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Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages

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U.S. Nuclear Regulatory Commission

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ABSTRACT

This report provides recommendations on preparing the criticality safety section of an application for approval of a transportation package containing fissile material. The analytical approach to the evaluation is emphasized rather than the performance standards that the package must meet. Where performance standards are addressed, this report incorporates the requirements of 10 CFR Part 71.

CONTENTS

Page

LIST OF FIGURES

LIST OF TABLES

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1 INTRODUCTION

1.1 BACKGROUND

This report provides recommendations on preparing the criticality safety section of an application for approval of a transportation package containing fissile material. This report was prepared in consultation with the staff of the Spent Fuel Project Office of the U.S. Nuclear Regulatory Commission (NRC).

Packages used to transport fissile and Type B quantities of radioactive material are designed and constructed to meet the performance criteria specified in Title 10 of the Code of Federal Regulations, *Part 71–Packaging and Transportation of Radioactive Material* (10 CFR Part 71).[1] To assist an applicant in preparing an application for approval of such packaging, the NRC issued Regulatory Guide 7.9, *Standard Format and Content of Part 71 Applications for Approval of Packaging for Radioactive Material* (Standard Format Guide).[2] The Standard Format Guide indicates the information to be provided in the application and establishes a uniform format for presenting that information. This report (NUREG/CR-5661) supplements Chapter 6, *Criticality*, of the Standard Format Guide. This report should not be considered a substitute for referring to the Standard Format Guide or to 10 CFR Part 71.

1.2 PURPOSE AND SCOPE

The purpose of this report is to clarify the design information and analysis information that should be included in the criticality safety section of an application for approval of a package. This report also recommends an acceptable analytical approach for performing the criticality safety evaluation. The criticality calculations performed herein use the SCALE code system[3] to illustrate the analysis approach. However, the report does not endorse any particular computational tool and stresses that any computational tools (SCALE system or any other code) used in the evaluation must be demonstrated as valid for the criticality safety analysis of the specific package design.

In this report, the performance requirements of 10 CFR Part 71 or the Standard Format Guide have not been emphasized; it is assumed that the reader is familiar with these documents. The completed criticality evaluation should address and demonstrate compliance with all applicable performance requirements, and the application should follow the Standard Format Guide. Sections 2 through 6 of this report have been compiled assuming that the recommendations in this report will be implemented in an application that has been prepared to demonstrate compliance with the requirements of 10 CFR Part 71 and in accordance with the Standard Format Guide.

1.3 SUMMARY RECOMMENDATIONS

This report recommends information and assumptions to be considered in the criticality section of an application for approval of a transportation package. A summary of these recommendations is listed below. The list provides the information and assumptions that should be considered; additional information and/or assumptions may need to be considered depending on the package design and the approach used in the safety evaluation.

1. Provide a complete description of the contents and the packaging (including maximum and minimum mass of all materials, maximum ^{235}U enrichment, physical parameters, type, form, and composition). See Sect. 2 for more details.

2. Provide a description (including sketches with dimensions and materials) of the calculational models, point out the differences between the models and actual package design, and discuss how these differences affect the calculations. See Sect. 3 for more details.

3. For packages equipped with fixed neutron absorbers, assume no more than 75% of the minimum neutron absorber content, unless comprehensive acceptance tests are implemented that are capable of verifying the presence and uniformity of the neutron absorber. See Sect. 3.1.3.

4. Demonstrate and consider the most reactive content loading and the most reactive configuration of the contents, the packaging, and the package array in the criticality evaluation. For spent fuel packages, assume unburned (fresh) fuel isotopic concentrations; however, do not take credit for any fixed burnable absorbers in the fuel. See Sects. 3.2–3.4 for more details.

5. Provide a description of the code(s) and cross-section data used in the safety analysis, together with references that provide complete information. Discuss software capabilities and limitations of importance to the criticality safety evaluations. See Sect. 4 for details.

6. Use appropriate validation procedures to justify the bias and uncertainties associated with the calculational method. In addition to the bias and uncertainties, the NRC position is that transportation packages should have a minimum administrative subcritical margin of 0.05 Δk. See Sect. 5 for more details.

7. For the following cases, demonstrate that the effective neutron multiplication factor (k_{eff}) calculated in the safety analysis is limited to 0.95 after consideration of appropriate bias and uncertainties (see Sect. 5.4).

   a. a **single package** with optimum moderation within the containment system, close water reflection, and the most reactive packaging and content configuration (consistent with the effects of normal conditions of transport or hypothetical accident conditions, whichever is more reactive);

   b. an **array of 5N undamaged packages** (packages subject to normal conditions of transport) with nothing between the packages and close water reflection of the array; and

   c. an **array of 2N damaged packages** (packages subject to hypothetical accident conditions) if each package were subjected to the tests specified in §71.73, with optimum interspersed moderation and close water reflection of the array.

   See Sects. 3.4 and 6.1–6.2 for more details.

8. Calculate and report the transport index (TI) for criticality control based on the value of N determined in the array analyses. See Sect. 6.3 for more details.

9. Provide sufficient information in the application to support independent analyses without reference to external documents.

2 PACKAGE DESCRIPTION

The criticality section of the application for approval of a transportation package should include a description of the packaging and its contents. Descriptions of the packaging and contents should be consistent with the engineering drawings and with other figures and text provided in other sections of the application. Other sections of the application may be referenced to ensure consistency and to limit duplication. However, a description of the package sufficient for understanding the criticality evaluation should be provided without reference to other sections. This description should focus on the package dimensions and material components that can influence k_{eff} (e.g., fissile material inventory and placement, neutron absorber material and placement, reflector materials), rather than structural information such as bolt placement and trunnions. This section of the report clarifies the information that is expected in the criticality safety section of the application.

2.1 CONTENTS

The criticality safety section of the application should have a complete and detailed description of the contents of the packaging. This should include content quantities, dimensions, and configurations that are most limiting in terms of criticality safety. The application should clearly state the full range of contents for which approval is requested. Thus parameter values (e.g., maximum ^{235}U enrichment, multiple fuel assembly types, fuel pellet diameter, fuel masses) needed to bound the packaging contents within prescribed limits should be provided. For packages with multiple loading configurations, each configuration should also be specifically described, including all possible partial-load configurations. The description of the contents should include

1. the type of materials (e.g., fissile and nonfissile isotopes, reactor fuel assemblies, packing materials, and neutron absorbers),

2. the form and composition of materials (e.g., gases, liquids, and solids as metals, alloys, or compounds),

3. the quantity of materials (e.g., masses, densities, ^{235}U enrichment, isotopic distribution, H/X, and C/X), including tolerances for any nominal values given, and

4. other physical parameters (e.g., geometric shapes, configurations, dimensions, orientation, spacing, and gaps), including tolerances for any nominal values given.

The criticality safety section of the application should also describe the configuration of the contents after the package has been subjected to the hypothetical accident conditions. Appropriate references to the structural and thermal sections of the application should be made. Any changes from the normal conditions content configurations should be described.

