water With a Low Specific Activity (< 0.1 Ci/L)**

Discussion and Conclusion

Information for tritiated water containing only tritium with a low specific activity was run on Radcalc for Windows. The H-3 activity was chosen to be 1,000 Ci and the package volume 10,100 L, yielding a specific activity of 0.099 Ci/L. Radcalc correctly classified the package as limited quantity, as shown in the accompanying printout, designated IIIA6a. When the activity was increased to 1010 Ci, Radcalc correctly identified the package as having exceeded the limited quantity limit, as shown in the printout designated IIIA6b.

Radcalc for Windows 1.0

Date: 09-22-95 13:56

Performed By: H. Harris

Checked By: _____

File: 111A6A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
H-3 1.00e+003

Waste Form: Normal
Physical Form: Tritiated Water
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.01e+007 cc
Waste Mass: 1.01e+007 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Limited Quantity of Tritiated Water with a
Low Specific Activity (111A6a)
Specific Activity < 0.1 Ci / liter and Total Activity =
1000 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.0337 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 1.0000)
Limited Quantity: Yes
LSA Determination: Yes (from LSA unity fraction 0.33003)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
H-3 1.00e+003

Source decayed to end of seal time:
Radionuclide: Curies:
H-3 9.95e+002

Radcalc for Windows 1.0

Date: 09-22-95 13:56

Performed By: H. Harris

Checked By: _____

File: IIIA6B.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
H-3 1.01e+003

Waste Form: Normal
Physical Form: Tritiated Water
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.01e+007 cc
Waste Mass: 1.01e+007 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Limited Quantity of Tritiated Water with a
Low Specific Activity (IIIA6b)
Specific Activity = 0.1 Ci / liter and Total Activity =
1010 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.0341 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 1.0100)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.33333)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
H-3 1.01e+003

Source decayed to end of seal time:
Radionuclide: Curies:
H-3 1.01e+003

**Case IIIA7: Limited Quantity Classification for Tritiated
Water With an Intermediate Specific Activity
(≥ 0.1 Ci/L and ≤ 1.0 Ci/L)**

Discussion and Conclusion

Information for tritiated water containing only tritium with an intermediate specific activity was run on Radcalc for Windows. The H-3 activity was chosen to be 100 Ci and the package volume 1,000 L, yielding a specific activity of 0.1 Ci/L. Radcalc correctly classified the package as limited quantity, as shown in the accompanying printout, designated IIIA7a. When the activity was increased to 101 Ci, Radcalc correctly identified the package as having exceeded the limited quantity limit.

Radcalc for Windows 1.0

Date: 09-22-95 13:58

Performed By: A. Harris

Checked By: _____

File: IIIA7A.RAD

===== Input Information =====

Source from input:
Radionuclide: H-3 Curies: 1.00e+002

Waste Form: Normal
Physical Form: Tritiated Water
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Limited Quantity of Tritiated Water with an
Intermediate Specific Activity (IIIA7a)
Specific Activity = 0.1 Ci / liter and
Total Activity = 100 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.00337 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.10000)
Limited Quantity: Yes
LSA Determination: Yes (from LSA unity fraction 0.33333)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: H-3 Curies: 1.00e+002

Source decayed to end of seal time:
Radionuclide: H-3 Curies: 9.95e+001

**Case IIIA8: Limited Quantity Classification for Tritiated
Water With a High Specific Activity (> 1.0 Ci/L)**

Discussion and Conclusion

Information for tritiated water containing only tritium with a high specific activity was run on Radcalc for Windows. The H-3 activity was chosen to be 1 Ci and the package volume 1 L, yielding a specific activity of 1.0 Ci/L. Radcalc correctly classified the package as limited quantity, as shown in the accompanying printout, designated IIIA8a. When the activity was increased to 1.01 Ci, Radcalc correctly identified the package as having exceeded the limited quantity limit.

Radcalc for Windows 1.0

Date: 09-22-95 13:59

Performed By: H. Harris

Checked By: _____

File: IIIA8A.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
H-3 1.00e+000

Waste Form: Normal
Physical Form: Tritiated Water
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+003 cc
Waste Mass: 1.00e+003 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Limited Quantity of Tritiated Water with a
High Specific Activity (IIIA8a)
Specific Activity = 1.0 Ci / liter and Total Activity = 1 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 3.37e-005 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.0010000)
Limited Quantity: Yes
LSA Determination: No (from LSA unity fraction 3.3333)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
H-3 1.00e+000

Source decayed to end of seal time:
Radionuclide: Curies:
H-3 9.95e-001

**Case IIIA9: Limited Quantity Classification for Tritiated
Water Containing Other Radionuclides**

Discussion and Conclusion

Information for tritiated water containing high specific activity tritium plus two other radionuclides was run on Radcalc for Windows. The H-3 activity was chosen to be 10 Ci and the package volume 10 L, yielding a specific activity of 1.0 Ci/L and a corresponding "H-3 limit" value of 100 Ci. The other two nuclides had a combined unity fraction of $9.0\text{E-}5$, which was 0.9 of 10^{-4} . When the ratio of the H-3 activity to the H-3 limit ($10\text{ Ci}/100\text{ Ci} = 0.1$) was added to the 0.9 , the result was 1.0 , which classifies the package as limited quantity. Radcalc correctly identified the package as limited quantity, as shown in the accompanying printout, designated IIIA9a. When the activity was increased to 10.1 Ci , Radcalc correctly identified the package as having exceeded the limited quantity limit.

