TECHNICAL EVALUATION REPORT FOR THE TOPICAL REPORT
"3R-STAT: A TC-99 AND I-129 RELEASE ANALYSIS COMPUTER CODE"
VERSION 3.0

Enclosure

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1.0 BACKGROUND

The U.S. Nuclear Regulatory Commission staff has reviewed a topical report (TR), prepared by Vance and Associates, Inc. (V&A), entitled, "Topical Report - 3R-STAT: A Tc-99 and I-129 Release Analysis Computer Code." The two intended uses of the 3R-STAT computer code are: (1) to analyze past fuel cycle data from operating plants to develop average ^{129}I and ^{99}Tc release rates as a basis for projecting future inventories of these two radionuclides; and (2) for use within waste management programs at nuclear power plants for providing more accurate estimates of the actual quantities of ^{129}I and ^{99}Tc in LLW shipped to disposal facilities. Use of the TR can lead to more realistic projections of the ^{129}I and ^{99}Tc inventories than the current methods that provide conservative bounding overestimates. This Technical Evaluation Report (TER) assesses: the methodology described in the TR; the accuracy of the predicted values; and the application of the approach to the regulated activities of low-level radioactive waste (LLW) generation and disposal.

This review has been coordinated with the Agreement States. Questions raised by the States during the review were incorporated into the requests for additional information (RAI) submitted to V&A. Questions received after the review schedule and RAI dispatch were forwarded to V&A for its consideration. If these later questions raised issues that were not previously identified in the NRC review, these questions were incorporated into the formal RAIs.

1.1 Regulations

By Federal Register notice dated December 27, 1982 (47 FR 57446), NRC promulgated 10 CFR Part 61, "Licensing Requirements for Land Disposal of Radioactive Material." This regulation requires LLW disposal facility operators to submit accurate and adequate information in their license applications. Specifically, 10 CFR 61.12(i) requires that the applicant provide a "...description of the kind, amount, classification and specifications of the radioactive material proposed to be received, possessed, and disposed of at the land disposal facility." This information is used by the licensing body in its review of the facility performance assessment (calculations used to demonstrate the potential impact of the disposal facility).

The "Standard Format and Content of a License Application for a Low-Level Radioactive Waste Disposal Facility" (NUREG-1199), and the "Standard Review Plan for the Review of a License Application for a Low-Level Radioactive Waste Disposal Facility" (NUREG-1200), provide additional guidance on the content of an application that would be found acceptable to NRC staff. Requirements and guidance relating to this TR are addressed in Section 3.1 of this TER.

1.2 Topical Report

As various States and compacts have proceeded with the tasks of siting and licensing LLW disposal facilities, preliminary performance assessments have demonstrated the potential importance of the long-lived, mobile isotopes. Specifically, ^{129}I and ^{99}Tc have been identified as isotopes that may impact a facility's ability to comply with the performance objectives of 10 CFR Part 61. Many factors influence the analysis of a facility's performance over the long term. These factors are discussed further in the staff's "Branch Technical Position on Performance Assessment for LLW Disposal Facilities" (currently in draft). A major factor can be the total quantity of individual isotopes in the disposed waste. Therefore, an estimate of this quantity should be provided by the applicant for a disposal facility license. Current inventory estimates are developed from historical manifest data received with the LLW shipments. A number of the estimates for specific radionuclides are based on scaling factors that relate measurable nuclide activities to activities of difficult-to-detect radionuclides. In the cases of ^{99}Tc and ^{129}I, the scaling factors are based on the minimum detectable activity (MDA) values of these "scaled" radionuclides. The use of scaling factors is discussed in more detail in Section 2.0 of this TER.

This TR provides an alternate technique for estimating ^{129}I and ^{99}Tc inventories at LLW disposal facilities from waste generated at nuclear power plants. Specifically, the TR estimates the total production and release of ^{129}I and ^{99}Tc from the fuel during reactor operation and conservatively assumes that all this material is contained in the LLW generated by the reactor, and consequently ends up in the LLW disposal facility. The scope of the TR is summarized in Section 2.0 of this TER.

The original TR was a three-volume proprietary report consisting of a main report, and five appendices. The TR was originally submitted to NRC under cover dated July 20, 1993, and was accepted for review on August 23, 1993. The TR was revised and submitted by V&A with a response to the first RAI (RAI-1), dated September 2, 1994. The revised TR consists of a main report, a validation and verification report, and tnree appendices. In addition, a non-proprietary version of the TR is available, consisting of a non-proprietary discussion of the analysis contained in the main report. Two further RAIs (RAI-2 and RAI-3) were generated as a result of the regulatory and technical reviews performed on the TR. The responses to these requests were submitted on December 1, 1994, and February 13, 1995, respectively.

1.3 Technical Evaluation

This TER assesses the methodology described in the TR, the accuracy of the predicted values, and the application of the approach to the regulated activities of LLW generation and disposal. Conditions prescribed by the TER must be met by the licensee using the methodology for the intended purpose as stated in the TR. The evaluation in this TER is based on the current state of the art and information provided by the applicant. Should NRC become aware of information indicating that the inventory estimates provided by the TR methodology are outside the bounds of regulatory acceptability, the basis for the TER findings would be reevaluated.

Review and approval of this TR certifies that the approach, model, and code are acceptable to NRC for providing reasonable assurance of compliance with the pertinent regulations. However, the use of a code by an independent third party (e.g., a licensee seeking to demonstrate accurate estimates of future disposal inventories) introduces the possibility of inappropriate use, application, or interpretation. This problem has been identified previously by NRC staff in the use of qualified codes by a third party. As a result, NRC issued Generic Letter (GL) 83-11, "Licensee Qualification for Performing Safety Analyses in Support of Licensing Actions," which specifies the regulatory interactions necessary to ensure adequate and appropriate use of such a code. This GL is discussed in the regulatory bases considered below.

The guidance in GL 83-11 does not provide the criteria necessary to determine the appropriate level of qualification necessary for third-party use of the 3R-STAT code. This TER will provide the criteria for qualification. Additionally, the TER will provide other conditions for approval of the use of this TR.

Finally, the quality assurance process used to develop the 3R-STAT code and the TR, and to provide for future revisions to the code and TR, were evaluated in this review. This process defines the development and maintenance procedures for updating the code and TR documentation.

2.0 SUMMARY OF TOPICAL REPORT

As stated above, the subject TR provides an alternate and more accurate method to determine ^{129}I and ^{99}Tc inventories at LLW disposal facilities from waste originating at nuclear power plants. ^{129}I and ^{99}Tc are important isotopes in the evaluation of the potential performance of an LLW disposal facility. These isotopes have long half-lives and are relatively mobile in the natural environment. Calculations performed to estimate potential radiological impacts at LLW disposal sites consider the facility's inventory of specific isotopes. Significant over-estimates of the inventory may lead to overly conservative analyses.

Current practices for quantifying and reporting ^{129}I and ^{99}Tc rely on the use of scaling factors and the MDA of the isotope. The scaling factors represent a ratio between the activities of measurable isotopes (e.g., ^{137}Cs, ^{60}Co) and difficult-to-detect isotopes (i.e., ^{129}I and ^{99}Tc). The licensee, using the scaling factor approach, determines the scaling factors using direct measurement techniques for ^{137}Cs and ^{60}Co. These direct measurements are generally insensitive to the weak beta and gamma emissions from the difficult-to-detect isotopes. As a result, the MDAs of ^{129}I and ^{99}Tc are used to generate the scaling factor (i.e., the scaling factor is the MDA divided by the measured activity of ^{137}Cs or ^{60}Co). This scaling allows the generator of waste to quantitatively bound difficult-to-detect isotopes quickly and easily without the excessive exposures to workers that could result from attempts to directly measure these isotopes through more costly or complex techniques. Scaling factors are generally updated or checked by analyzing specific wastes, on a periodic basis, to ensure that appropriate values are being used. It has been estimated that this method of determining the quantities of the difficult-to-detect isotopes overestimates actual quantities by factors ranging from 100 to 10,000 times.

The isotopes ^{129}I and ^{99}Tc are required to be quantified by total activity on waste manifests. Manifests are records that must accompany waste shipped for disposal at land disposal facilities. The NRC guidance on quantifying and reporting isotopic constituents in LLW is contained in the 1983 "Branch Technical Position on Waste Classification and Waste Form." This NRC guidance suggests that in classifying waste, the concentrations of specific isotopes in the waste should be accurate to within a factor of 10. Current inventory estimates at the disposal sites are sums of the activities reported on individual shipment manifests. NRC recently updated the guidance to provide acceptable methods for calculating the average activity concentrations of the isotopes in the waste for comparison with the regulations.

The TR details a methodology for inventory calculations independent of the waste classification methodology described above. The TR methodology, model, assumptions, and validation are described in the sections that follow.

2.1 Methodology

The TR describes an alternate method for calculating the total activity of ^{129}I and ^{99}Tc generated in nuclear power plants and shipped to a disposal facility. The methodology focuses on the source and release of these isotopes into a reactor's waste rather than basing estimates on "scaled" waste concentrations. The source of ^{129}I and ^{99}Tc is the fission of fuel in the reactor and, in the case of ^{99}Tc, the activation of deposits in the reactor coolant. The release of these isotopes (to the reactor coolant and ultimately to the reactor's LLW) is modeled using a computer code to calculate the average release rate of the difficult-to-detect isotopes. This average release rate value can be used either to predict total quantities expected to be received at a waste disposal facility (e.g., as a predictive tool for licensing) or to estimate the actual quantities received at the disposal site (e.g., as a verification and monitoring tool). The methodology assumes that <u>all</u> the contamination released into the reactor's coolant system ends up in the LLW, which is subsequently shipped to the disposal site.