2.2 PACKAGING

The criticality section of the application should include a description of the packaging with emphasis on the design features pertinent to the criticality safety evaluation. The features that should be emphasized are

1. the materials of construction and their relevance to criticality safety,

2. pertinent dimensions and volumes, including tolerances and allowable deviations,

3. the limits on design features relied on for criticality safety (e.g., minimum dimensions for fixed neutron absorbers, minimum loading of neutron absorber material, minimum separation distances), and

4. other design features that contribute to criticality safety.

The application should also describe the configuration of the packaging after the package has been subjected to the hypothetical accident conditions. Appropriate references to the structural and thermal sections of the application should be made. Any changes from the normal condition packaging configuration which may affect the criticality evaluation should be described.

2.3 SPECIFICATION OF TRANSPORT INDEX

The application should specify the TI for criticality control. The TI is the dimensionless number (rounded up to the next tenth) that designates the degree of control (e.g., limits package accumulation) to be provided by the carrier. The TI is defined by 10 CFR Part 71 to address concerns for radiation protection (TI value is maximum dose in millirem per hour at 1 m from the package surface) and criticality control. The TI for criticality control is calculated by dividing 50 by the number "N." The number "N" used to determine the TI for criticality control is derived from separate consideration (see Sects. 6.2 and 6.3) of the number of damaged and undamaged packages that can be adequately subcritical in an array subject to the conditions of 10 CFR § 71.59(a).

3 CRITICALITY SAFETY ANALYSIS MODELS

The application for approval of transportation packages should provide specific information on all calculational models used to perform the criticality safety evaluation. This section provides recommendations on the information that should be provided for each calculational model.

3.1 GENERAL

The applicant should perform criticality safety analysis for single packages and arrays of packages. In each case, the package conditions under normal conditions of transport (i.e., an undamaged package) and the package conditions under hypothetical accident conditions (i.e., damaged package) should be considered. For each evaluation, a calculational model should be developed. An exact model of the package may not be necessary. However, the calculational models should explicitly include the physical features important to criticality safety. Also, any modeling approximations should be shown to be conservative or essentially neutral relative to a more exact model.

The applicant should provide three types of calculational models: contents models, the single-package models, and package array models. The contents models should include all geometric and material regions out to the containment boundary (or to a convenient boundary, such as the strongback of a fresh fuel assembly package). Each contents model should dimensionally fit inside the undamaged and damaged package models used in the single-package and package array evaluations. Additional calculational models may be needed to describe the range of contents or the various array configurations or damage configurations that should be analyzed.

The criticality section of the application should contain a detailed description of the calculational models. Sections 3.1.1 through 3.1.4 discuss the items that should be included with the description of the calculational models.

3.1.1 Sketches

The criticality section of the application should include simplified, dimensioned sketches of the calculational models. Sketches drawn specifically for the various portions of the model are preferable to engineering drawings. However, the sketches should be consistent with the engineering drawings. Any differences with the engineering drawings, or with other figures in the application, should be noted and explained.

The sketches should be simplified by limiting the dimensional features on each sketch and by providing multiple sketches, with each sketch building on the previous one. Multiple sketches for each calculational model may be necessary to show sufficient detail. Also, multiple sketches may be necessary to show different undamaged and damaged package configurations.

3.1.2 Dimensions

The sketches discussed in Sect. 3.1.1 should show the dimensions that are used in the calculations (see examples in Appendix A). Any difference between dimensions used in the sketches and those in the engineering drawings, or other figures of the application, should be noted and explained. The dimensions on the sketches should be specified in both SI and English units.

The criticality section should address dimensional tolerances of the packaging, including components containing neutron absorbers. When developing the calculational models, adjustments should be made for tolerances that tend to add conservatism (i.e., produce higher k_{eff} values). For example, subtraction of the negative tolerance from the nominal wall thickness of steel should be conservative for array calculations and may have no significant effect on the single-package calculation.

3.1.3 Materials

The range of material specifications (including tolerances and uncertainties) for the packaging and contents should be addressed in the criticality section of the application. Specifications and tolerances for all fissile materials, neutron-absorbing materials, materials of construction, and moderating materials should be confirmed with the engineering drawings of the packaging or the specified design criteria. The range of material specifications should be used to select parameters that produce the highest k_{eff} value consistent with normal and hypothetical accident conditions. For example, the ^{235}U enrichment of the fuel should be maximized, while the ^{10}B enrichment of a neutron poison component should be minimized. In practice, the effect of small variations in dimensions or material specifications may also be considered by determination of a reactivity allowance that covers the k_{eff} change due to the parameter changes under consideration. This additional reactivity allowance should be positive and included as an additional element of the calculational uncertainty (see Sect. 5.4).

For each calculational model, the atom density of any neutron absorber (e.g., boron, cadmium, or gadolinium) added to the packaging for criticality control should be limited to 75% of the minimum neutron absorber content specified in the application. This minimum neutron absorber content should be verified by chemical analysis, neutron transmission measurements, or other acceptable methods. A percentage of neutron absorber material greater than 75% may be considered in the analysis only if comprehensive acceptance tests, capable of verifying the presence and uniformity of the neutron absorber, are implemented. The adequacy of these tests will be considered on a case-by-case basis. Use of independent tests that verify the presence of the absorber material and adequate demonstration that the tests have appropriate sensitivity to the quantities of concern (presence and uniformity of absorber constituents) are issues that should be considered.

Limiting added absorber material credit to 75% without comprehensive tests is based on concerns for potential "streaming" of neutrons due to nonuniformities. It has been shown that boron carbide granules embedded in aluminum permit channeling of a beam of neutrons between the grains and reduce the effectiveness for neutron absorption. The experimental work of Refs. 4 and 5 shows that for a monoenergetic neutron beam, the granulated boron carbide areal density of 0.040 g/cm^2 of ^{10}B is equivalent to a homogeneous areal density of 0.033 g/cm^2 of ^{10}B. The efficiency of boron as a neutron absorber allows credit for only 75% of the poison to be a manageable value for most transportation package designs. The 75% value demonstrated by this work is conservative for several reasons: (1) many neutron poisons tend to be distributed homogeneously through a component of the packaging and are not distributed in a granular fashion, and (2) the experimental work is based on the use of a monodirectional beam of neutrons, while in most package designs an isotropic source of neutrons will be impinging on the wall (thus reducing the potential for intragranular transmission). Nevertheless, the 75% value is a prudent value consistent with demonstrated percentages found in experimental work.

A table should be provided in the application that identifies all of the different material regions in the criticality safety calculational models. This table should list the following for each region: the material in each region, the density of the material, the constituents of the material, the weight percent and atom density of each constituent, the region mass represented by the model, and the actual mass of the region (consistent with the contents and packaging description discussed in Sect. 2). The materials, densities, and masses provided in the sketches should be consistent with the corresponding items in the engineering drawings and should have the same numerical values used in the input of the calculational method. For each sketch representing a portion of the calculation model, there should be a corresponding subsection discussing the material compositions and densities of each region shown in the sketch. All density values that are used, whether input by the analyst or retrieved by the code from a software database, should be reported in the application.

The source of all material density values should be reported. If a density value other than that found in standard references (e.g., materials or engineering handbook) is used in the calculation, the applicant should explain why the density is different, how the value was determined, and how the value affects the k_{eff}. Compositional differences should also be discussed.