Radcalc for Windows 1.0

Date: 09-22-95 14:00

Performed By: A. Harris

Checked By: _____

File: IIIA9A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
H-3	1.00e+001
Na-22	4.00e-004
Eu-152	4.00e-004

Waste Form:	Normal
Physical Form:	Tritiated Water
Container Type:	30 Gallon Drum

Package Void Volume:	2.17e+005 cc
Waste Volume:	1.00e+004 cc
Waste Mass:	1.00e+004 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	12:00 Sep. 5, 1995
Date container sealed:	12:00 Sep. 5, 1995
Date container received:	12:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Limited Quantity of Tritiated Water
Containing Two Other Radionuclides (IIIA9a)
Specific Activity = 1.0 Ci / liter and H-3 Limit = 100 Ci

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	0.000346 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	A (from unity fraction 0.010090)
Limited Quantity:	Yes
LSA Determination:	No (from LSA unity fraction 3.3336)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
H-3	1.00e+001
Na-22	4.00e-004
Eu-152	4.00e-004

Source decayed to end of seal time:

Radionuclide:	Curies:
H-3	9.95e+000
Na-22	3.91e-004
Eu-152	3.98e-004

**Case IIIA10: Low Specific Activity Classification for a
Type A Package With Low A_2 Values (≤ 0.05 Ci)**

Discussion and Conclusion

Information for a Type A package containing four radionuclides, all with A_2 values less than 0.05 Ci, was run on Radcalc for Windows. The activities of the four radionuclides were chosen so that their associated mCi/g to low specific activity limit ratios were exactly 0.25, so that the combined low specific activity unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA10a) shows that the package was correctly identified as low specific activity. When one of the activities was increased slightly, raising the combined low specific activity unity fraction to 1.01, Radcalc correctly identified the package as having exceeded the low specific activity limit, as shown in the printout designated IIIA10b.

Radcalc for Windows 1.0

Date: 09-22-95 14:02

Performed By: A. Harris

Checked By: _____

File: IIIA10A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Ac-227	2.50e-004
Th-228	2.50e-004
Pu-242	2.50e-004
Cf-252	2.50e-004

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+004 cc
Waste Mass:	1.00e+004 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Low Specific Activity Type A Package
(IIIA10a)
All A2 Values < 0.05 Ci and
Combined LSA Unity Fraction = 1.0

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	2.46e-005 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	A (from unity fraction 0.22569)
Limited Quantity:	No
LSA Determination:	Yes (from LSA unity fraction 1.0000)
MRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
Ac-227	2.50e-004
Th-228	2.50e-004
Pu-242	2.50e-004
Cf-252	2.50e-004

Source decayed to end of seal time:

Radionuclide:	Curies:
Ac-227	2.49e-004
Th-227	1.65e-004
Ra-223	1.04e-004
Po-215	1.04e-004
Pb-211	1.03e-004

Bi-211	1.03e-004
Tl-207	1.03e-004
Fr-223	3.44e-006
Th-228	2.43e-004
Ra-224	2.43e-004
Pb-212	2.43e-004
Bi-212	2.43e-004
Pu-242	2.50e-004
U-238	3.19e-015
Cf-252	2.45e-004

Radcalc for Windows 1.0

Date: 09-22-95 14:02

Performed By: Al. Harris

Checked By: _____

File: IIIA10B.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Ac-227	2.60e-004
Th-228	2.50e-004
Pu-242	2.50e-004
Cf-252	2.50e-004

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+004 cc
Waste Mass:	1.00e+004 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Low Specific Activity Type A Package
(IIIA10b)

All A2 Values < 0.05 Ci and

Combined LSA Unity Fraction = 1.01

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	2.46e-005 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	A (from unity fraction 0.22903)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 1.0100)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
Ac-227	2.60e-004
Th-228	2.50e-004
Pu-242	2.50e-004
Cf-252	2.50e-004

Source decayed to end of seal time:

Radionuclide:	Curies:
Ac-227	2.59e-004
Th-227	1.72e-004
Ra-223	1.08e-004
Po-215	1.08e-004
Pb-211	1.08e-004

Bi-211	1.08e-004
Tl-207	1.07e-004
Fr-223	3.58e-006
Th-228	2.43e-004
Ra-224	2.43e-004
Pb-212	2.43e-004
Bi-212	2.43e-004
Pu-242	2.50e-004
U-238	3.19e-015
Cf-252	2.45e-004

Case IIIA11: Low Specific Activity Classification for a
Type B Package With Intermediate A_2 Values
(> 0.05 Ci and ≤ 1.0 Ci)

Discussion and Conclusion

Information for a Type B package containing four radionuclides, all with A_2 values between 0.05 and 1.0 Ci, was run on Radcalc for Windows. The activities of the four radionuclides were chosen so that their associated mCi/g to low specific activity limit ratios were exactly 0.25, so that the combined low specific activity unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA11a) shows that the package was correctly identified as low specific activity. When one of the activities was increased slightly, raising the combined low specific activity unity fraction to 1.01, Radcalc correctly identified the package as having exceeded the low specific activity limit.