Reactor coolant data are input to a computer code to model the core release conditions that allow determination of activity release estimates. These estimates are validated against measured isotope activities. Based on review of the TR, NRC staff concluded that the 3R-STAT model and validation methodology are appropriate.

2.2 Models and Assumptions

The model, embodied in the code, is described in pp. 2-1 - 2-4 of the non-proprietary version of the TR. However, to aid in understanding the model, the three fundamental bases of the approach are described as follows. First, the mechanism specific release fractions (q_i) for ^{131}I can be determined (as functions of time). Second, the release ratios of $^{131}I/^{129}I$ and $^{131}I/^{99}Tc$ can be established for the specific release mechanisms. Third, the production rate of ^{99}Mo (the parent of ^{99}Tc) can be established based on the plant specific $^{99}Mo/^{60}Co$ ratio.

The first basis involves a series of complex calculations to solve non-linear equations (equating the measured short-lived iodine ratios to the release fractions) by sampling two parameters (the failed fuel fraction and the escape rate coefficient) and using a least-squares-fitting approach to solve for the best fit results. A major aspect of this basis is the use of the short-lived iodine ratios to determine the release characteristics of the fuel loading within the reactor. These characteristics are grouped by release mechanism: recoil, diffusion, and knockout. These mechanisms are considered for both tramp fuel and defective fuel (i.e., fuel with pin failures). This approach is discussed in the technical bases evaluated below.

The second basis uses information, calculated outside of 3R-STAT, to determine the ratios of ^{131}I to the isotopes of concern. The ratios are determined from literature and models external to the 3R-STAT code, but incorporated by reference in the TR. Ratios for diffusion, knockout, and recoil are referenced, and terms are included in the code's equations, to implement these ratios. Certain aspects of this information are discussed in the technical bases evaluated in this TER.

The third basis estimates the ^{99}Tc produced by activation. This term is independent of the model used to calculate the production of ^{99}Tc by fission. The term is developed from plant specific activation ratio data. The fraction of ^{99}Tc produced by activation is added to the fraction produced by fission, calculated by 3R-STAT in the same manner as for ^{129}I.

Specific technical assumptions and model conditions are addressed in detail in this TER. Only those issues identified as being crucial to the model, or having an impact on the regulatory acceptability of the TR, are included in this TER. Other assumptions and model conditions reviewed are identified in the review questions and responses to be included in the final TR.

2.3 Model Validation

The TR uses a set of validation measurements and calculations to support the argument that the model is more accurate than the current practice of using scaling factors. These validation comparisons use measurements of the difficult-to-detect radionuclides made with a sensitive mass spectrometry technique. This technique is more sensitive to the weak beta emitting isotopes than the methods generally used to determine scaling factors. As a result, few of the sample measurements made in the validation study were below the lowest limit of detection for this measurement technique.

The general approach used by V&A (i.e., developing a model and using actual data to validate that model) is acceptable. The TR identifies uncertainties in the model predictions based on the validation data. This TER provides a regulatory mechanism for dealing with the model uncertainty.

3.0 SUMMARY OF REGULATORY EVALUATION

3.1 Summary of Regulatory Bases Considered

3.1.1 Low-Level Waste Disposal Facility Licensing

3.1.1.1 ^{129}I and ^{99}Tc Inventory Calculations (10 CFR 61.12(i))

An application for a license to dispose of LLW under the regulations promulgated at Part 61, or an equivalent Agreement State regulation, must provide information on the bases for the proposed facility's radionuclide inventory. Specifically, an applicant is required, under 10 CFR 61.12(i), to provide an accurate estimate of the quantity of radioactive material to be disposed of in the facility. The current mechanism for making this estimate is based on summations of waste manifest information. The applicant for a waste disposal facility license may use the inventory estimate to support an analysis of potential impacts to the public and the environment. The analysis must conclude that there is reasonable assurance that the site will comply with the performance objectives of Part 61 (10 CFR 61.41-10 CFR 61.44).

The impacts from the potential migration of radionuclides from the waste can be calculated using a variety of methodologies. Generally, groundwater impacts are conservatively determined using a methodology that uses the total inventory of contaminant as the "source" term. Thus, for the sake of analyzing the groundwater pathways (which may dominate the entire impact analysis), the total site inventory of certain radionuclides can be important. As a result, NRC requires that generators who send wastes containing certain long-lived, highly mobile (in the natural groundwater environment) isotopes, such as ^{129}I and ^{99}Tc, report the total activities of these isotopes on waste manifests.

Although the regulations at 10 CFR 61.12(i) address all waste and all isotopes projected to be disposed of at a LLW disposal facility, this TR provides a methodology for estimating the quantity of two important radionuclides: ^{129}I and ^{99}Tc. The long-term potential impacts of LLW disposal can be intrinsically tied to the longer lived, more mobile radionuclides. Therefore, the use of this TR by a licensee, to estimate the amount of ^{129}I and ^{99}Tc to be accepted at a disposal site, has the potential to greatly influence the ability of the facility to demonstrate compliance with the performance objectives of Part 61.

3.1.1.2 Incorporation by Reference in an LLW Disposal Facility Application and User Qualification for an LLW Disposal Facility Applicant (NUREG 1200, Section 1.5 and Generic Letter 83-11)

The stated intent of the TR is to provide a method for LLW disposal facility license applicants and licensees (once the application is approved and license issued) to support their estimates of ^{129}I and ^{99}Tc inventories. Because an applicant for such a license can incorporate information in its application by reference (NUREG-1200, Section 1.5), V&A has proposed that the TR can be used in this manner.

The use of a TR by a particular applicant or licensee should be qualified by NRC. The staff has previously provided guidance on the qualification of licensees using TRs in GL 83-11. Therefore, any disposal facility applicant wishing to use 3R-STAT, Version 3.0, should follow the guidance contained in GL 83-11.

3.1.2 Waste Generator Licensing

3.1.2.1 Waste Classification (10 CFR Part 20, Appendix F, III. A. 1)

The TR provides an analysis (response to question B1 of RAI-2) to demonstrate that ^{99}Tc and ^{129}I concentrations, on a per-package basis, do not have an impact on waste classification. This analysis uses ^{99}Tc data from a historical data base to demonstrate that this isotope has minimal impact on waste classification. Also, V&A provides an analysis using a conservative estimate of ^{129}I production, and incorporation of this isotope in a waste resin filter, to demonstrate the minimal impact of ^{129}I concentration on waste classification determinations. As a result, V&A suggests that the determination of waste classification should be conservatively based on current practices.

3.1.2.2 Waste Manifesting (10 CFR Part 20, Appendix F, I.)

The total quantities of ^{129}I and ^{99}Tc are required to be reported to the waste disposal facility operator by the LLW generator under the requirements of 10 CFR Part 20, Appendix F. This manifest requirement allows waste disposal site operators to quickly and selectively determine the total site inventory of these specific isotopes.

V&A proposes, in the TR, that to implement consistent tracking of the ^{129}I and ^{99}Tc inventories, generators using the TR provide manifest data (as they do currently) and then provide corrected manifest totals for these isotopes on an annual or "fuel cycle" basis. This approach would allow generators to comply with the manifest requirements, while ^{129}I and ^{99}Tc inventories could be tracked using the 3R-STAT methodology. Disposal facilities could then reflect the more accurate total inventories of ^{129}I and ^{99}Tc in performance assessments.

This TR provides an alternate mechanism to allow waste disposal site operators to determine more realistic totals for these isotopes. The TR does not replace the manifest reporting, because the TR results are not used to provide estimates on a waste package or waste shipment basis. Both approaches may be used for determining site inventories; however, in some cases, the manifest reporting approach may be dictated, either because the generator does not use the TR approach or because the waste was not generated under the physical conditions considered in the TR. In addition, under routine application, the TR is applied retroactively to estimate a total inventory for a specified period, rather than a per package or per shipment basis.

3.1.2.3 User Qualification for a Reactor Licensee (Generic Letter 83-11)

The TR states that individual utilities may use 3R-STAT to assess isotope generation and release in their individual plants. This option could be required by disposal site operators. Use of the code by the generator after waste generation could greatly enhance knowledge regarding realistic quantities of ^{129}I and ^{99}Tc shipped to any disposal facility. The use of this methodology would be based on a generator-specific demonstration of its capability to correctly and adequately apply the methodology as discussed below.

The use of a TR by a reactor licensee should be qualified by NRC. The staff has previously provided such guidance in GL 83-11. Therefore, any reactor licensee wishing to revise technical specifications to incorporate the use of 3R-STAT, version 3.0, should follow the guidance contained in GL 83-11.