3.1.4 Differences Between the Models and the Actual Package Configuration

The calculational models described in the criticality safety section of the application should be consistent with the undamaged and damaged package configurations as described in other sections (general, structural, thermal) of the application. Any differences (e.g., in dimensions, material, geometry) between the calculational models and the package configurations should be identified. The applicant should show how these different values (in dimensions, densities, etc.) were determined and justify the values used in the calculational models. Also, the applicant should discuss and explain how the differences impact the calculated k_{eff} values.

3.2 CONTENTS MODELS

The contents model should provide a detailed description of the packaging contents as they are assumed to be configured in the single-package and package array calculations. Models that show the contents under normal conditions of transport and under hypothetical accident conditions should be included in the application. A contents model representing each of the different loading configurations (full- and partial-load configurations) should also be provided. A single-contents model that will encompass different loading configurations should be considered only if the justification is clear and straightforward.

Each contents model should provide a description of the fissile contents of a package in its most reactive configuration, consistent with its physical and chemical form within the containment vessel under the normal or hypothetical accident conditions considered by the model. If the contents can vary over some parameter range (e.g., mass, enrichment, spacing), the criticality safety analysis should demonstrate that the model describes and uses the parameter specification that provides the maximum k_{eff} value under normal and hypothetical accident conditions. In designing the calculational models, tolerances that tend to add conservatism (i.e., produce higher k_{eff} values) should be included. Any assumed fissile material distribution that limits the maximum k_{eff} of the package contents should be justified.

The contents models for packages that transport loose pellets should ensure that variations in pellet size and spacing are considered in determining the configuration that produces the maximum k_{eff} value. The maximum pellet enrichment should be considered in the criticality safety evaluation. Fuel elements should consider the actual fuel pin spacing provided by the element.

At this time, the NRC does not accept burnup credit for spent fuel transportation packages. Therefore, unburned (fresh) fuel isotopics should be considered in the evaluation of packages containing spent fuel; however, no credit should be taken for any fixed burnable absorbers in the fuel when the fuel has been irradiated.

Other fissile materials should assume a particle spacing that results in maximum reactivity. Packages that transport isotopic waste containing fissile material should ensure that the limiting concentration and/or mix of fissile material is used in the safety analysis. Contents that are unknown or uncertain must be assumed to have a value that maximizes k_{eff}.

3.3 SINGLE-PACKAGE MODELS

The single-package models, together with the contents model(s), should depict the configuration of the packaging and contents under normal conditions of transport and under hypothetical accident conditions. These models should be those used to demonstrate that a single package remains adequately subcritical (see Sect. 5.4) per the requirements of 10 CFR § 71.55. The calculational model (single-package and contents model) for the single-package evaluation should consider the following items:

1. The undamaged single-package model should represent the physical condition of a package subjected to the test specified in 10 CFR § 71.71 (normal conditions of transport).

2. The damaged single-package model should represent the physical condition of a package subjected to the tests specified in 10 CFR § 71.73 (hypothetical accident conditions).

3. The packaging and contents should be in the most reactive configuration consistent with the chemical and physical form of the material. Determination of the most reactive configuration should account for the effects of both the normal and hypothetical accident conditions. In development of the damaged package models, the applicant should consider (a) the change in internal and external dimensions due to impact; (b) loss of material, such as neutron shield or wooden overpack, due to the fire test; (c) rearrangement of fissile material or neutron absorber material within the containment system due to impact, fire, or immersion; and (d) the effects of temperature changes on the package material and/or the neutron interaction properties.

4. Water moderation should be considered to occur to the most reactive extent possible. Partial flooding or preferential flooding (i.e., uneven flooding among the regions of a package to the most reactive extent), if possible, should be considered. If the contents are cladded fuel rods, flooding of the pellet-to-clad-gap regions should be considered. If fuel rods or pellets are annular, flooding of the annulus should also be considered, even if the rods or pellets are cladded. Moderation by other packaging materials should also be considered.

5. The containment system should be reflected closely on all sides by at least 30 cm of water. Package materials that are present and are better reflectors than water should be considered. For example, a lead shield around the containment system may provide more effective reflection than water.

In many cases, one model can be used to envelop both the undamaged and the damaged single-package models. If only one model is used in the single-package analysis, the applicant should justify that this model bounds the most reactive undamaged and damaged configuration of the package.

3.4 PACKAGE ARRAY MODELS

The package array models should depict the arrangements of packages that are used in the calculations necessary to fulfill the requirements of 10 CFR § 71.59. At least two array models are needed: an array of

5N undamaged packages (normal conditions of transport) and an array of 2N damaged packages (hypothetical accident conditions). The configuration of the individual packages (undamaged and damaged) used in the respective array models should be the worst case for the array of packages, which may not be the same as the worst case for a single package. The dimensions of the array that provides the limiting subcritical k_{eff} value should be determined as described in Sect. 6.2. The calculational models for the array analysis should consider the following items:

1. The applicant should demonstrate that the most reactive array configuration has been considered in the criticality safety evaluation. The exact lattice arrangement may be represented by a simplified arrangement if justification is provided.

2. The applicant should consider all types of array arrangements. Often an array model that provides the lowest surface-to-volume ratio (typically one with equal dimensions on each side of the array) is a good initial arrangement because this model should minimize neutron leakage from the array (see Sect. 6.2).

3. The array of packages should be reflected on all sides by a close-fitting water reflector at least 30 cm thick.

4. The following criteria for moderation in the containment system should be assessed and separately applied for normal conditions of transport and hypothetical accident conditions. Optimum moderation is the condition that produces the highest k_{eff} value over the range of moderation conditions. Sources of moderation in the containment system are water leaking into the containment system, and the packaging materials and contents inside the containment system.

   Typically, the analysis for the array of undamaged packages can assume that the packages are dry internally, provided that there is no water leakage into the package, including the containment system, when the package is subjected to the tests specified in 10 CFR § 71.71.

   The analysis for the array of damaged packages should assume water leakage into the containment system to the most reactive degree. For those cases where water inleakage is not assumed, the application must adequately demonstrate that water inleakage would not occur under hypothetical accident conditions. The adequacy of such demonstrations will be assessed on a case-by-case basis. The acceptance criteria for these demonstrations are beyond the scope of this report.

   Regardless of whether water inleakage is assumed, internal moderation provided by the materials and contents (e.g., plastics, foam, impurities, or residual moisture in the fuel) in the package should be considered when determining optimum moderation. If the moderation provided by the packaging materials or contents overmoderates the package contents, and by its physical and chemical form cannot leak from the containment vessel, then its overmoderating properties can be considered in the model. For example, a solid moderator which is shown to overmoderate the fissile material can be considered in the calculational model if its continued presence is demonstrated under normal conditions of transport and hypothetical accident conditions.

5. If there can be leakage of water into the package, then partial and preferential flooding should be considered in determining optimum moderation. For fuel with pellet-to-clad gaps, flooding of the gap region should be considered.