Radcalc for Windows 1.0

Date: 09-22-95 14:03

Performed By: H. Harris

Checked By: _____

File: IIIA11A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Th-227	1.25e-001
U-230	1.25e-001
U-236	1.25e-001
Pu-241	1.25e-001

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+005 cc
Waste Mass:	1.00e+005 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Low Specific Activity Type B Package

(IIIA11a)

All A2 Values > 0.05 Ci and < 1.0 Ci

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	0.0124 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 3.7500)
Limited Quantity:	No
LSA Determination:	Yes (from LSA unity fraction 1.0000)
HRC Quantity Determination:	No
Fissile Quantity:	0.0012092 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
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Source decayed to start of seal time:

Radionuclide:	Curies:
Th-227	1.25e-001
U-230	1.25e-001
U-236	1.25e-001
Pu-241	1.25e-001

Source decayed to end of seal time:

Radionuclide:	Curies:
Th-227	4.11e-002
Ra-223	5.36e-002
Po-215	5.36e-002
Pb-211	5.37e-002
Bi-211	5.37e-002
Tl-207	5.35e-002

U-230	4.60e-002
Po-214	4.60e-002
Pb-210	2.01e-004
Bi-210	1.66e-004
Po-210	1.11e-005
U-236	1.25e-001
Th-232	5.06e-013
Ra-228	2.15e-015
Pu-241	1.25e-001
Am-241	1.64e-005
Np-237	2.75e-013
Pa-233	6.09e-014
U-233	4.36e-021
U-237	2.91e-006

**Case IIIA12: Low Specific Activity Classification for a
Type B Package With High A_2 Values (> 1.0 Ci)**

Discussion and Conclusion

Information for a Type B package containing three radionuclides, all with A_2 values greater than 1.0 Ci, was run on Radcalc for Windows. The activities of the three radionuclides were chosen so that their associated mCi/g to low specific activity limit ratios were exactly 0.333, so that the combined low specific activity unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA12a) shows that the package was correctly identified as low specific activity. When one of the activities was increased slightly, raising the combined low specific activity unity fraction to 1.01, Radcalc correctly identified the package as having exceeded the low specific activity limit.

Radcalc for Windows 1.0

Date: 09-22-95 16:05

Performed By: J. Harris

Checked By: _____

File: IIIA12A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
S-35	1.00e+001
Mn-56	1.00e+001
I-131	1.00e+001

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+005 cc
Waste Mass: 1.00e+005 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Low Specific Activity Type B Package
(IIIA12a)
All A2 Values > 1.0 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.186 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 3.1667)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 1.0000)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:

Radionuclide:	Curies:
S-35	1.00e+001
Mn-56	1.00e+001
I-131	1.00e+001

Source decayed to end of seal time:

Radionuclide:	Curies:
S-35	7.90e+000
Mn-56	0.00e+000
I-131	7.53e-001

**Case IIIA13: Low Specific Activity Classification for
a Type A Package With Mixed A_2 Values**

Discussion and Conclusion

Information for a Type A package containing three radionuclides, each having an associated A_2 value in a different range, was run on Radcalc for Windows. The activities of the three radionuclides were chosen so that their associated mCi/g to low specific activity limit ratios were exactly 0.5, 0.25, and 0.25, so that the combined low specific activity unity fraction was exactly 1.0. The accompanying printout of the Radcalc for Windows Input and Calculated Results sheet (designated IIIA13a) shows that the package was correctly identified as low specific activity. When one of the activities was increased slightly, raising the combined low specific activity unity fraction to 1.01, Radcalc correctly identified the package as having exceeded the low specific activity limit.

Radcalc for Windows 1.0

Date: 09-22-95 14:04

Performed By: H. Harris

Checked By: _____

File: IIIA13A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Cr-51	1.50e+001
Th-227	1.25e-001
Am-241	2.50e-003

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+005 cc
Waste Mass:	1.00e+005 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Low Specific Activity Type A Package
(IIIA13a)
Mixed A2 Values

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	0.00796 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	A (from unity fraction 0.96250)
Limited Quantity:	No
LSA Determination:	Yes (from LSA unity fraction 1.0000)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
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Source decayed to start of seal time:

Radionuclide:	Curies:
Cr-51	1.50e+001
Th-227	1.25e-001
Am-241	2.50e-003

Source decayed to end of seal time:

Radionuclide:	Curies:
Cr-51	7.08e+000
Th-227	4.11e-002
Ra-223	5.36e-002
Po-215	5.36e-002
Pb-211	5.37e-002
Bi-211	5.37e-002
Tl-207	5.35e-002
Am-241	2.50e-003
Np-237	6.65e-011
Pa-233	2.01e-011
U-233	2.56e-018

**Case IIIA14: Highway Route Controlled Quantity Classification
for a Package in Which All Radionuclides Are
Limited by 3,000 A_2**

Discussion and Conclusion

Information for a Type B package containing two radionuclides with a total activity less than 30,000 Ci was run on Radcalc for Windows. The A_2 values were chosen to be less than 10, so that the limiting values used by Radcalc to calculate the highway route controlled quantity (HRCQ) unity fraction were both equal to 3,000 times A_2 . The activities of the radionuclides were chosen so that the ratio of each activity to the corresponding limiting value was exactly one-half, making the combined HRCQ unity fraction exactly equal to 1. The accompanying printout, designated IIIA14a, shows that Radcalc correctly identified the package as not requiring highway route control. When one of the activities was increased slightly, raising the combined HRCQ unity fraction to 1.01, Radcalc correctly identified the package as requiring highway route control, as shown in the accompanying printout designated IIIA14b.