3.2 Summary of Technical Bases Considered and Findings

3.2.1 3R-STAT Models

To determine the steady-state reactor coolant concentrations of ^{129}I and ^{99}Tc, 3R-STAT performs a fuel cycle-dependent analysis of the release of the iodine and tellurium precursor radionuclides from both tramp fuel (i.e., fuel particles external to the fuel rod cladding) and defective fuel rods. In this analysis, 3R-STAT performs a calculation in which the fuel is represented by an equivalent core-average fuel rod and tramp particle, rather than a calculation based on the isotope releases on an individual fuel rod and tramp particle basis. The steady-state nuclide concentrations are determined by balancing the fuel releases with: (1) the losses through the reactor coolant purification system and steam carryover; and (2) the decay of the nuclide inventory.

Each of these steps employs relatively complex modeling of the various processes and mechanisms involved. The 3R-STAT models used to perform these calculations, as described in the TR and in the responses to the RAIs, have been reviewed in detail. This review focused on the applicability of the various assumptions in the models, the accuracy of the specific representations, and the consistency with the present state-of-the-art. The major issues raised during this review are summarized in the following sections.

3.2.1.1 Evaluation of Mechanism-Specific Release Fractions for ^{131}I (q_i)

Table 1 identifies the parameters used in the 3R-STAT model to represent the release rate fractions.

Table 1
^{131}I Release Fractions

Parameter designation	Release mechanism and source	Value	Derivation
q_1	Recoil, tramp	Fixed	$q_1+q_2+q_3=1$
q_2	Diffusion, tramp	Fixed	Literature
q_3	Knockout, tramp	Fixed	Literature
q_4	Recoil, defects	Constrained	Calculated
q_5	Diffusion, defects	Constrained	Calculated
q_6	Knockout, defects	Constrained	$q_4+q_5+q_6=1$
ϵ	Escape rate coeff.	Constrained	Sampled
a	Tramp fuel source	Constrained	Sampled
b	Failed fuel source	Constrained	a+b=1

A critical element of the methodology is the determination of release rate fractions for ^{131}I (q_i). The ^{131}I analysis is used to determine the release rates of the long-lived isotopes. The release analysis for ^{131}I is based on the ratios of the short-lived iodine release rates. The activities of the short-lived iodine isotopes are routinely and easily measured. Specifically, the measured (average) activity ratios for the five short-lived iodine isotopes are combined with a theoretical description of the activity ratios as a function of the release mechanisms. Next, various assumptions discussed below are made to solve the problem for the release rate fractions (q_i) for ^{131}I. After these fractions have been calculated for each mechanism, mechanism-specific release rate ratios are used to calculate the release of the long-lived isotopes in question.

However, the release mechanisms and their specific release rate fractions for ^{131}I are not simply determined. Three release mechanisms are considered from each of two fuel sources, leading to a total of six release rate fractions. The release mechanisms are diffusion, recoil, and knockout. The sources are defects in the fuel cladding and tramp fuel. Three of the fractions are prescribed in the model, based on calculations and information external to the 3R-STAT computer code. The other three release fractions, and three final variables, are calculated by the 3R-STAT code. These calculations are performed using an iterative solution technique that employs sampled values for two of the three variables, with the final variable constrained by the sampling.

<u>Finding</u>: The mechanism-specific release fractions for ^{131}I are adequate as described in the TR.

3.2.1.2 Chemical and Isotopic Dependence of the Escape Rate Coefficient

In 3R-STAT, the activity release from the fuel rod gap is determined by the fuel rod escape rate coefficient, ϵ. The escape rate coefficient, ϵ, is a free parameter (variable) for ^{131}I in the 3R-STAT model and is determined in part by the short-lived iodine input measurement data. In the response to question A10 of RAI-1, V&A notes that the transport properties within the fuel rod gap depend on the chemical species, but do not have a significant dependence on the specific isotope. Consequently, all the iodine isotopes will be released at the same fractional rate from the fuel rod gap.

<u>Finding</u>: The escape rate coefficient, as modeled in the TR, is acceptable to describe the release of the iodine isotopes.

3.2.1.3 Diffusion Release Modeling

In determining the release of the tellurium precursors from the fuel, 3R-STAT assumes that tellurium diffusion from the fuel to the coolant is inconsequential. The data included in the American Nuclear Society (ANS) 5.4 Working Group report (NUREG/CR-2507) and the radionuclide transport model proposed by Olander (see Ref. 1) suggest that (at elevated temperatures) the diffusion rate of tellurium may be as much as a factor of 4 larger than for iodine. To evaluate this assumption, V&A has modified the 3R-

STAT model to include tellurium diffusion. The V&A calculations based on this updated model, reported in the response to question A11 of RAI-1, indicate that the increase in ^{129}I is negligible when the tellurium diffusion rate is increased to 5 times the diffusion rate of iodine. 3R-STAT cites the Turnbull (see Ref. 2) diffusion coefficient as a basis for the model for the diffusion release. The Turnbull diffusion coefficient consists of three terms: (1) a temperature-dependent term; (2) a vacancy term; and (3) a volumetric fission rate term. In 3R-STAT, the fission rate term is neglected in the calculation of diffusion, but is accounted for explicitly in the knockout release. This approximation enters in the calculation of q_2 for the tramp fuel. V&A, in the response to question A17 of RAI-2, has evaluated the effect of this approximation for a plant having no failed fuel rods and has shown that the effect on the ^{129}I release is negligible.

The diffusion of the radionuclides varies by several orders of magnitude because of the fuel temperature differences between the average and peak power locations within the fuel. 3R-STAT neglects this spatial dependence and uses a single core-average diffusion coefficient to calculate the release of ^{129}I. V&A has evaluated this approximation (response to question A9 of RAI-2) by comparing the ^{129}I release from a set of high- and low-powered fuel pins with the release calculated from the 3R-STAT composite pin. This comparison indicates that the release from the 3R-STAT composite pin is within approximately 30 percent of the explicit pin calculation.

Finding: The uncertainty associated with the diffusion release modeling is small compared to the expected 3R-STAT calculational uncertainty and is included in the uncertainty derived from the benchmark comparisons.

3.2.1.4 Equivalent Pin Representation

Because of the lack of information concerning the individual fuel rod conditions, and to simplify the analysis, 3R-STAT represents the entire core as a composite or representative fuel rod. The release of radionuclides from the defective fuel rods is determined using core-average fuel rod parameters. To evaluate this assumption, V&A has performed a series of sensitivity calculations in which the fuel rod release parameters were varied over a range that would be expected in a typical core. The variations included the mechanism release fractions q_i, fuel rod burnup, and escape rate coefficient ϵ. Six cases, each consisting of three substantially different fuel rods, were calculated. In each case the individual fuel rod releases were summed and compared to the release that 3R-STAT would calculate, assuming a single composite fuel rod. The 3R-STAT predictions of the ^{129}I release agreed with the sum of the individual fuel rod releases to within approximately 50 percent in all six cases (response to question A18 of RAI-1).

Finding: This uncertainty is small compared to the expected 3R-STAT calculational uncertainty and is included in the uncertainty derived from the benchmark comparisons.

3.2.1.5 Representative Tramp Fuel Particle

In determining the release from the tramp fuel, 3R-STAT assumes a composite tramp fuel particle having a surface-to-volume ratio (S/V) of 3000 m^{-1}, corresponding to a spherical particle of 10 μm radius, and a fuel burnup of 700 effective full power days (EFPDs). It is noted, however, that since all three release mechanisms are proportional to S/V, and 3R-STAT only requires the fractional releases, the 3R-STAT predictions are independent of this assumption.

In 3R-STAT, an underestimate of the tramp fuel burnup may result in a non-conservative under-prediction of the ^{129}I and ^{99}Tc releases. To evaluate the effect of assuming a 700-EFPD tramp fuel burnup, V&A has accessed the industry-wide Part 61 waste sample data base and determined the distribution of tramp fuel burnups. The data suggests that only approximately 5 percent of the pressurized-water reactor (PWR) fuel cycles have tramp fuel exposures greater than 700 EFPD, which will result in a 3R-STAT under-prediction. In the case of boiling-water reactors (BWRs), less than half of the plants have burnups greater than the assumed 700-EFPD tramp fuel burnup. In addition, the responses to question A7 of RAI-1 and question A8 of RAI-2 demonstrate that the tramp fuel burnup assumption has minimal impact, when looking only at the tramp fuel contribution. When looking at the contribution from other mechanisms, the impact of this assumption is reduced further.

Finding: Based on the above analysis, the modeling of the tramp fuel is adequate as described by the representative tramp fuel particle.

3.2.1.6 Determination of the Fuel Burnup by the $^{134}Cs/^{137}Cs$ Ratio

3R-STAT determines the fuel burnup using a correlation of the $^{134}Cs/^{137}Cs$ ratio to fuel burnup. This correlation assumes that the measured ^{137}Cs is released from the defective fuel rods and not the exposed tramp fuel. In the response to question A28 of RAI-2, V&A has provided iodine and cesium measurements taken during Cycle-9 of Beaver Valley-1, and during Cycles 1 and 3 of Beaver Valley-2 nuclear power plants. These data support the assumption and indicate a substantial correlation between the cesium concentrations and the fuel defects. The cesium concentrations were less than detectable during the periods of no failures, but increased abruptly above the detectable threshold during the periods, later in the cycle, when defects had occurred.