6. Optimum interspersed hydrogenous moderation should be determined in the evaluation of arrays of damaged packages. Optimum interspersed moderation is the degree of hydrogenous moderation between packages that results in the highest k_{eff} value. In addition to interspersed moderation, moderation in regions of the package outside the containment system should also be considered if these regions consist of voids, hydrogenous or other moderating materials, or water-absorbing materials (e.g., foam, wood). The overmoderating or "isolating" effect of a packaging material may be considered, provided that the material remains in place and maintains its overmoderating or "isolating" properties under hypothetical accident conditions. Note that moderation between packages, moderation in regions of the package outside the containment system, and moderation within the containment system need to be considered concurrently to the most reactive extent.

4 METHOD OF ANALYSIS

This section of the report discusses the information that should be supplied on the computer code, nuclear cross-section data, and technique used to complete the criticality safety evaluation.

4.1 COMPUTER CODE SYSTEM

The computer codes used in the safety evaluation should be identified and described in the application or adequate references should be included. Verification that the software is performing as expected is important. The applicant should identify all hardware and software (titles, versions, etc.) used in the calculations as well as pertinent configuration control information. Correct installation and operation of the computer code should be demonstrated by performing and reporting (in the application or by reference) the results of the sample problems or general validation problems provided with the software package. Capabilities and limitations of the software that are pertinent to the calculational models should be discussed with particular attention to limitations that may affect the calculated k_{eff} value.

Computational methods that fully consider the anisotropic angular terms of the Boltzmann radiation transport equation are preferred for use in criticality safety analysis. The deterministic discrete-ordinates technique and the Monte Carlo statistical technique are the most rigorous and flexible techniques available to consider the anisotropic scattering terms. These techniques solve, respectively, the differential and integral eigenvalue (e.g., the k_{eff} value) form of the Boltzmann equation. Monte Carlo analyses are prevalent because these codes can better model the geometry detail needed for most criticality safety analyses. Well-documented and well-validated computational methods, such as those provided in the SCALE code system,[3] may require less description than a limited-use and/or unique computational method. The use of computational methods that limit or eliminate the angular terms in the Boltzmann equation (e.g., diffusion theory) or use simpler methods to estimate k_{eff} should be thoroughly justified.

When using a Monte Carlo code, the applicant should consider the imprecise nature of the k_{eff} value provided by the statistical technique. Every k_{eff} value should be reported with a standard deviation, σ. Typical Monte Carlo codes provide an estimate of the standard deviation of the calculated k_{eff}. The applicant may wish to obtain a better estimate for the standard deviation (Monte Carlo code estimates typically underpredict σ) by repeating the calculation with different valid random numbers and using this set of k_{eff} values to estimate σ_o. If fewer than 20 to 25 k_{eff} values are provided in the set, the estimation of σ should be calculated using the student-t distribution formula. Also, because of the statistical nature of Monte Carlo methods, this method should not be used to determine changes in k_{eff} due to small problem parameter variations. The change in k_{eff} due to a parameter change should be statistically significant (greater than at least 3σ) to indicate a trend in k_{eff}.

The geometry model limitations of deterministic discrete-ordinates methods typically restrict their applicability to calculation of bounding, simplified models and investigation of the sensitivity of k_{eff} to changes in system parameters. These sensitivity analyses can use a model of a specific region of the full problem (e.g., a fuel pin or homogenized fissile material unit surrounded by a detailed basket model) to demonstrate changes in reactivity with small changes in model dimensions or material specification. Applicants should consider such analyses when necessary to ensure or demonstrate that the full package model has utilized conservative assumptions relative to calculation of the system k_{eff} value. For example, a one-dimensional fuel pin model may be used to demonstrate the reactivity effect of tolerances in the clad thickness.

4.2 CROSS SECTIONS AND CROSS-SECTION PROCESSING

The calculational method consists of both the computer code and the neutron cross-section data used by the code. The criticality safety evaluation should be performed using cross-section data that are derived from measured data involving the various neutron interactions (e.g., capture, fission, and scatter). Although not infallible, unmodified data processed from compendiums of evaluated nuclear data (e.g., the various versions of the Evaluated Nuclear Data Files in the United States or the Joint European Files) should be considered as the major sources of such data.

The neutron cross-section data and any codes used to process the data for the criticality safety analyses should be identified, described, and referenced in the application. The codes used to process the data are subject to the same recommendations provided in the initial paragraph of Sect. 4.1. The application should identify the source of the neutron cross-section data (e.g., specific version of an evaluated nuclear data file) and supply pertinent references that document the content of the cross-section library, the procedure used to generate the cross-section library, and its range of applicability. Verification that the data library consists of the cross-section data described and referenced in the application is important. The applicant should demonstrate correct installation and operation of the data library by performing and reporting the results of any sample problems or general validation problems provided with the software package. Capabilities and limitations of the data library that are pertinent to the calculational models should be discussed with particular attention to discussing limitations that may affect the calculations. For example, the 123-group library once provided in the SCALE code package did not have resonance data for ^{235}U. Although not an issue for low-enriched, well-moderated systems that the library was generated to analyze, this lack of data made the library inappropriate for high-enriched, low-moderation systems.[6]

Continuous energy and multienergy-group (multigroup) cross-section libraries are acceptable. The number of energy groups and the energy boundaries of each group should be specified for a multigroup library. Known limitations (e.g., omission or limited range of resonance data, limited order of scattering) that may affect the analysis should be provided. The temperature range over which the cross-section data are applicable needs to be considered in the analyses and specified in the application. For multigroup cross sections, the order of scatter available on the library and applied in the calculation should be indicated. For continuous energy data, the number of points in the nuclide set should be specified. Computer programs and methods used to perform functions such as cross-section mixing for problem materials, problem-dependent resonance self-shielding, or cell-weighting of mixtures to represent heterogeneous configurations should be identified and discussed consistent with the recommendations of Sect. 4.1.

Any special techniques used in the analysis to improve the adequacy or use of the cross-section data should be discussed. For example, the SCALE system sequences automatically perform a problem-dependent resonance calculation for only one type of unit cell within a lattice. If deemed important, resonance-corrected data for materials outside the lattice, or for other types of unit cells within the lattice, can be calculated separately and provided via an optional input field.

4.3 CODE INPUT

All major code input parameters or options used in the criticality safety analysis should be identified and discussed in the application. This identification and discussion of code input should be provided in addition to the actual case inputs (or at least a sampling of the inputs for the various types of calculational models). For a Monte Carlo analysis, the applicant should indicate, among other things, the neutron starting distribution, the number of histories tracked (number of generations and particles per generation), boundary conditions selected, order of scatter selected (for multigroup codes), any special reflector treatment, and any special biasing option. For a discrete-ordinates analysis, the applicant should specify the spatial mesh used in each region, the angular quadrature used, the order of scatter selected, the boundary conditions selected, and the flux convergence criteria. Any of these input parameters can influence the accuracy of the results; therefore, the selection of the input values should be carefully considered and, to the extent possible, be consistent with the data used in the validation analyses.