Radcalc for Windows 1.0

Date: 09-25-95 10:41

Performed By: H. Harris

Checked By: _____

File: IIIA14A2.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
Na-24 7.50e+003
Pd-107 4.50e+003

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:

Test Case for a Highway Route Controlled Quantity (IIIA14a)
HRCQ Unity Fractions Limited by 3000 A2
Total Activity < 30000 Ci
HRCQ Unity Fraction = 1

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 208. Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 3000.0)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 40.000)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
Na-24 7.50e+003
Pd-107 4.50e+003

Source decayed to end of seal time:
Radionuclide: Curies:
Na-24 2.66e-011
Pd-107 4.50e+003

Radcalc for Windows 1.0

Date: 09-25-95 10:42

Performed By: H. Harris

Checked By: _____

File: IIIA14B2.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Na-24	7.65e+003
Pd-107	4.50e+003

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Highway Route Controlled Quantity (IIIA14b)
HRCQ Unity Fractions Limited by 3000 A2
Total Activity < 30000 Ci
HRCQ Unity Fraction = 1.01

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	212. Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 3030.0)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 40.500)
HRC Quantity Determination:	Yes
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
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Source decayed to start of seal time:

Radionuclide:	Curies:
Na-24	7.65e+003
Pd-107	4.50e+003

Source decayed to end of seal time:

Radionuclide:	Curies:
Na-24	2.72e-011
Pd-107	4.50e+003

**Case IIIA15: Highway Route Controlled Quantity Classification
for a Package in Which All Radionuclides Are Limited
by 30,000 Ci**

Discussion and Conclusion

Information for a Type B package containing two special-form radionuclides with a total activity of 30,000 Ci was run on Radcalc for Windows. The A_1 values were chosen to be greater than 10, so that the limiting value used by Radcalc to calculate the HRCQ unity fraction was 30,000 Ci for both. The activities of the radionuclides were set equal to 15,000 Ci, making the combined HRCQ unity fraction exactly equal to 1. The accompanying printout, designated IIIA15a, shows that Radcalc correctly identified the package as not requiring highway route control. When one of the activities was increased slightly, raising the combined HRCQ unity fraction to 1.01, Radcalc correctly identified the package as requiring highway route control.

Additionally, the A_2 values of both radionuclides were chosen to be less than 10, so that when the form was changed to normal, the limiting values used to calculate the HRCQ unity fraction switched to 3,000 times A_2 . When the program was run with 15,000 Ci of each radionuclide in normal form, Radcalc correctly identified the package as requiring highway route control, indicating that it used the correct set of values (A_2 instead of A_1) to perform the HRCQ determination.

Radcalc for Windows 1.0

Date: 09-25-95 10:47

Performed By: A. Harris

Checked By: _____

File: IIIA15A2.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Sn-123	1.50e+004
I-129	1.50e+004

Waste Form:	Special
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Highway Route Controlled Quantity (IIIA15a)
HRCQ Unity Fraction Limited by 30000 Ci (for Special Form)
Total Activity = 30000 Ci
HRCQ Unity Fraction = 1

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	53.9 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 65.000)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 100.00)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
Sn-123	1.50e+004
I-129	1.50e+004

Source decayed to end of seal time:

Radionuclide:	Curies:
Sn-123	1.28e+004
I-129	1.50e+004

**Case IIIA16: Highway Route Controlled Quantity Classification
for a Package in Which One Radionuclide Is Limited
by 30,000 Ci and a Second Is Limited by 3,000 A₂**

Discussion and Conclusion

Information for a Type B package containing two radionuclides with a total activity less than 30,000 Ci was run on Radcalc for Windows. The A₂ values were chosen so that one was greater than 10 and the second was less than 10, requiring Radcalc to set one limiting value to 30,000 Ci and the second to 3,000 times A₂. The activities of the radionuclides were chosen so that the ratio of each activity to the corresponding limiting value was exactly one-half, making the combined HRCQ unity fraction exactly equal to 1. The accompanying printout, designated IIIA16a, shows that Radcalc correctly identified the package as not requiring highway route control. When one of the activities was increased slightly, raising the combined HRCQ unity fraction to 1.01, Radcalc correctly identified the package as requiring highway route control.

Radcalc for Windows 1.0

Date: 09-25-95 10:53

Performed By: A. Harris

Checked By: _____

File: IIIA16A2.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
Br-82	9.00e+003
Pt-197	1.50e+004

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Highway Route Controlled Quantity (IIIA16a)
HRCQ Unity Fraction Limited by Both 3000 A2 and 30000 Ci
Total Activity < 30000 Ci
HRCQ Unity Fraction = 1

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	173. Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 2250.0)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 80.000)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
Br-82	9.00e+003
Pt-197	1.50e+004

Source decayed to end of seal time:

Radionuclide:	Curies:
Br-82	6.53e-003
Pt-197	1.36e-008

Case IIIA17: Fissile Excepted Classification**Discussion and Conclusion**

Information for a normal form solid containing all five fissile radionuclides was run on Radcalc for Windows. The activities of the radionuclides were chosen so that their associated fissile masses were as close to 3.0 g as possible. The total fissile mass was adjusted to be just under 15.0 g. The accompanying printout, designated IIIA17a, shows that Radcalc correctly identified the package as fissile excepted. When one of the activities was increased slightly, raising the total fissile mass just above 15.0 g, Radcalc correctly identified the package as having exceeded the fissile excepted standard, as shown in the printout designated IIIA17b.