For the case where no cesium measurement data are available, 3R-STAT allows the user to input cesium data based on trend values or defaults from the plant setup data files. These trend or default cesium values can result in up to a factor of 3 under-prediction of the ^{129}I release (response to question A14 of RAI-2). However, the situation in which the under-prediction may occur is that in which no defective fuel is releasing ^{129}I. In these situations, the ^{129}I release is lowest and, therefore, the impact on the inventory estimate at a waste disposal site is least (response to question B5 of RAI-2).

Finding: Use of the $^{134}Cs/^{137}Cs$ ratio is adequate for determining the burnup of the fuel. Use of the trend or default cesium ratio is acceptable for determining the burnup when the conditions (i.e., no measurable cesium released) reflect a low failed fuel fraction.

3.2.1.7 Coolant Purification and Steam Carryover Constants

The coolant purification constant (ß) and the steam carryover constant (θ) control the non-decay radionuclide losses from the reactor coolant. These input modeling parameters are plant-specific and may involve a substantial degree of uncertainty. In addition, the 3R-STAT predictions are functions of these parameters. To quantify the effect of the uncertainty in these parameters, V&A has performed a series of sensitivity calculations. Assuming variations in the coolant iodine purification constant β_I and the steam carryover fraction θ_I of 10 percent and a factor of 2, respectively, the ^{129}I and ^{99}Tc releases varied by less than approximately 30 percent (response to question A25 of RAI-2).

Finding: Based on the above analysis, the coolant purification and steam carryover constants are adequately described and modeled.

3.2.1.8 Impact of Assuming Steady State Conditions

The equations used in the TR and code are all based on an assumed steady state equilibrium condition. This assumption neglects the periods during start-up and shutdown, and during transient power spikes, when changes in the release conditions are known to occur. The TR is based on an assumption that the steady state analysis is representative and adequate for the period of analysis (response to question A8 of RAI-1).

The V&A TR suggests that the reactor coolant data should be ignored during periods of observed transient fluctuations. Specifically, data should be eliminated during start-up, shutdown, and any "spiking" events. Spiking is a term used to describe the phenomenon of localized power transients that cause sharp increases in the observed activities of short-lived isotopes in the reactor coolant system.

Finding: The steady state conditions adequately represent the core conditions for the purpose of estimating the release to the coolant during the reactor operating cycle. Therefore, the reactor coolant data collected during transients should be ignored.

3.2.2 Validation of the 3R-STAT Methodology

The 3R-STAT analysis of the tramp and defective fuel rod release of ^{129}I and ^{99}Tc is a complex calculation that uses measured and calculated input that typically involves inherent uncertainties. The analysis requires knowledge of the conditions in the fuel pellet and fuel rod gap, as well as the condition of the fuel rod cladding. In 3R-STAT, these fuel rod conditions are inferred using a detailed description of the tramp fuel release mechanisms, together with cycle-specific plant measurements of the short-lived iodine concentrations. In addition, the calculation of the steady-state concentrations employs plant and nuclide-dependent values of the coolant system purification and steam carryover fractions.

Because the detailed fuel conditions, purification and carryover fractions, and short-lived concentration measurements typically involve uncertainties, the 3R-STAT predictions of ^{129}I and ^{99}Tc are subject to uncertainty.

Consequently, the review of the TR addressed the validation of 3R-STAT. The specific focus concerned the completeness and accuracy of the benchmark comparisons, as well as the estimated statistical uncertainty limits on the 3R-STAT predictions. The major issues resulting from this review are summarized in the following sections.

3.2.2.1 Fuel Rod Parameters

The benchmark comparisons included in the TR Validation and Verification Report are purported to provide the validation for the application of 3R-STAT to operating reactors. Seventeen operating reactors, including both PWRs and BWRs, have been analyzed. The TR suggests that these comparisons justify the 3R-STAT fuel rod release models for application to all slightly enriched uranium oxide light-water reactor (LWR) fuel. Applications to fuel types (e.g., highly enriched uranium) not included in this data base will require additional validation (response to question A7 of RAI-1).

In 3R-STAT, the fuel burnup of the defective fuel rods, used to determine the burnup-dependent radionuclide yields, is determined based on the ratio of ^{134}Cs to ^{137}Cs. 3R-STAT assumes that when both ^{134}Cs and ^{137}Cs are measured in the reactor coolant, it is a result of defective fuel rods, and the fuel rod burnup is inferred from the measured $^{134}Cs/^{137}Cs$ ratio using a precalculated (approximately) linear correlation. The validation for this method is provided in the benchmark comparisons. These comparisons include a range of burnups from, approximately, 150 to 950 EFPD, which covers the typical range of LWR fuel rod burnups. Plants with no defective fuel rods, as well as plants with multiple defects, were included. The Cs-ratios varied from 0.3 to 1.4; this range was typical of a sample taken on 160 fuel cycles (response to questions A8 of RAI-2 and A7 of RAI-1).

Although the 3R-STAT fuel release models include a dependence on the fuel burnup, no explicit dependence on the fuel rod power is included. The range of fuel rod powers, included in the benchmark comparisons, has not been provided. V&A has performed a series of sensitivity calculations (response to question A7 of RAI-1) to determine the effect of the fuel rod power dependence on the benchmark comparisons. These calculations indicate that the 3R-STAT ^{129}I and ^{99}Tc benchmark predictions will change by less than 10 percent, when the fuel rod power is varied over the range of rod powers that typically occurs in an LWR.

Finding: The TR is applicable to all slightly enriched (approximately 3 percent) uranium oxide LWR fuel in nuclear power plant reactors at normal operating power conditions.

3.2.2.2 Benchmark Calculations and Uncertainty

The comparison statistics (mean values, standard deviations, etc.) determined from the benchmark calculations provide the uncertainty estimates for the 3R-STAT ^{129}I and ^{99}Tc predictions. To ensure that these uncertainty estimates provide a true measure of the 3R-STAT prediction accuracy, Brookhaven National Laboratory (BNL) and NRC reviewed and recalculated all of the benchmark calculations. This evaluation identified several errors and/or inconsistencies in the calculations. In the response to questions A23 of RAI-

1 and question A2 of RAI-2, V&A has corrected the benchmark calculations, and updated the comparison statistics (in responses to questions A22(m) of RAI-1, B11 of RAI-1, and A12A of RAI-2). The revised calculation-to-measurement bias and standard deviation are 1.49 and 2.63, respectively, for ^{129}I, and 2.29 and 7.08, respectively, for ^{99}Tc. The corresponding 95 percent probability limits for under-prediction are 3.28 and 10.8 for ^{129}I and ^{99}Tc, respectively (response to question B11, RAI-1).

The 3R-STAT predictions of ^{129}I and ^{99}Tc are sensitive to the assumed tellurium removal rate constant β_T, especially for high tramp fuel fractions. To reduce the effect of this sensitivity, 3R-STAT calculates the tellurium removal rate constant internally when the tramp fuel fraction "a" is ≥ 0.35. To determine the effect of the uncertainty in β_T, V&A has performed a series of sensitivity calculations. For the case where β_T is not calculated internally, the ^{129}I and ^{99}Tc predictions vary by less than 25 percent and 1 percent, respectively, for a typical range of β_T uncertainty. For the case where β_T is calculated internally, the ^{99}Tc variation was less than approximately 12 percent and the ^{129}I varied by a factor of 3 (response to question A27 of RAI-2). Although the effect on the ^{129}I prediction is large, it is included in the benchmark comparisons and is consistent with the derived 3R-STAT uncertainties, stated above.

With 95 percent confidence, the 95 percent under-prediction factors, for the ^{129}I and ^{99}Tc predictions for individual fuel cycles, are 5.88 and 40.1, respectively (see Table 2, p.15, and Appendix A to this TER). However, the ^{99}Tc validation results include large calculation-to-measurement (C/M) differences between the 3R-STAT calculations and measurements for the PWR plants. The PWR data suggest a factor of approximately 16 over-prediction of the ^{99}Tc release, and a very large standard deviation of a factor of approximately 25 between the calculations and measurements.[1] V&A has suggested that the over-prediction of the PWR ^{99}Tc releases may be due to "plate-out" of technetium on core surfaces and/or "break through" in the measurement resin column. However, no quantitative analysis of the specific reduction in the measured ^{99}Tc has been provided. As a result, there is a large degree of uncertainty (biased to over-prediction) in the PWR ^{99}Tc measurements and their relation to the 3R-STAT predictions.

Although these measurements include many of the operational aspects of the 3R-STAT application, the accuracy and completeness of the plant measurement data base are limited. To provide an independent estimate of the 3R-STAT prediction uncertainty, V&A has performed a detailed Monte Carlo uncertainty analysis. The first step in this analysis includes an estimation of the uncertainty in the important modeling and input parameters. The effect of the uncertainty in these parameters was determined by randomly varying each uncertain input/modeling parameter and calculating the corresponding 3R-STAT ^{129}I and ^{99}Tc releases. The uncertainty in the ^{129}I and ^{99}Tc predictions was determined from the distribution of the 3R-STAT calculated results. The V&A Monte Carlo uncertainty analysis indicated 95 percent probability upper limits

1. These values were determined using the actual C/M data and the definitions of the mean and standard deviation, rather than fitting the data to the lognormal distribution.

of 2.64 and 2.91 on the ^{129}I and ^{99}Tc predictions, respectively (response to question A21 of RAI-2). This ^{129}I limit is in general agreement with the 3.28 value determined by the validation; however, the ^{99}Tc value is substantially less than the value of 10.8 inferred from the benchmark comparisons. The reduced ^{99}Tc 95 percent limit determined by the Monte Carlo uncertainty analysis (relative to the benchmark comparisons) may be caused by the type of plant assumed in the Monte Carlo analysis (i.e., BWR versus PWR), measurement uncertainties, or underestimates of the ^{99}Tc release parameter uncertainties.