4.4 ADEQUACY OF CALCULATION

The criticality safety section of the application should review and discuss calculational issues that are important in ensuring an accurate k_{eff} value is obtained. Adequate problem-dependent treatment of multigroup cross sections, use of sufficient cross-section energy groups (multigroup) or data points (continuous energy), and proper convergence of the numerical results are examples of issues the applicant may need to review and discuss in the criticality section of the application. To the degree allowed by the code, the applicant should demonstrate or discuss any checks made to confirm that the calculational model prepared for the criticality safety analysis is consistent with the code input. For example, code-generated plots of the geometry models and outputs of material masses by region may be beneficial in this confirmation process. The statistical nature of Monte Carlo calculations is such that there are no fixed rules, criteria, or tests for judging when calculational convergence has occurred. Thus the applicant should discuss the code output or other measures used to confirm the adequacy of convergence. For example, many Monte Carlo codes provide output edits that should be reviewed to determine adequate convergence, including:

1. the k_{eff} by generation run,
2. plot of average k_{eff} by generation run,
3. final k_{eff} edit table by generation skipped,
4. plot of k_{eff} by generation skipped, and
5. frequency distribution bar graph.

Other conditions in the output that may indicate a convergence problem should be reviewed, for example,[7]

1. upward or downward trends in k_{eff} by generation run over the last half of the total generations,
2. upward or downward trends in k_{eff} by generation for the first half of generations skipped,
3. sudden changes of greater than one standard deviation in either k_{eff} plot,
4. abnormally high or low generation k_{eff} (±20% of calculated mean), and
5. a calculated result that is not consistent with expected results based on previous experience (may be indicative of other problems).

It is also advisable to check for adequate sampling of isolated fissile regions by examining the printed regionwise fission event data and associated statistics.

If necessary, the applicant should review the code documentation as well as literature (such as Refs. 7 and 8) to obtain practical discussions on the uncertainties associated with Monte Carlo codes used to calculate k_{eff} and advice on output features and trends that should be observed. If convergence problems were encountered by the applicant, a discussion of the problem and the steps taken to obtain an adequate k_{eff} value should be provided. For example, calculational convergence may be achieved by selecting a different neutron starting distribution or running additional neutron histories. Modern personal computers and workstations allow a significant number of particle histories to be tracked; a minimum of 200,000 histories is now typical.

As a minimum, portions of output (such as the plots of k_{eff} by generation run and k_{eff} by generation skipped) from selected cases should be included in the application. In selecting the output to provide, the applicant should consider that the goal is to demonstrate that the calculations have been performed as described and run to successful completion.

5 VALIDATION OF CALCULATIONAL METHOD

The application should demonstrate that the calculational method (codes and cross-section data) used to establish criticality safety has been validated against measured data that can be shown to be applicable to the package design characteristics. The validation process should provide a basis for the reliability of the calculational method and should justify that the calculated k_{eff} , plus bias and uncertainties, for the necessary package conditions will ensure an actual package $k_{eff} \leq 0.95$.

The applicant should comply with the following guidelines[9] in performing and documenting the validation process:

1. bias and uncertainties should be established through comparison with critical experiments that are applicable to the package design;

2. the range of applicability for the bias and uncertainty should be based on the range of parameter variation in the experiments;

3. any extension of the range of applicability beyond the experimental parameter field should be based on trends in the bias and uncertainty as a function of the parameters and use of independent calculational methods; and

4. a margin of subcriticality should be included. The NRC currently regards 0.05 Δk as the minimum administrative margin of subcriticality that should be considered for transportation packages.

Although significant reference material is available to demonstrate the performance of many different criticality safety codes and cross-section data combinations, the application needs to demonstrate that the specific calculational method used by the applicant (e.g., code version, cross-section library, and computer platform) is validated in accordance with the above process. The remainder of this section of the report provides recommendations on the assumptions that should be made and the information that should be provided in performing and documenting the validation process.

5.1 SELECTION OF CRITICAL EXPERIMENTS

The first phase in the validation process should be to establish an appropriate bias and uncertainty for the calculational method by using well-defined critical experiments that have parameters (e.g., materials, geometry, etc.) that are characteristic of the package design. The single-package configuration, the array of packages, and the normal and hypothetical accident conditions should be considered in selecting the critical experiments for the validation process. Ideally, the set of experiments should match the package characteristics that most influence the neutron energy spectrum and reactivity. These characteristics include:

1. the fissile isotope (^{233}U, ^{235}U, ^{238}Pu, ^{239}Pu, and ^{241}Pu according to the definition of 10 CFR 71), form (e.g., homogeneous, heterogeneous, metal, oxide, fluoride), and isotopic composition of the fissile material;

2. hydrogenous moderation, consistent with the normal conditions of transport and hypothetical accident conditions, in and between packages that results in maximum k_{eff} (if substantial amounts of other moderators such as carbon or beryllium are in the package, these should also be considered);

3. the type (e.g., boron, cadmium), placement (between, within, or outside the contents), and distribution of absorber material and materials of construction;

4. the single-package contents configuration (e.g., homogeneous or heterogeneous) and packaging reflector material (e.g., lead, steel); and

5. the array configuration including spacing, interstitial material, and number of packages.

Unfortunately, it is unlikely that the complete combination of package characteristics will be found from available critical experiments, and critical experiments for large arrays of packages do not currently exist. Thus the applicant should model a sufficient variety of critical experiments to demonstrate the capability of the calculational method in predicting k_{eff} for each individual experiment that has characteristics that are also judged to be important to the k_{eff} of the package (or array of packages) under normal conditions of transport and hypothetical accident conditions.

Reference 10 provides general guidance on selecting critical experiments and provides descriptions of a significant number of critical experiments appropriate for low-enriched lattice systems. The critical experiments that are selected by the applicant should be briefly described in the application with references provided for detailed descriptions. The applicant should indicate any deviation from the reference experiment description including the basis for the deviation (e.g., discussions with experimenter, experiment log books). Since validation and supporting documentation may result in a voluminous report, it is acceptable to summarize the results in the application and reference the validation report for specific information.

5.2 ESTABLISHMENT OF BIAS AND UNCERTAINTY

For validation using critical experiments, the bias in the calculational method is the difference between the calculated k_{eff} value of the critical experiment and unity (1.0). Typically, a calculational method is termed to have a positive bias if it overpredicts the critical condition (i.e., calculated $k_{eff} > 1.0$) and a negative bias if it underpredicts the critical condition (i.e., calculated $k_{eff} < 1.0$). A calculational methodology should have a bias that either has no dependence on a characteristic parameter or is a smooth, well-behaved function of characteristic parameters. The applicant should analyze a sufficient number of critical experiments to determine if trends may exist with parameters important in the validation process [e.g., hydrogen-to-fissile ratio (H/X), ^{235}U enrichment, neutron absorber material]. As indicated in Sect. 4.1, the k_{eff} values should change by at least 3σ to indicate any type of parametric trend. The bias for a set of criticals should be taken as the difference between the best fit of the calculated k_{eff} data and 1.0. Where trends exist, the bias will not be constant over the parameter range. If no trends exist, the bias will be constant over the range of applicability. For trends to be recognized, they must be statistically significant.