Radcalc for Windows 1.0

Date: 09-26-95 08:56

Performed By: H. Harris

Checked By: _____

File: IIIA17A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.49e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Waste Form:	Normal
Physical Form:	Solid
Container Type:	30 Gallon Drum

Package Void Volume:	2.17e+005 cc
Waste Volume:	1.00e+003 cc
Waste Mass:	1.00e+003 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	11:00 Aug. 30, 1995
Date container sealed:	11:00 Aug. 30, 1995
Date container received:	11:00 Aug. 30, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	0.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Fissile Exempt Quantity (IIIA17a)
Masses of All Five Fissile Isotopes = 3 g (Approximately)
and Total Fissile Mass < 15 g

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	Not Calculated

Heat Generated:	1.72 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 20327.)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 5.7787e+005)
HRC Quantity Determination:	Yes
Fissile Quantity:	14.998 g
15g Fissile Radionuclides or Less:	Yes
(Fissile Excepted per 49CFR173.453(a))	

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.49e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Source decayed to end of seal time:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.49e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Radcalc for Windows 1.0

Date: 09-26-95 08:57

Performed By: H. Harris

Checked By: _____

File: IIIA17B.RAD

***** Input Information *****

Source from input:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.50e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Waste Form:	Normal
Physical Form:	Solid
Container Type:	30 Gallon Drum

Package Void Volume:	2.17e+005 cc
Waste Volume:	1.00e+003 cc
Waste Mass:	1.00e+003 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	11:00 Aug. 30, 1995
Date container sealed:	11:00 Aug. 30, 1995
Date container received:	11:00 Aug. 30, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	0.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for a Fissile Exempt Quantity (IIIA17b)
Masses of All Five Fissile Isotopes = 3 g (Approximately)
and Total Fissile Mass > 15 g

***** Calculated Results *****

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	Not Calculated

Heat Generated:	1.72 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	B (from unity fraction 20327.)
Limited Quantity:	No
LSA Determination:	No (from LSA unity fraction 5.7787e+005)
HRC Quantity Determination:	Yes
Fissile Quantity:	15.003 g

15g Fissile Radionuclides or Less: No
(Fissile Excepted per 49CFR173.453(a))

Note: Transportation classifications assume three significant figures.

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.50e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Source decayed to end of seal time:

Radionuclide:	Curies:
U-233	2.89e-002
U-235	6.50e-006
Pu-238	5.14e+001
Pu-239	1.86e-001
Pu-241	3.10e+002

Case IIIA18: Radioactive Material Classification**Discussion and Conclusion**

Information for a Type A package containing four radionuclides was run on Radcalc for Windows. The activities of the four radionuclides were chosen so that their specific activities were exactly $0.5\text{E-}3 \mu\text{Ci/g}$, so that their combined specific activity was exactly $2.0\text{E-}3 \mu\text{Ci/g}$. The accompanying printout for the Radcalc for Windows Input and Calculated results sheet (designated IIIA18a) shows that the package was correctly identified as not containing radioactive material. When one of the activities was increased slightly, raising the combined specific activity to $2.02\text{E-}3 \mu\text{Ci/g}$, Radcalc correctly identified the package as containing radioactive material, as shown in the accompanying printout designated IIIA18b.

Radcalc for Windows 1.0

Date: 09-22-95 14:10

Performed By: H. Harris

Checked By: _____

File: IIIA18A.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
As-77	5.00e-004
Rb-86	5.00e-004
Gd-153	5.00e-004
Hg-197	5.00e-004

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for Radioactive Material Classification (IIIA18a)
Combined Specific Activity = 0.002 uCi/g

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	3.77e-006 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	No
Type Determination:	A (from unity fraction 4.9167e-005)
Limited Quantity:	Yes
LSA Determination:	Yes (from LSA unity fraction 6.6667e-006)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
As-77	5.00e-004
Rb-86	5.00e-004
Gd-153	5.00e-004
Hg-197	5.00e-004

Source decayed to end of seal time:

Radionuclide:	Curies:
As-77	1.30e-009
Rb-86	1.64e-004
Gd-153	4.59e-004
Hg-197	2.31e-007

Radcalc for Windows 1.0

Date: 09-22-95 14:10

Performed By: H. Harris

Checked By: _____

File: IIIA18B.RAD

===== Input Information =====

Source from input:

Radionuclide:	Curies:
As-77	5.10e-004
Rb-86	5.00e-004
Gd-153	5.00e-004
Hg-197	5.00e-004

Waste Form:	Normal
Physical Form:	Solid
Container Type:	4 x 4 Liner

Package Void Volume:	1.36e+006 cc
Waste Volume:	1.00e+006 cc
Waste Mass:	1.00e+006 g
Waste Void Volume:	0.000 cc

Date to begin source decay:	9:00 Sep. 5, 1995
Date container sealed:	9:00 Sep. 5, 1995
Date container received:	9:00 Oct. 5, 1995
Days to decay source before seal time:	0.00 days
Days container is sealed:	30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test case for Radioactive Material Classification (IIIA18B)
Combined Specific Activity > 0.002 uCi/g

===== Calculated Results =====

H2 Percent Concentration:	0.000 %
H2 Volume:	0.000 cc
H2 Generation Rate:	0.000 cc/hour

Heat Generated:	3.79e-006 Watts
Partial Pressure (H2):	0.000 kPa
Total Pressure (H2 and Air):	101. kPa

Radioactive:	Yes
Type Determination:	A (from unity fraction 4.9667e-005)
Limited Quantity:	Yes
LSA Determination:	Yes (from LSA unity fraction 6.7000e-006)
HRC Quantity Determination:	No
Fissile Quantity:	0.00000 g
Less than 15g Fissile Radionuclides:	Yes
(Fissile Excepted per 49CFR173.453(a))	
Note: Transportation classifications assume three significant figures.	