The statistical parameters for the individual fuel cycles, the derivations of which are discussed in Appendix A to this TER, are identified in Table 2 below. The statistical parameters are discussed in response to question A12A of RAI-2. The 95 percent/95 percent limits are the levels below which at least 95 percent of the C/M values fall with 95 percent confidence.

Table 2
Statistical Limits (Under-Prediction)

Iso-topes	Standard Deviation	95% Under-Prediction	95%/95% Under-Prediction
^{99}Tc	7.08	10.9	40.1
^{129}I	2.65	3.29	5.88

Applicants for LLW disposal facility licenses and licensees (generators) using the code should identify and justify the statistical limits proposed for their specific application of the TR. A generator may determine (and justify) that it should perform some independent validation and quantify its under-prediction uncertainty uniquely.

<u>Finding</u>: The uncertainties identified by the waste generator must be justified by the generator and included with the reported TR calculated inventory. The values in the table represent the uncertainties based on the benchmark calculations and comparisons, calculated using the methodology described in Appendix A to this TER. These values may be used (if justified by the generator) in cases where no additional validation is available or provided.

3.2.2.3 3R-STAT Coding Verification

As part of the verification, independent hand calculations were performed to test the 3R-STAT coding. In the response to question A7 of RAI-2, V&A provided a calculation, with the 3R-STAT sample steps reduced, to provide the highly precise 3R-STAT solution required for this test. In addition, V&A provided a spreadsheet, in response to question 8 of RAI-3, of a hand calculation that illustrated iteration in steps equivalent to those of 3R-STAT.

<u>Finding</u>: The numerical comparisons provided demonstrate agreement for both the PWR and BWR calculations and verify the 3R-STAT coding.

3.2.2.4 Dependence of the Prediction Uncertainty on the Core Conditions

The TR uncertainty analysis and the Monte Carlo uncertainty analysis of the response to question A21 of RAI-2 assume the calculational uncertainty is the same for both BWR and PWRs, and for plants with and without fuel failures. The method used to calculate the releases, however, suggests that the 3R-STAT calculational uncertainty depends on these plant conditions. The BWR ^{99}Tc release is determined using a ^{60}Co measurement together with a precalculated $^{99}Mo/^{60}Co$ ratio, whereas the PWR ^{99}Tc release is determined using an estimated knockout release fraction from tramp fuel, q_3. Consequently, in the case of the ^{99}Tc release, the BWR uncertainty is due to the uncertainty in the ^{99}Mo calculation, while the PWR uncertainty is primarily influenced by the uncertainty in the tramp fuel knockout release fraction, q_3. In determining the ^{129}I release, the (low "a") high fuel failure calculation is performed using the short-lived iodine measurements to calculate the release fractions and determine the ^{129}I release. Alternatively, for the (high "a") no-failures calculation, the ^{129}I release is a function of the estimated tramp fuel release fractions. Consequently, the uncertainty in the high fuel failure calculation is heavily influenced by the uncertainty in the short-lived iodine measurements, whereas the no-fuel failures calculational uncertainty is more sensitive to the uncertainties in the tramp fuel fractional releases: q_1, q_2, and q_3. In view of the substantial differences between the BWR and PWR calculations and also between the high failure and no-failure calculations, it is concluded that the individual fuel cycle calculational uncertainty will have a substantial dependence on reactor type (BWR vs. PWR) and the number of fuel failures (low "a" vs. high "a"), as shown in Tables 3 and 4.

The validation data presented in the "Validation and Verification Report" of the TR, and the uncertainty analysis presented in the response to question A21 of RAI-2 do not account for the plant and fuel failure dependence of the 3R-STAT calculation uncertainty for individual fuel cycles. All plant types and core conditions are combined and average accuracy statistics are determined for the disposal facility application. This type of analysis can result in optimistic estimates of the prediction accuracy for individual fuel cycles. For example, if the PWR and BWR C/M ^{99}Tc release data in the "Validation and Verification Report" are separated, the BWR data suggest a factor of approximately 1.6 over-prediction and a standard deviation of approximately 3.0, whereas the PWR data suggest a factor of approximately 16 over-prediction and a standard deviation of approximately 25.[2] These differences are not surprising, in view of the differences in the sensitivities of the model.

V&A, in the response to question 2 of RAI-3, states that the model is not substantially different for different reactors (PWR vs. BWR) or different at all for different core conditions (high exposed fuel fraction vs. low exposed fuel fraction). Rather, from the same input data, the code determines the core conditions, and the sensitivities of the model are based on the core

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2. These values were determined using the actual C/M data and the definitions of the mean and standard deviation, rather than fitting the data to a lognormal distribution. If a lognormal distribution is assumed, the PWR over-prediction and standard deviation are 16 and 28, respectively, and the corresponding BWR statistics are 2.1 and 8.5.

conditions. V&A suggests that the only input required is the plant type, to allow calculation of steam carryover in BWRs.

Table 3
^{129}I Sensitivity

Reactor Type	Failed Fuel Fraction	Key Parameters	Rel. Release Rate	Relative Uncert.	Impact on LLW Inv.*
PWR	Low "a"**	q_4, q_5, q_6	High	Low	High
	High "a"	q_1, q_2, q_3	Low	High	Low
BWR	Low "a"	q_4, q_5, q_6	High	Low	High
	High "a"	q_1, q_2, q_3	Low	High	Low

* Assumes waste at the LLW disposal facility is from a combination of all four types of core conditions (i.e., low "a" and high "a" from PWRs and BWRs).

** Low "a" refers to a large failed fuel fraction.

Table 4
^{99}Tc Sensitivity

Reactor Type	Failed Fuel Fraction	Key Parameters	Rel. Release Rate	Relative Uncert.	Impact on LLW Inv.*
PWR	Low "a"**	q_3	Equal	High	Equal
	High "a"	q_3	Equal	High	Equal
BWR	Low "a"	^{99}Mo/^{60}Co	Equal	Low	Equal
	High "a"	^{99}Mo/^{60}Co	Equal	Low	Equal

* Assumes waste at the LLW disposal facility is from a combination of all four types of core conditions (i.e., low "a" and high "a" from PWRs and BWRs).

** Low "a" refers to a large failed fuel fraction.

Finding: The benchmark comparisons adequately represent the range of core conditions identified in the TR. The model is sufficient to evaluate the range of core conditions discussed in the TR.

3.2.3 Application of 3R-STAT

The 3R-STAT methodology has a substantial degree of user flexibility with respect to the processing of measured data, input requirements, modeling parameters, and numerical procedures. The licensee plant-specific treatment of these inputs and procedures can affect the accuracy of the 3R-STAT predictions. To ensure the applicability of the upper tolerance uncertainty limits (derived in the "Validation and Verification Report") in specific licensee applications, a detailed review of the plant-specific features of the 3R-STAT Methodology was performed. The major issues resulting from this review are summarized in the following sections.

3.2.3.1 Uncertainty in Waste Disposal Facility Inventory

In the response to question A22(m) of RAI-1, V&A has indicated that in calculating the uncertainty in the total waste disposal inventory, it assumes that the 3R-STAT calculational errors resulting from the use of individual cycle waste batch data are random and independent. As a result, the 3R-STAT calculational uncertainty for the total waste inventory is expected to decrease as the number of fuel cycles received at the disposal facility increases. To take advantage of the cancellation of errors implied by this assumption, it must be shown that the 3R-STAT errors made in the individual batches are independent. V&A, in the response to question 6 of RAI-3, provides three bases for the assumption that the uncertainties of individual fuel cycles or batches are independent.

The uncertainty in the inventory at an LLW disposal facility can be calculated from the uncertainties of the incoming fuel cycle data. V&A described an example of such a calculation for the response to question A22(m) of RAI-1. In the example provided by V&A, the following under-prediction factors were developed from the individual uncertainties in the fuel cycle estimates (see Table 5).

Table 5
LLW Disposal Facility Uncertainty (Under-Prediction)

Isotope	Under-Prediction Factor
^{99}Tc	5
^{129}I	2

The statistical treatment of the results from individual fuel cycles provides the LLW disposal facility operator with additional information after the waste has been received and a sum total inventory calculated. This incoming fuel-cycle-specific information will be based on actual data and will be plant-specific. The treatment described above used the standard deviations of the data to identify a 95 percent prediction interval in the summed total facility inventory received from these fuel cycles.

Finding: The LLW disposal facility should calculate a total inventory from the sums of the incoming fuel cycle estimates from LLW generators using the code. The LLW disposal facility will be able to calculate an uncertainty associated with the inventory from the statistical data presented by the LLW generator. The TR provides only an adequate criterion for evaluating the total facility inventory. Appendix A to this TER provides an adequate methodology to demonstrate that this criterion has been identified. Use of the methodololgy described in Appendix A to theis TER is acceptable for calculating LLW disposal site inventory uncertainty.