The applicant should consider three general sources of uncertainty: the experimental data or technique, the calculational method, and the particular analyst and calculational models. Examples of uncertainties in experimental data are uncertainties reported in material or fabrication data or uncertainties due to an inadequate description of the experimental layout. Examples of uncertainties in the calculational method are uncertainties in the approximations used to solve the mathematical equations, uncertainties due to solution convergence, and uncertainties due to cross-section data or data processing. Interpretation of the calculated results, individual modeling techniques, and selection of code input options are possible sources of uncertainty due to the analyst or calculational model.

In general, all of these sources of uncertainty should be cumulatively observed in the variability of the calculated k_{eff} results obtained for the critical experiments. The variability should include the Monte Carlo standard deviation in each calculated critical experiment k_{eff} value as well as any change in the calculated value caused by the consideration of experimental uncertainties. Thus these uncertainties will be included in the bias and uncertainty in the bias. This variation or uncertainty in the bias should be established by a valid statistical treatment of the calculated k_{eff} values for the critical experiments. Methods exist (see Ref. 10) that allow the bias and uncertainty in the bias to be evaluated as a function of changes in a selected characteristic parameter.

Calculational models used to analyze the critical experiments should be provided or adequate references to such discussions should be provided. Input data sets used for the analysis should be provided along with an indication of whether these data sets were developed by the applicant or obtained from other identified sources (e.g., published references, data bases). Known uncertainties in the experimental data should be identified, along with a discussion of how (or if) they were included in the establishment of the overall bias and uncertainty for the calculational method. The statistical treatment used to establish the bias and uncertainty should be thoroughly discussed in the application with suitable references where appropriate. Relative to experimental uncertainties, the applicant should provide a discussion on the approach used to model the experiments (i.e., with nominal dimensions and material compositions or with conservative tolerances, with simplifications in the geometry and material specifications, etc.).

5.3 ESTABLISHMENT OF RANGE OF APPLICABILITY

As an integral part of the code validation effort, the applicant should define the range of applicability for the established bias and uncertainty. The applicant should demonstrate that, considering both normal and hypothetical accident conditions, the package is within this range of applicability and/or the applicant should define the extension of the range necessary to include the package. The range of applicability should be defined by identifying the range of important parameters (see Ref. 10 for guidance on identifying important parameters) and/or characteristics for which the code was (or was not) validated. The procedure or method used to define the range of applicability should be discussed and justified in the application for approval. For example, the method of Ref. 10 indicates the range of applicability to be the limits (upper and lower) of the characteristic parameter used to correlate the bias and uncertainties. The characteristic parameter may be defined in terms of, for example, the hydrogen-to-fissile ratio (e.g., H/X = 10 to 500), the average energy causing fission, the ratio of total fissions to thermal fissions (e.g., F/F_{th} = 1.0 to 5.0), or the ^{235}U enrichment.

Use of the bias and uncertainty for the evaluation of a package with characteristics beyond the defined range of applicability is endorsed by consensus guidance.[9] This guidance indicates the extension should be based on trends in the bias as a function of system parameters and, if the extension is large, confirmed by independent calculational methods. However, the applicant should consider that extrapolation can lead to a poor prediction of actual behavior. Even interpolation over large ranges with no experimental data can be misleading (see Ref. 6 for an example). The applicant should also consider the fact that comparisons with other calculational methods can illuminate a deficiency or provide concurrence; however, given discrepant results from independent methods, it is not always a simple matter to determine which result is "correct" in the absence of experimental data (see Ref. 11 for an illustration).

The applicant should recognize that there is no available guidance on what constitutes a "large" extension, nor any guidance on how to extend trends in the bias. In fact, it is not just the trend in the bias that the applicant should consider, but the trend in the uncertainties and bias. The paucity of experimental data near one end of a parameter range may cause the uncertainty to be larger in that region. (Note: Any extension of the uncertainty using the method of Ref. 10 should consider the behavior of the uncertainty as a function of the parameter, not just the maximum value of the uncertainty.) Proper extension of the bias and uncertainty means the applicant should determine **and understand** the trends in the bias and uncertainty. The applicant should exercise extreme care in extending the range of applicability and provide in the application a detailed justification for the need for an extension, along with a thorough description of the method and procedure used to estimate the bias and uncertainty in this extended range.

5.4 ESTABLISHMENT OF ACCEPTANCE CRITERIA

The criticality safety section of the application should demonstrate how the bias and uncertainty determined from the comparison of the calculational method with critical experiments are used to establish a minimum k_{eff} value [i.e., upper subcritical limit (USL)] so that similar systems with a higher calculated k_{eff} are considered to be critical. The USL should be established with an additional margin of subcriticality (often termed a safety margin) included.[9] The following general relationship (see Ref. 10) for establishing the acceptance criteria should be used in the application for approval:

$$k_c - \Delta k_u \geq k_{eff} + 2\sigma + \Delta k_m ,$$

where

- k_c = mean value of k_{eff} resulting from the calculation of benchmark critical experiments using a specific calculational method and data;
- Δk_u = an allowance for the calculational uncertainty;
- Δk_m = a required margin of subcriticality (minimum of 0.05 for applications of approval for packaging);
- k_{eff} = the calculated value obtained for the package or array of packages;
- σ = is the standard deviation of the k_{eff} value obtained with Monte Carlo analysis.

If the calculational bias β is defined as $\beta = k_c - 1$, then the bias is negative if $k_c < 1$ and positive if $k_c > 1$. Thus the acceptance criteria may be rewritten as

$$1.00 + \beta - \Delta k_u \geq k_{eff} + 2\sigma + 0.05,$$

or

$$k_{eff} + 2\sigma \leq 0.95 - \Delta k_u + \beta \ .$$

The maximum USL that should be used for a package evaluation is

$$USL = 0.95 - \Delta k_u + \beta \ .$$

The uncertainty, Δk_u, will always be greater than or equal to zero, whereas the bias, β, can be positive or negative. However, a positive bias is not recommended; therefore, the equation should be revised to

$$USL = 0.95 - \Delta k_u + \bar{\beta}$$

where $\bar{\beta} = \begin{cases} \beta \text{ if } \beta \leq 0 \\ 0, \text{ if } \beta > 0 \ . \end{cases}$.

The applicant should consider that the value for Δk_m (=0.05) may need to be increased by an arbitrary amount if there is a lack of sufficient critical data to adequately determine the calculational bias and uncertainty. The statistical method of Ref. 10 provides a technique to estimate Δk_u and Δk_m based on available data. This estimate for Δk_m can be used to demonstrate that the value of 0.05 for the margin of subcriticality is adequate for the given set of critical experiments used in the validation. A paucity of critical experiment data or the need to extend beyond the range of applicability may indicate the applicant should consider the adequacy of the 0.05 value. Also, for high-reactivity worth systems where the value of k_{eff} is particularly sensitive to parameter changes in the package, a margin of subcriticality greater than 0.05 Δk should be considered by the applicant.

6 CRITICALITY CALCULATIONS AND RESULTS

This section of the report describes the criticality calculations that should be performed and documented in the criticality safety section of the application for approval of a package. The criticality safety evaluation should demonstrate the subcriticality of a single package and an array of packages during normal conditions of transport and hypothetical accident conditions, and determine the TI for criticality control of a shipment. For the purposes of this evaluation, the applicant should consider the term "subcriticality" to mean that the calculated k_{eff} value (including any Monte Carlo standard deviation) is less than the USL defined by Sect. 5.4.