Bulk Density:	1.00 g/cc
---------------	-----------

Source decayed to start of seal time:

Radionuclide:	Curies:
As-77	5.10e-004
Rb-86	5.00e-004
Gd-153	5.00e-004
Hg-197	5.00e-004

Source decayed to end of seal time:

Radionuclide:	Curies:
As-77	1.33e-009
Rb-86	1.64e-004
Gd-153	4.59e-004
Hg-197	2.31e-007

IV OTHER RADCALC FEATURES

IVA UNIT CONVERSION

The units used internally by Radcalc for Windows are in terms of centimeters, grams, and curies. Cases IVA1 - IVA3 test conversions from other units available in Radcalc for Windows to units in terms of centimeters and grams. Case IVA4 tests the conversion of becquerels to curies and curies to becquerels. Case IVA5 investigates the unit conversions that take place within Radcalc for Window's container dialogue box.

Case IVA1: Feet/Pounds to Centimeters/Grams

Discussion and Conclusion

In case IB2 presented previously, volumes are entered in cubic feet and mass in pounds. The Radcalc for Windows Input and Calculated Results sheet shows that these values have been correctly converted to cubic centimeters and grams. The bulk density has also been calculated correctly in g/cm^3 from the waste volume in cubic feet and the waste mass in pounds.

Case IVA2: Inches/Pounds to Centimeters/Grams

Discussion and Conclusion

In case IC1B printed previously, volumes are entered in cubic inches and mass in pounds. The Radcalc for Windows Input and Calculated Results sheet shows that these values have been correctly converted to cubic centimeters and grams. The bulk density has also been calculated correctly in g/cm^3 from the waste volume in cubic inches and the waste mass in pounds.

Case IVA3: Meters/Kilograms to Centimeters/Grams

Discussion and Conclusion

In case IB4 printed previously, volumes are entered in cubic meters and mass in kilograms. The Radcalc for Windows Input and Calculated Results sheet shows that these values have been correctly converted to cubic centimeters and grams. The bulk density has also been calculated correctly in g/cm^3 from the waste volume in cubic meters and the waste mass in kilograms.

Case IVA4: Becquerels to Curies**Discussion and Conclusion**

Radcalc for Windows performs calculations in terms of curies for activity. When the user enters a radionuclide inventory in terms of becquerels, Radcalc for Windows converts activities into units of curies for calculations. The resulting radionuclide inventories calculated by Radcalc for Windows at the beginning and end of seal time are then converted to becquerels in the Radcalc for Windows Input and Calculated Results sheet if the initial radionuclide inventory was specified in becquerels. The conversions from and to becquerels were checked by making two Radcalc for Windows runs. The first uses a radionuclide inventory entered in terms of becquerels. The second uses the same inventory entered in terms of curies. Results from both cases are consistent, indicating proper conversions have taken place. The two cases, designated IVA4a and IVA4b, follow.

Radcalc for Windows 1.0

Date: 09-25-95 09:23

Performed By: A. Harris

Checked By: _____

File: IVA4A.RAD

===== Input Information =====

Source from input:
Radionuclide: Becquerels:
S-35 3.70e+010

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for Bq/Ci and Ci/Bq Conversions (IVA4a)
Activity = 3.7E10 Bq

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.000288 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.016667)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.0033333)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Becquerels:
S-35 3.70e+010

Source decayed to end of seal time:
Radionuclide: Becquerels:
S-35 2.92e+010

Radcalc for Windows 1.0

Date: 09-25-95 09:24

Performed By: H. Harris

Checked By: _____

File: IVA48.RAD

===== Input Information =====

Source from input:
Radionuclide: Curies:
S-35 1.00e+000

Waste Form: Normal
Physical Form: Solid
Container Type: 4 x 4 Liner

Package Void Volume: 1.36e+006 cc
Waste Volume: 1.00e+006 cc
Waste Mass: 1.00e+006 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 9:00 Sep. 5, 1995
Date container sealed: 9:00 Sep. 5, 1995
Date container received: 9:00 Oct. 5, 1995
Days to decay source before seal time: 0.00 days
Days container is sealed: 30.00 days

Entered G Values:
G Alpha G Beta G Gamma
0 0 0

Comments:
Test Case for Bq/Ci and Ci/Bq Conversions (IVA4b)
Activity = 1.0 Ci

===== Calculated Results =====

H2 Percent Concentration: 0.000 %
H2 Volume: 0.000 cc
H2 Generation Rate: 0.000 cc/hour

Heat Generated: 0.000288 Watts
Partial Pressure (H2): 0.000 kPa
Total Pressure (H2 and Air): 101. kPa

Radioactive: Yes
Type Determination: A (from unity fraction 0.016667)
Limited Quantity: No
LSA Determination: Yes (from LSA unity fraction 0.0033333)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 1.00 g/cc

Source decayed to start of seal time:
Radionuclide: Curies:
S-35 1.00e+000

Source decayed to end of seal time:
Radionuclide: Curies:
S-35 7.90e-001

Case IVA5: Container Information Dialog Box Unit Conversions**Discussion and Conclusion**

Container and waste descriptions can be entered in terms of centimeters, meters, feet, inches, grams, kilograms, and pounds. When the user changes units through use of the units box, values for the package void volume, waste volume, waste mass, waste void volume, and waste true density convert to the new units chosen. The following conversions, representing all possible conversions in the container dialog box, show agreement with hand calculations. Note that Radcalc for Windows uses four significant digits for these conversions.