3.2.3.2 Measurement of Short-lived Radionuclides

The short-lived iodine measurement data are used to determine the fuel rod release mechanisms, escape rate coefficient (ϵ), and the tramp fuel fraction. The short-lived cesium measurement data are used to determine the fuel rod burnup. The 3R-STAT ^{129}I and ^{99}Tc predictions are sensitive to these measurement data, and it is important that the measurement error be minimized. The factors contributing to the measurement uncertainty include: (1) the minimum time allowed for flushing the sample line; (2) the sampling frequency; and (3) the decay time between sample collection and counting. No specific procedures were used to control these factors in the short-lived iodine and cesium measurements used in the benchmark calculations. To ensure that, in 3R-STAT licensing applications, the measurement uncertainty is within the limits derived from the benchmark comparisons, in response to RAI-1, V&A has added additional recommendations to the Users Manual, to control these factors (response to question A4 of RAI-1). These recommendations include: (1) a minimum 180-minute flush of the sample line; (2) a sampling frequency of at least every other day or three times per week; and (3) times between sampling and counting should be between 1 and 2 hours for ^{132}I, ^{133}I, ^{134}I, and ^{135}I, and between 4 and 8 hours for ^{131}I.

Finding: The methodology described in the TR is acceptable for sampling the short-lived iodine isotopes.

3.2.3.3 Determination of the $^{99}Mo/^{60}Co$ Ratio

The ^{99}Tc produced by the decay of ^{99}Mo is an important, and sometimes dominant, contribution to the ^{99}Tc in the reactor coolant. The isotope ^{99}Mo is produced by the activation of the corrosion product ^{98}Mo. 3R-STAT determines the coolant concentration of ^{99}Mo using a predetermined $^{99}Mo/^{60}Co$ ratio. In the benchmark calculations, a constant nominal value of the $^{99}Mo/^{60}Co$ ratio was used. To ensure that, in 3R-STAT licensing applications, the ^{99}Tc prediction uncertainty is within the limits derived from the benchmark comparisons, V&A has provided specific recommendations in the Users Manual on the procedures to be used in the determination of the $^{99}Mo/^{60}Co$ ratio. These recommendations include: (1) the ratio should be determined using a large number of coolant samples (approximately 30 to 40); (2) the ^{99}Mo and ^{60}Co measurements should be made during steady-state conditions; and (3) the ratio should be reviewed and updated on an annual basis (response to question A6, RAI-1).

Finding: Determination of the $^{99}Mo/^{60}Co$ ratio is acceptable as described in the TR.

3.2.3.4 Input Measurement Data

3R-STAT may be run using several code options. These include: (1) averaging the input data and using a single data set input to 3R-STAT; (2) averaging of the daily analysis results; and (3) the batch analysis option. The batch analysis option uses the curve-smoothing feature in order to eliminate random variability and reduce the uncertainty in the input measurement data.

3R-STAT uses the measured iodine, cesium, and cobalt data to determine the fuel rod release fractions and burnup, and the ^{99}Tc contribution from the corrosion products. The individual sample measurements typically include a relatively high level of variability. To reduce the effect of this variability on the predictions, 3R-STAT performs a regression fit of the input measurements. If the regression fit is not performed correctly, the prediction uncertainty may increase beyond the uncertainty limits derived from the benchmark comparisons. To ensure the applicability of the uncertainty limits in licensing applications, V&A has provided specific recommendations in the Users Manual on the procedures to be used in performing the regression fit. These recommendations include: (1) the selected time span should not exceed a single cycle, should include the maximum number of measurements, and should provide an accurate data fit; (2) the selected time span should avoid discontinuities in the ratio data and abrupt slope changes in the trend data; (3) measurements made within 2 weeks of a return to power should be avoided; (4) any large outlier in the middle of the span should be removed; and (5) the iodine ratios should be reviewed for continuity before batch analysis.

In the response to question A21 of RAI-2, V&A quantitatively evaluated the sensitivity because of the input data. This evaluation demonstrated that the overall prediction uncertainty because of input sensitivity was consistent with the model uncertainty based on the benchmark calculations.

Finding: The input data measurements are sufficient to adequately characterize the fuel-cycle when determined in accordance with the procedures identified in the TR.

3.2.3.5 Limit on Residual Error

In 3R-STAT, the fuel rod release parameters and tramp fuel fraction are determined by a least-squares-fit of the fuel rod model to the short-lived iodine measurement data. The residual error, edited by 3R-STAT, is a measure of the goodness of the fit and the numerical accuracy of the solution. (It is noteworthy that this error does not include the error introduced by uncertainty in the input measurements and model parameters.) The residual error in each of the benchmark calculations is less than the V&A selected value of 0.20. To ensure the applicability of the uncertainty limits determined from the benchmark comparisons, in licensing applications of 3R-STAT, the residual error should be less than the 0.20 value selected by V&A in the benchmark calculations.

Finding: The limit on the residual error should not exceed the 0.20 value used in the benchmark calculations. The TR has been modified to include a routine in the 3R-STAT code for aborting calculations exceeding this limit.

3.2.4 3R-STAT Manuals

The 3R-STAT manuals are intended to help the licensee implement the code, prepare model and measurement input data, and interpret the results. The 3R-STAT manuals have been reviewed in detail to ensure that the manuals provide the necessary methodology documentation and user instruction to reliably perform these aforementioned tasks. The focus of the review was to ensure that the 3R-STAT manuals provide a true representation of the actual coding, an accurate and clear description of the methodology, and a sufficiently complete description of the application of 3R-STAT. The major issues resulting from this review are summarized in the following sections.

3.2.4.1 3R-STAT Sample Problem Solutions

Appendices C and D of the Volume-2 3R-STAT Manuals provide BWR and PWR sample problem definitions and solutions. This information allows the user to test and validate his code implementation and calculational procedures. As part of the evaluation of the TR, BNL implemented the 3R-STAT coding and calculated the Volume-2 sample problems. The intial comparison of the V&A and BNL sample problem solutions indicated that the V&A calculations were not performed with Version 3.0 of 3R-STAT, which V&A provided for review. In the response to question A1 of RAI-1, V&A has provided updated sample problem input and solutions.

Finding: These updated V&A solutions are in agreement with the corresponding BNL calculations.

3.2.4.2 3R-STAT Documentation

To ensure the reliable and valid application of 3R-STAT, it is important that the description of the models, numerical solution methodology, validation, and coding provided in the 3R-STAT manuals be accurate. As part of the BNL review, several inconsistencies and errors were identified in the manuals. In the responses to questions A22 of RAI-1 and A1 of RAI-2, V&A has provided the modifications and corrections necessary to update the manuals. In addition, V&A has increased the users' capability to confirm the proper application of 3R-STAT and perform diagnostics by adding a description of the "runtime errors" to Section 7 of the Users Manual.

Finding: The 3R-STAT documentation is acceptable. The TR should be re-issued incorporating this TER and the review questions and responses, as appendices.

3.2.4.3 Quality Assurance

The TR provides the quality assurance procedures to be applied to the development and maintenance of the code and TR. This TER reflects a review of Version 3.0 of the 3R-STAT code. Only this version of the code is qualified by this report. Any substantive changes to the code or TR should be made in accordance with the procedures, described in Volume 4 (Section C) of the TR, and will require reevaluation. Non-substantive and editorial changes to the TR for clarification should be controlled. Controlled copies should be distributed to users and all qualified recipients. Non-substantive changes must meet the following criteria: (1) no changes to the code are necessary; and (2) no revalidation is necessary. Revalidation would be required in those instances where changes in the code or model affect comparison of the benchmark calculations as provided in the final TR.

Finding: The 3R-STAT quality assurance program is acceptable with the procedures in place. The transmittal of the final TR should be controlled in accordance with VA-QA-001.

3.2.5 Technical Evaluation Summary

In summary, the models used in the physical representation of the system are acceptable. In conjunction with the validation, and as applied in the specific manner discussed in the TR, the model can provide an adequate estimate of the inventories of ^{129}I and ^{99}Tc at an LLW disposal facility. The code accurately executes the mathematical models described in the TR. In addition, the data provided with the report, and in response to the questions generated during this review, better quantify the associated uncertainty beyond those data currently available for use by an applicant for a LLW disposal facility license. The application is appropriate and the documentation sufficient to ensure the proper use of the code in licensing applications.

4.0 REGULATORY POSITION

The TR and code provide an acceptable method of calculating ^{129}I and ^{99}Tc at LLW disposal facilities. The information provided by the TR methodology can be used in a disposal facility licensing. Finally, waste classification and manifesting are not impacted by this TR. This section provides the staff regulatory position on the use of this TR.

4.1 Low-Level Waste Disposal Facility Licensing

License applicants should use the following guidance in determining adequacy of information used for LLW license applications. The primary burden is on the applicant to justify the use of the code as appropriate and adequate within the scope of the license application.

4.1.1 ^{129}I and ^{99}Tc Inventory Calculations

This TR and the code associated with it provide an acceptable method of calculating ^{129}I and ^{99}Tc to be transferred for disposal from operating commercial power reactors to an LLW disposal facility. The calculations, including the uncertainties discussed in the TR and this TER, provide a more accurate estimate of the inventories expected at the LLW disposal facilities than is currently available. An applicant may use the TR to calculate or predict the total inventory of ^{129}I and ^{99}Tc received or expected at the disposal site. A licensee may use the TR to calculate the total inventory sent to a disposal site in LLW.