The calculations that the applicant should include in the criticality safety section will depend on the various parameter changes and conditions that should be considered, the packaging design and features, the contents, and the damaged condition of the package. The calculated results should be presented in a tabular form with a case identifier, a brief description of the conditions for each case, and the case results. Values of k_{eff} obtained from Monte Carlo codes should always indicate the estimated standard deviation. Additional information should be included in the table if it supports and simplifies the description in the text. The case description should be clearly presented in the tables to permit easy cross-reference between the table and the text. Tables 1 and 2 show an example of the format desired to summarize the results of single-package and package array calculations.

The following subsections present a logical, generic approach to the calculational effort that should be described in the application for approval. Two series of calculational cases should be performed: (1) a series of single-package cases and (2) a series of array cases. Both series should consider normal and hypothetical accident conditions. Subsets of the array series for different size arrays or different package arrangements may also be necessary. Each array series should include calculations to determine the number of undamaged packages that will ensure subcriticality of an array under normal conditions of transport, as well as calculations to determine the number of damaged packages that ensure subcriticality of an array under hypothetical accident conditions. A TI for criticality control should be derived (see Sect. 6.3) from these array sizes based on the prescription of 10 CFR § 71.59.

6.1 SINGLE PACKAGE

The applicant should perform a series of calculations to demonstrate that the single package remains subcritical under normal conditions of transport and hypothetical accident conditions (per the requirements of 10 CFR § 71.55).

The single-package calculations also provide useful points of reference for subsequent calculations involving variations of certain parameters.

The single-package series of calculations must consider a model of the single containment vessel fully reflected by water (a 30-cm-thick region of full-density water is recommended). The containment vessel should be optimally moderated with the fissile content in its most reactive credible configuration. This water-reflected, optimally moderated containment vessel analysis should be compared with one where the water reflector is replaced by the package material (including water flooding in voids) that surrounds the containment system. Package materials such as lead may provide better reflection of the containment system than water. Demonstration that these two single, undamaged cases are adequately subcritical satisfies the requirements of 10 CFR § 71.55(b).

Table 1 Example format of table for single-package calculations

Case	Water reflected[a]	Internal moderation[b]	$k_{eff} \pm \sigma^c$
SU1	No	0.0	
SU2	Yes	0.0	
SU3	Yes	0.001	
SU4	Yes	0.003	
.	.	.	
.	.	.	
SUx	Yes	1.0	
SUy	No	1.0	

[a]When fully reflected, water should be at least 30-cm thick on all faces.
[b]Internal moderation is the specific gravity water equivalent of hydrogenous content within all void spaces inside the package, including the containment vessel.
[c]σ is one standard deviation of the calculated Monte Carlo result.

Table 2 Example format of table for array calculations

Case[a]	Array size	Internal moderation[b]	Interspersed moderation[c]	$k_{eff} \pm \sigma^d$
IA1	Infinite	0.0	0.0	
IA2	Infinite	0.0	0.001	
IA3	Infinite	0.0	0.003	
.				
.				
IAx	Infinite	0.0	1.0	
FA1	7 × 7 × 7			
FA2	7 × 7 × 7			
FA3	7 × 7 × 7			
.				
.				
FA10	5 × 5 × 5			
FA11	5 × 5 × 5			
.				
.				

[a]Case identifier IA represents infinite arrays and FA represents finite arrays; all finite arrays should be reflected by at least 30 cm of water on all faces.
[b]Internal moderation is the specific gravity water equivalent of hydrogenous content within all void spaces inside the package, including the containment vessel.
[c]Interspersed moderation is the specific gravity water equivalent of hydrogenous content between packages.
[d]σ is one standard deviation of the calculated Monte Carlo result.

The remaining single-package cases provided in the application should systematically investigate progressive states of water flooding and package reflection representative of the normal and hypothetical accident conditions. If the hypothetical accident conditions cause damage to the contents or packaging, the damaged configuration of the package should be considered. If a package has multiple void regions, including regions within the containment system, flooding each region independently and consecutively should be considered. Variations in the flooding sequence should be considered by the applicant [e.g., partial flooding, variations caused by the package lying in horizontal or vertical orientations, flooding (moderation) at less than full-density water, progressively flooding regions from the inside out]. Water flooding of cladded fuel rod gap regions should be considered. The final case of this single-package series should represent a package completely water-flooded and water-reflected. The primary objectives of the single-package cases should be

1. to demonstrate that a single package is subcritical when subjected to the normal conditions of transport and hypothetical accident conditions as specified by 10 CFR § 71.55, and

2. to identify the specific conditions that produce the highest k_{eff} value.

For packages with different fissile material loading configurations (including partial-load configurations), the applicant should use a similar approach for each different loading, unless a limiting-contents model is developed and demonstrated in the application to provide a bounding reactivity for the different loadings. The results of the single-package calculations can influence the approach and the number of calculations required for the array series calculations, particularly if there are different content loading configurations.

6.2 EVALUATION OF PACKAGE ARRAYS

The applicant should perform the package array calculations to obtain the information needed to determine the TI for criticality control as prescribed by 10 CFR § 71.59. The applicant may consider beginning the array calculations with an infinite array model because, if the infinite array is adequately subcritical under normal and hypothetical accident conditions, no additional array calculations should be necessary. If the infinite array under normal and hypothetical accident conditions is shown to be above the USL, a large (number of packages) finite array should be selected and all cases recalculated. Successively smaller finite arrays may be required until the array sizes for normal and hypothetical accident conditions are found to be below the USL. As an alternative, an applicant may initiate the analyses using any array size–for example, one that is based upon the number of packages planned to be shipped on a vehicle.

Care should be taken so that the most reactive array configuration of packages has been considered in the criticality safety assessment. In investigating different array arrangements, the competing effects of leakage from the array system and of interaction between packages in the array should be considered. Array arrangements that minimize the surface-to-volume ratio decrease leakage and should, in simplistic terms, maximize k_{eff}. Preferential geometric arrangement of the packages in the array should be considered. For example, consider packages where the fissile material is loaded off-center. In this case, the need to optimize the interaction may mean that an array is more reactive when packages are grouped in a single or double layer. The effect of the external water reflector also needs to be considered. For some array cases there may be little moderator present within the array, so increasing the surface area may lead to more moderation and possibly higher reactivity. The exact package arrangement may be represented by a simplified arrangement if adequate justification is provided. For example, Appendix A demonstrates a case where a triangular-pitch arrangement of packages can, in simple cases, be represented by using an appropriately modified package model within a square-pitch lattice arrangement. In more complex cases, the effect of having a triangular pitch may be important, since interaction between three triangularly pitched packages could be a dominating factor. Because there are so many competing effects, any simplifications made in the assessment need to be justified; something that is obvious from the point of view of array leakage may not be as obvious from the point of view of package interaction. All finite arrays of packages should be reflected on all sides by a close-fitting, full-density water reflector at least 30 cm thick.