- cubic centimeters, grams and grams per cubic centimeter to
- cubic meters, kilograms and kilograms per cubic meter
- cubic inches, pounds and cubic inches per pound
- cubic feet, pounds and cubic feet per pound

- cubic meters, kilograms and kilograms per cubic meter to
- cubic centimeters, grams and grams per cubic centimeter
- cubic inches, pounds and cubic inches per pound
- cubic feet, pounds and cubic feet per pound

- cubic inches, pounds and cubic inches per pound to
- cubic centimeters, grams and grams per cubic centimeter
- cubic meters, kilograms and kilograms per cubic meter
- cubic feet, pounds and cubic feet per pound

- cubic feet, pounds and cubic feet per pound to
- cubic centimeters, grams and grams per cubic centimeter
- cubic meters, kilograms and kilograms per cubic meter
- cubic inches, pounds and cubic inches per pound

Container dimensions listed under the container selection list were checked against, and found to agree with, those reported in Table 3-2 of this document.

IVB TARGET PERCENT SPECIFIED

Cases IVB1 and IVB2 are used to ensure that Radcalc for Windows calculations where a target percent is specified return a seal time and hydrogen volume that are consistent. Each case is first run with a specified target percent. The seal time returned by the first run is then used in a second run. The hydrogen volume calculated by the two runs should be consistent.

Case IVB1: Target Percent Reached

Discussion and Conclusion

In the first run with this case, a 5.00% target percent is specified. The first run yields a seal time of 0.54 days and a hydrogen concentration of 5.00%. The second run uses 0.54 days as the seal time, resulting in a hydrogen concentration of 4.99%. The slight discrepancy is attributed to the round-off error in knowing the number of days to only two significant figures, as given by the Radcalc for Windows output. The Radcalc for Windows Input and Calculated Results sheet for the first run, designated IVB1, follows.

Radcalc for Windows 1.0

Date: 09-23-95 13:10

Performed By: K. Hildes

Checked By: _____

File: IVB1.RAD

***** Input Information *****

Source from input:
Radionuclide: Becquerels:
Sr-90 1.00e+010
M.F.P. 1.00e+010

Waste Form: Normal
Physical Form: Solid
Container Type: Sample Pig Carrier

Package Void Volume: 1.00 cc
Waste Volume: 265. cc
Waste Mass: 264. g
Waste True Density: 1.00 g/cc

Days to decay source before seal time: 30.00 days
Calculate number of days sealed until 5.00% hydrogen is reached.

Entered G Values:

G Alpha	G Beta	G Gamma
0	0.5	0

Comments:

Test Case for Target Percent Reached (IVB1)

***** Calculated Results *****

The sealed container will generate 5.00 % hydrogen in 0.54 days
H2 Volume: 0.105 cc
H2 Generation Rate: 0.00811 cc/hour

Heat Generated: 0.00181 Watts
Partial Pressure (H2): 5.33 kPa
Total Pressure (H2 and Air): 107. kPa

Radioactive: Yes
Type Determination: B (from unity fraction 1.3500)
Limited Quantity: No
LSA Determination: No (from LSA unity fraction 409.10)
HRC Quantity Determination: No
Fissile Quantity: 0.00000 g
Less than 15g Fissile Radionuclides: Yes
(Fissile Excepted per 49CFR173.453(a))
Note: Transportation classifications assume three significant figures.

Bulk Density: 0.996 g/cc

Source decayed to start of seal time:
Radionuclide: Becquerels:
Sr-90 9.98e+009
Y-90 9.98e+009
M.F.P. 1.00e+010

Source decayed to end of seal time:
Radionuclide: Becquerels:
Sr-90 9.98e+009
Y-90 9.98e+009
M.F.P. 1.00e+010

Case IVB2: Target Percent Not Reached**Discussion and Conclusion**

In this case, the target percent hydrogen specified lies outside of the one-hour to 36,500-day range considered for Windows in a calculation to target percent. In the first run with this case, a 3.00% target percent is specified. The first run reports that at 36,500 days, which corresponds to 0 hours, February 3, 2100, the hydrogen percent concentration reached only 2.41%. The second run specifies 0 hours, February 3, 2100 as the end of the seal time, resulting in a hydrogen concentration of 2.41%, as expected. The first run for this case is printed as IC5 in Section IC.

IVC DATING ROUTINE**Case IVC1: Length of Month****Discussion and Conclusion**

The number of days for each month of the year used by Radcalc for Window's dating routine was checked. The following Radcalc for Windows Input and Calculated Results sheet, designated IVC1, shows how the number of days in January and February were checked during a leap year. This process was repeated for all months in both a leap year (1996) and a non-leap year (1995). The number of days reported in all cases were as expected.

Radcalc for Windows 1.0

Date: 09-23-95 13:10

Performed By: K. Hillebrand

Checked By: _____

File: IVC1.RAD

***** Input Information *****

No source entered

Waste Form: Normal
Physical Form: Solid
Container Type: 30 Gallon Drum

Package Void Volume: 0.000 cc
Waste Volume: 0.000 cc
Waste Mass: 0.000 g
Waste Void Volume: 0.000 cc

Date to begin source decay: 16:00 Jan. 10, 1996
Date container sealed: 16:00 Feb. 10, 1996
Date container received: 16:00 Mar. 10, 1996
Days to decay source before seal time: 31.00 days
Days container is sealed: 29.00 days

← Days for Jan.