This TR provides an acceptable method of assessing an LLW facility inventory of ^{129}I and ^{99}Tc from generators that certify their use of the TR. To evaluate a future LLW facility inventory, the applicant should conduct an inventory analysis using representative, fuel cycle specific uncertainty ranges from generator's estimates of inventory contributions. The development of the LLW facility uncertainty ranges should be based on an analysis of potential waste inventory, such as that described in Section 3.2.3.1, above.

After receiving LLW containing these isotopes from generators using 3R-STAT, the disposal facility will be able to develop a statistical representation of the uncertainty in the calculated inventory, e.g., the 95 percent under-prediction value from the standard deviations on the fuel cycle specific inventory estimates provided by the generators. The statistical treatment of the results from individual fuel cycles will provide the LLW disposal facility operator with additional information after the waste has been received. This information will be based on actual data and will be plant-specific. The treatment should use the standard deviations of the data to identify the uncertainty in the actual facility inventories.

As discussed in the technical evaluation above, the model provides results with broad uncertainty ranges. For the low failed fuel fraction estimates, the uncertainty is substantially greater than for high failed fuel fraction estimates. However, the uncertainty in the low failed fuel estimates becomes less significant when combined with high failed fuel cycles. In addition, the code overestimates low-failed fuel cycles, i.e. the actual inventory from low failed fuel cycles will likely be less than that calculated by the code. However, for high failed fuel cycles, the code provides more realistic estimates, and therefore, the uncertainty associated with these cycle specific projections is less (see Tables 3 and 4, section 3.2.2.4). Indubitably, waste streams from both high and low failed fuel cycles have historically been disposed of at LLW facilities.

Should future waste, going to an individual LLW disposal facility, be entirely derived from low failed fuel cycles, the waste will contain significantly less total inventory than determined by this TR methodology. Normally, averaging the data from the many fuel cycles anticipated and accepted during the facility's lifetime will result in 3R-STAT over-predicting the actual inventory. As a result, there is a small probability that the TR could under-predict the amount of ^{129}I and ^{99}Tc in some disposal facility inventories. While there is a small probability that the estimate from 3R-STAT could under-predict the inventory, the TR provides reasonable assurance that the inventory of ^{129}I and ^{99}Tc will be adequately described and meet the requirements of 61.12(i) for wastes from the specific generators using this TR.

4.1.2 Incorporation by Reference in an LLW Disposal Facility Application and LLW Disposal Facility User Qualification

The directions provided in the NRC guidance (NUREG-1200) state that the applicant should provide a discussion of the use of reference materials in the context of their application and the reference's pertinence and limitations. An applicant for a LLW disposal facility license should provide such discussion when referencing this TER and TR. The discussion should specify how the facility's proposed waste acceptance criteria will ensure that all waste generators that choose to use the TR do so appropriately; address the inventory expected from generators not using the TR (e.g., other power reactors, research reactors, sealed sources, and other possible sources); and specify the inventory control mechanism to be employed to ensure that the inventories are accurately tracked.

As discussed above, the user of the TR is required to qualify its use of the code if the code is used in support of a licensing action (GL 83-11). This qualification should be demonstrated by the user in conjunction with the request for consideration of the code results in an LLW disposal facility licensing action.

4.2 Use by Waste Generators

The waste generators who will use this TR are nuclear power plant licensees who operate reactors under the conditions described in the TR.

4.2.1 Waste Classification

The TR provides total inventory values for fuel cycles from contributing generators. Waste packages and waste shipments to LLW disposal facilities require classification in accordance with NRC regulations at 10 CFR Part 20, Appendix F.

The TR does not provide an alternate mechanism for waste classification. For waste classification, the waste generator should use conservative values (based on the scaling factors) consistent with the current practice. This would mean that the disposal facility would still be provided or capable of calculating a total ^{129}I or ^{99}Tc activity from waste manifests. This total will be replaced using the 3R-STAT inventory values provided periodically by the generators using the V&A code and added to the inventory from other sources. This mechanism is necessary because the TR does not provide a mechanism for identifying waste shipment specific estimates of radionuclide content or concentrations. The information from the 3R-STAT TR is provided on a fuel-cycle-specific basis and may not be provided until after the waste has been shipped and disposed of in the disposal facility. Additionally, the licensee should be able to verify that any shipped waste does not contain ^{129}I and ^{99}Tc in concentrations sufficient to cause the waste to be classified as "Greater Than Class C." This can be achieved by continuing the current conservative approach for estimating ^{129}I and ^{99}Tc concentrations for classification purposes.

4.2.2 Reporting of Waste Inventories (Waste Manifesting)

Incoming waste manifests would still contain the conservative values based on the scaling factors. As a result, the disposal facility would still be capable of calculating a total ^{129}I or ^{99}Tc activity through summations of data from waste manifests. This total may be adjusted periodically using information supplied by the generators, using the 3R-STAT code.

The 3R-STAT results, reported by a reactor licensee, should include the 3R-STAT analysis result report, as described in the TR on page 5-9 of the Users Manual, and a description of the uncertainty. Specifically, the user should supply the standard deviations, 95 percent uncertainty limits, and 95 percent/95 percent limits associated with the estimates and the basis for those values (i.e., either the TR values or other values, based on additional validation). Providing this information to the disposal site operator will maximize the flexibility that the disposal site operator has in analyzing the disposal facility inventory uncertainty, as discussed in sections 4.1.1. and 3.2.3.1.

Corrected waste inventories should be clearly identified by the waste generator. The corrected information should be provided to the waste disposal facility operator, who should have appropriate procedures in place to ensure that the adjusted inventory information is provided to any regulatory or oversight group tracking the waste disposed at the disposal site.

4.2.3 Waste Generator User Qualification

As discussed above, the user of the TR should qualify its use of the code, if the code is used by the disposal facility operator in support of a licensing action, as described in GL 83-11.

The reactor user can use the code without performing additional validation, if justification is provided. When a licensee does no additional validation, the user should report the standard deviation, 95 percent uncertainty limits, and 95 percent/95 percent limits identified in Table 2, together with the adjusted inventory estimates generated by 3R-STAT. Alternatively, the reactor user can perform additional validation to quantify the uncertainty associated with plant conditions and measurement techniques that provide the code's input data.

A licensee intending to use 3R-STAT should submit information substantiating that the code can be properly used. Specifically, licensees should commit to the training program outlined in the TR. The licensee should provide a rationale for its suggested frequency of refresher training. The licensee should identify the format and content (i.e., statistics or uncertainties) of the information to be provided to the LLW disposal site operator. The licensee should identify the manner, frequency, and identification of inventory information being adjusted.

4.3 Summary of TR Uses

This section identifies the specific actions necessary for use of the 3R-STAT code.

4.3.1 Waste Generator Licensee (Nuclear Power Plant) Usage

A nuclear power plant licensee should certify their use of the code with the NRC in accordance with GL 83-11.

A nuclear power plant licensee should conduct validation testing, if necessary, as described in 3.1.2.3 and GL 83-11.

A nuclear power plant licensee should classify waste being shipped to disposal sites using actual measurements of ^{129}I and ^{99}Tc activities or estimates conservatively using scaling factors, as they have in the past.

A nuclear power plant licensee should provide manifests with waste shipments. These manifests should be prepared in the same way manifests have been prepared in the past and in accordance with NRC's uniform manifest requirements (60 FR 15649).

A nuclear power plant licensee should collect short lived iodine data over the operating cycle in accordance with the procedures in the TR and as discussed in detail, below.

A nuclear power plant licensee should calculate the ^{129}I and ^{99}Tc released from its reactor during the fuel cycle using the 3R-STAT code. The code will provide $\mu Ci/sec$ or $\mu Ci/MWD$ results which should be appropriately converted to total μCi release estimates.

A nuclear power plant licensee should evaluate the uncertainty associated with the release calculated by 3R-STAT.

A nuclear power plant licensee should report the calculated release, indicate which manifests represent the wastes containing this inventory, provide the uncertainty on the estimate, and provide the justification for the uncertainty to the disposal site operator.

A nuclear power plant licensee certified to use the code, as described in 4.2.3 above, will analyze plant reactor coolant system measurement data using the 3R-STAT code. Specifically, the licensee will follow the procedures in the Users Manual to analyze batch data. The data should have been collected according to the procedures identified in the TR. The licensee will calculate the average release rate for the time period of interest and a total release for each isotope for each time period of interest. The time periods of interest may be less than the entire fuel cycle due to changing core conditions. However, the analysis will generally take place at the end of the fuel cycle.

Upon calculating the total inventory release, the licensee will determine, based on the commitments made during qualification of the use of the code, the uncertainty associated with the calculated inventory. If the licensee commits to a program of additional validation, the license should provide the calculated uncertainty value in accordance with its commitment. If the licensee justifies the use of the values in this TER as uncertainty estimates, then the licensee would estimate the uncertainty using these multipliers.

4.3.2 LLW Disposal Facility Operator/Applicant Usage

An LLW disposal facility applicant or operator should certify that they are using the 3R-STAT TR in accordance with the provisions of this TER, in a letter to the NRC or the applicable Agreement State regulatory authority.

An LLW disposal facility applicant should contact operating reactors for historical short-lived iodine sample data. Using these data the applicant should calculate the historical release rate from the representative reactors.

Using these historical release rates the applicant should estimate the future activity of ^{129}I and ^{99}Tc expected at the disposal site during the operating period.

An applicant should identify and justify the use of uncertainty estimates on the fuel-cycle-specific release rates generated in the estimate of future inventories.

An applicant should calculate an uncertainty associated with the total inventory calculated by 3R-STAT and ensure that the requirements of 61.12(i) regarding waste description have been fulfilled.

An applicant should consider and estimate quantities of these isotopes to be received from other generators, not using 3R-STAT.

The applicant should identify and justify the use of the estimate and uncertainty in the license application.

An LLW disposal facility operator should ensure waste received from a generator using the TR is classified and manifested in accordance with the regulations and guidance.

An operator should identify waste manifest data which are superseded by data provided by generators using this TR.

An operator should add the 3R-STAT inventories reported to the inventory of these isotopes received from other generators that do not or cannot use 3R-STAT.

An operator should evaluate the uncertainty of the 3R-STAT estimates and justify the use of the values used in such an evaluation.

An operator should describe and justify the use of the estimate, and the uncertainty on the estimate, in its reports to the appropriate regulatory authority (e.g., in site closure performance assessments).

An LLW disposal facility operator or applicant using the code in support of a licensing action will generate, based on either historical information provided by nuclear power plant licensees or on estimates of fuel-cycle-specific released inventories, an estimate of the facility inventory of ^{129}I and ^{99}Tc. This facility inventory will be the sum of the independent fuel-cycle-specific inventories provided or assumed along with the estimates based on waste manifests from other generators (non-3R-STAT users). The uncertainty of the facility estimate will depend on the uncertainty on the individual fuel-cycle-specific estimates, the estimates, and the number of estimates, in addition to any uncertainty on the manifest information being used.

The LLW disposal facility operator calculating current inventory will collect the information provided by the generators using 3R-STAT and calculate a sum of those independent fuel-cycle-specific estimates to determine total inventory from these generators. This inventory will be added to the inventory from generators not using 3R-STAT and a total site inventory determined. The LLW disposal facility operator should justify and calculate an uncertainty with regard to the inventory from the 3R-STAT users; justification for using the uncertainty estimates/ranges reported with the inventory estimates should be provided.

4.3.3 3R-STAT Vendor Usage/Requirements

The 3R-STAT vendor, Vance and Associates, Inc. (V&A), should maintain a control log of the 3R-STAT users.

V&A should submit a change to the code, using the procedures described in the TR, providing a routine to implement the limit on residual error discussed in section 3.2.3.5.

V&A should submit an application to NRC for each modification to the code which falls outside the scope of the criteria identified in section 3.2.4.3.

V&A should distribute to those receiving controlled copies of the TR any changes that fall within the scope of the criteria identified in section 3.2.4.3.

V&A should provide the final TR to NRC incorporating the TER and review questions and all the changes identified in this TER.

5.0 REFERENCES

1. Olander, D. R., "Combined Grain-Boundaries and Lattice Diffusion in Fine-Grained Ceramics," Advances in Ceramics, Vol. 17, 1986.

2. Turnbull, J., et al., "The Diffusion Coefficients of Gaseous and Volatile Species during the Irradiation of Uranium Dioxide," Journal of Nuclear Materials, Vol. 107, 1982.

APPENDIX A

Uncertainty in a LLW Disposal Facility Inventory Calculated Using the 3R-STAT TR Methodology

BACKGROUND

The 3R-STAT TR provides a methodology for quantifying the uncertainty in fuel cycle specific estimates of two isotopes. The uncertainty in the estimates generated in the topical report is based on the calculated geometric means and geometric standard deviations of the multiplicative bias for I-129 and Tc-99 based on pairs of code calculations and measurements. The V&A approach has a shortcoming; it does not reflect the uncertainty in the data. The V&A TR provides 95 percent one-sided underprediction intervals for individual fuel cycle biases, assuming that the calculated geometric means and standard deviations are the **true** values. As the reported values are **sample** values, a correct approach is a tolerance interval approach, which reflects the uncertainty in the estimated geometric means and standard deviations.

The 3R-STAT TR suggests a similar methodology for quantifying the uncertainty in LLW disposal facility inventories of two isotopes. According to the TR, the uncertainty in LLW inventories expected at LLW disposal sites is based on values of fuel cycle-specific information coming from waste generators. According to the TR approach, the uncertainty in the calculated LLW disposal facility inventory (the sum of the individual fuel cycle specific values) would be appropriately quantified, i.e., with a 95 percent prediction interval. However, a correct methodology must be used to calculate such an interval. The TR provides an example of such a quantification. However, because insufficient detail is provided, it is not possible to evaluate the methodology used in the TR.

As described in the technical evaluation report (TER), a LLW disposal facilty applicant should provide a description and justification for the uncertainty associated with ^{129}I and ^{99}Tc inventories calculated using the TR methodology. The TR suggests that the appropriate quantification is a 95 percent one-sided prediction interval applied to the calculated total facility inventory, based on individual fuel cycle-specific information, from power reactor waste generators in a compact. The methodology for calculating such a prediction interval, based on the bias in the incoming shipments, is described in this discussion. The assessment of the total inventory using $\bar{r}$ and s from the TR in an application should follow this discussion.

DISCUSSION

1. Individual Fuel Cycle Bias

Given:

$c_i(\Delta t_i)$ = calculated value for fuel cycle (i) based on Δt_i
$m_i(\Delta t_i)$ = measured value for fuel cycle (i) based on Δt_i.

The bias in the calculated fuel cycle value ($r_i(\Delta t_i)$), indexed by (i)[1], is:

$$r_i(\Delta t_i) = \frac{c_i(\Delta t_i)}{m_i(\Delta t_i)} \quad . \tag{1}$$

Assume that the biases (r_i) (we drop the (Δt_i) for convenience) have a lognormal distribution. Then equation (1) can be expressed:

$$\ln r_i = \ln c_i - \ln m_i \quad . \tag{2}$$

Further, the geometric mean $\bar{r}$ of the sample is given by:

$$\ln \bar{r} = \frac{1}{n} \sum_i \ln r_i \tag{3}$$

where n is the number of observations[2],

and the geometric standard devation (s) of the sample is given by:

$$s^2 = \frac{1}{n-1} \sum_i (\ln r_i - \ln \bar{r})^2 \quad . \tag{4}$$

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[1] These values come from the fuel cycles which were actually measured in the TR validation. These values should be justified by the applicant.

[2] Based on the TR validation data.

Assume that the bias r has a lognormal distribution. Then ln (r) has a normal distribution. Using the sample values as though they were the true mean and standard deviation of ln (r), an approximate lower 95% prediction interval for the observed value of ln (r) is given by:

$$L(95\%) = \ln(\bar{r}) - 1.645\,(s) \tag{5}$$

where:

1.645 = the 95th percentile of a standard normal distribution.

Equation (5) yields an approximate prediction interval because ln ($\bar{r}$) and s are only approximations of the true values.

A comparison between the approximate 95% prediction interval and a 95%/95% tolerance interval for individual fuel cycle bias values demonstrates that the approximate underprediction interval is the same order of magnitude as the tolerance interval. These values have been converted to multiplicative factors. From the review of the TR:

	^{129}I	^{99}Tc
sample size (n)	23	20
approx. 95% one sided prediction interval	3.29	10.9
95%/95% tolerance interval	5.88	40.1

2. Total Disposal Facility Bias

We now show how the total bias can be estimated based on the calculated fuel cycle values only. Let c_j be the calculated value for entire fuel cycle (j).

The calculated total inventory is:

$$C = \sum_j c_j \tag{6}$$

Similarly, the measured total inventory is:

$$M = \sum_j m_j \tag{7}$$

where m_j is the hypothetical measured value.

The bias (R) in the total inventory is defined by:

$$R = \frac{C}{M} \quad . \tag{8}$$

From equations (1), (7), and (8), the bias in the total facility inventory is:

$$R = \frac{C}{\sum_j \frac{c_j}{r_j}} \quad . \tag{9}$$

Equation (9) defines the bias (R) as a function of the individual fuel cycle biases (r_j). We wish to find an underprediction bound (B) such that:

$$\text{Prob}\ \{\ R > B\ \} = .95 \quad .$$

Since

$$\text{Prob}\ \{\ R < B\ \} = .05$$

B is the 5th percentile of the distribution of the bias R. This distribution can be approximated in one of two ways.

(1) Assume the r_j in equation (9) are independently and lognormally distributed with geometric mean and geometric standard deviation given by $\bar{r}$ and s. Then evaluate the distribution by simulation and estimate B.

(2) Assume the r_j in equation (9) have the same empirical distribution given by the (n) values of $r_i(\Delta t_i)$. Then evaluate the distribution by simulation and estimate B.

SUMMARY

As can be seen, the relative difference between the individual fuel cycle approximate prediction and tolerance intervals are between a factor of 2 and 4 for iodine and technecium, respectively. However, for the purposes of providing uncertainty estimates on individual fuel cycles the differences are not significant. Additionally, in finding an underprediction bound for the total inventory from multiple independent fuel cycles, the error in using the sample values as though they were true values is likely to be less.