← Days for Feb.

Entered G Values:

G Alpha	G Beta	G Gamma
0	0	0

Comments:

Test Case for Length of Months (IVC1)

***** No Results Calculated *****

Case IVC2: Leap Years**Discussion and Conclusion**

The identification of leap years in Radcalc for Windows was checked against the dating routine used by Microsoft's⁴ Excel spreadsheet program. The intervals checked were:

February 28, 1960 (leap year) to January 5, 2003 (non-leap year)
Both give 15,652 days

January 17, 1961 (non-leap year) to December 16, 1993 (non-leap year)
Both give 12,021 days

October 4, 1995 (non-leap year) to February 29, 1996 (leap year)
Both give 148 days

January 1, 1996 (leap year) to January 2, 2000 (leap year)
Both give 1,462 days

The use of hours entered was checked by hand. Both Radcalc for Windows and the hand calculation yielded a time of 366.96 days as the time that elapses between 3 a.m., February 28, 1996, and 2 a.m., March 1, 1997.

**Case IVC3: Calculation of End Date Given Start Date
and Time Interval****Discussion and Conclusion**

Radcalc for Windows is capable of calculating the number of days to reach a target hydrogen gas concentration. The corresponding end date is also calculated if a start date was entered by the user. Case IC5 from Section IC is an example of this sort. The end date given by IC5 was compared against Excel spreadsheet dating routine results using the same starting date and time interval. The date returned by the spreadsheet calculation was the same as given by Radcalc for Windows.

CASE IVD: BULK DENSITY**Discussion and Conclusion**

The bulk density is calculated from the waste mass divided by the waste volume. In cases IB1, IB2, IB3, IB4, IC2, IC3, IC4, and IC5 from Sections IB and IC, the bulk densities calculated by Radcalc for Windows match spreadsheet calculations.

⁴Microsoft is a registered trademark of Microsoft Corporation.

CASE IVE: HEAT GENERATION

Discussion and Conclusion

Radcalc for Windows reports the heat generation rate based on the total recoverable energy at the start of shipment. The total recoverable energy for each radionuclide available in Radcalc for Windows was checked against that of the ORIGEN2 database in the verification of the FENDL/D-1.0 database, as discussed in Chapter 3.0. Also, the heat generation rate calculated by Radcalc for Windows was compared with results of Excel spreadsheet calculations. The spreadsheets calculate the heat generation rate using the Radcalc for Windows methodology and decay energy data (FENDL/D-1.0) as outlined in Chapter 2.0. In cases IB1, IB2, IB3, IB4, IC2, IC4, and IC5, results were found to be identical between the spreadsheets and Radcalc for Windows calculations within the three significant figures available in Radcalc for Windows.

IVF PRESSURE

Case IVF1: Partial Pressure of Hydrogen

Discussion and Conclusion

The partial pressure of hydrogen calculated by Radcalc for Windows is compared against Excel spreadsheet calculations. The spreadsheets are set up to use Radcalc for Windows methodology and decay energy data in the calculation of hydrogen volume, as was done for the cases listed under Section IB. The spreadsheets calculate the partial pressure of hydrogen, as outlined in Chapter 2.0. Calculations for the partial pressure of hydrogen from Radcalc for Windows were compared to spreadsheet calculations for cases IB1, IB2, IB3, IB4, IC2, IC3, IC4, and IC5 found under Sections IB and IC. In all cases, output from Radcalc for Windows was the same as that given by the spreadsheets within the three significant figures reported by Radcalc for Windows.

Case IVF2: Total Pressure

Discussion and Conclusion

The total pressure calculated by Radcalc for Windows is compared against Excel spreadsheet calculations. The spreadsheets are set up to use Radcalc for Windows methodology and decay energy data in the calculation of hydrogen volume, as was done for the cases listed under Section IB above. The spreadsheets calculate the total pressure as outlined in Chapter 2.0. Calculations for the total pressure of hydrogen from Radcalc for Windows were compared to spreadsheet calculations for cases IB1, IB2, IB3, IB4, IC2, IC3, IC4, and IC5 found under Sections IB and IC. In all cases, output from Radcalc for Windows was the same as that given by the spreadsheets within the three significant figures reported by Radcalc for Windows.

APPENDIX F

CHANGE REPORT AND PROBLEM REPORT FORM

Change Request and Problem Report

		CR/PR Number: _____
1.	Software/Document Identification (Name): _____	Rev: _____
2.	Prepared by: _____	Date: _____
	System Name: _____	TPCN, W/O: _____
3.	CR/PR Type: ☐ Change Request ☐ Problem Report	Requested Completion Date: _____
4.	Description: _____	
5.	Justification If Change Request: _____	
6.	Submitter's Priority ☐ High ☐ Medium ☐ Low	
7.	Change Authority: _____ ☐ Accept ☐ Modify ☐ Reject ☐ Defer Until: _____	
8.	Assigned to: _____	Planned Release Date: _____
9.	Solution Comments	Cost/Schedule Estimate: _____ / _____
10.	Software/Documents Affected: _____	
11.	Approvals Indicate CR is Complete or PR is Resolved.	
	Software Developer: _____	Date: _____
	Cognizant Manager: _____	Date: _____
	CR or PR Preparer: _____	Date: _____
	Other: _____	Date: _____

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