Each array model for undamaged packages is not required to include interspersed moderation; however, moderation built into the packaging (e.g., due to hydrogenous packaging materials) or added to the packaging due to normal conditions of transport (e.g., the spray test) should be included to the most reactive extent possible under normal conditions. For damaged packages, varying amounts of hydrogenous moderation should be added in all regions that can be flooded within (see discussion of Sect. 6.1 for single package) and between the packages (i.e., interspersed moderation) by varying the density of water in these regions. If water in-leakage is considered (see Sect. 3.4), then the water density should be varied from zero to full density in increments such that the optimum moderator density is determined. The applicant should provide a plot of the k_{eff} value as a function of the moderator density to demonstrate the trend and the location of the highest k_{eff} value.

As an interspersed moderator is added to the region between packages, the spacing of the packages may become important because of the amount of moderator that may be present. For this reason, it is sometimes convenient to model an infinite array of packages using an array unit cell consisting of the individual package and a tight-fitting repeating boundary. If the k_{eff} response to increasing interspersed moderator density for this array with the units in contact has an upward trend (positive slope) at full-density moderation, the applicant should consider increasing the size of the unit cell and recalculating k_{eff} as a function of moderation density. Increasing the size of the unit cell provides an increased edge-to-edge spacing between packages and makes more volume available for the interspersed moderator. The applicant should stop this procedure only after confirming that the packages are isolated and that added interstitial space is only providing additional water reflection.

To illustrate this recommended procedure, consider a cylindrical shipping package with a diameter of one unit and a height (or length) of two units. With a tight-fitting cuboid around the cylinder, 21.5% of the cuboid's volume is outside the package and is available for an interspersed moderator. By increasing the cuboid's dimensions so that the edge-to-edge spacing between the packages in all directions is 10% of the package diameter, then 38.2% of the cuboid's volume is outside the package and is available for an interspersed moderator. This small increase in edge-to-edge spacing corresponds to a 126% increase in volume available for the interspersed moderator. Therefore, if the k_{eff} value is increasing at full water density with the packages in contact, then increasing the packaging spacing to permit additional interspersed moderation may be necessary.

The applicant should consider combinations of density and spacing variation (consistent with normal and hypothetical accident conditions) that may cause a higher k_{eff} value to be calculated and should provide a discussion in the application that demonstrates the maximum k_{eff} value has been determined. Figure 1 depicts some typical plots of k_{eff} versus interspersed water moderator density illustrating the moderation, absorption, and reflection characteristics that may be encountered in packaging safety evaluations. These curves represent changes in array moderation for a fixed package spacing. Curves A, B, and C represent arrays for which an array of packages at the selected spacing is overmoderated and increasing water moderation only lowers (curves B and C) or has no effect (curve A) on the k_{eff} value. Curves D, E, and F represent arrays for which the array is undermoderated at zero water density, and increasing the moderator density causes the k_{eff} value to

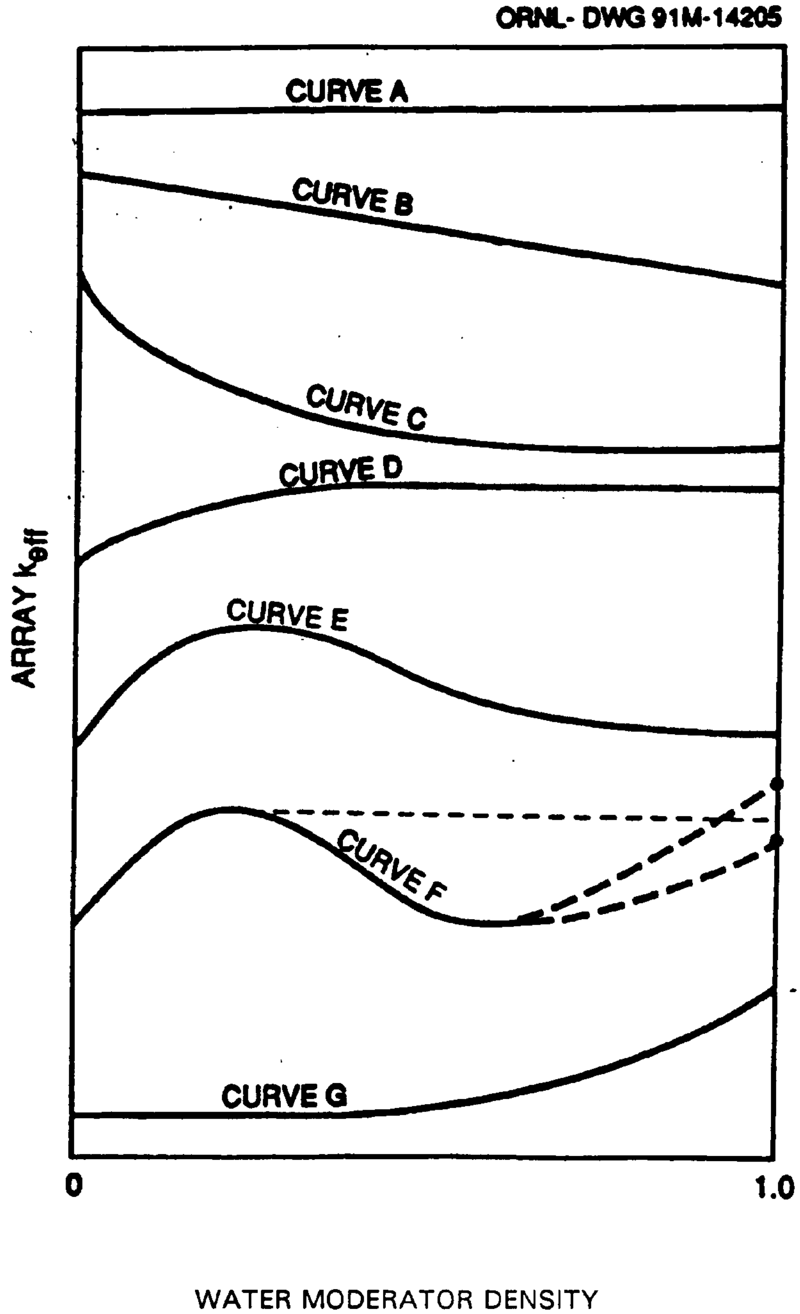

Figure 1 Typical plots of array k_{eff} vs interspersed water moderator density

increase. Then as the water density increases further, neutron absorption comes into effect, neutron interaction between packages decreases, and the k_{eff} value levels out (curve D) or decreases (curves E and F). The applicant should consider that peaking effects such as seen in curves E and F frequently occur at very low moderator density (e.g., 0.001 to 0.1 fraction of full density). Therefore, the applicant should exercise care when selecting the values of interspersed moderator density to calculate in the search for the maximum k_{eff} value.

As indicated above, optimum moderation conditions for the array of packages represented by curves D, E, and F have been obtained; and the only mechanism that could make the k_{eff} value of curve D, E, or F rise above the value at full-density water is increased reactivity due to increased reflection provided by more interspersed water (i.e., additional spacing between packages). If the array k_{eff} at full-density moderation is less than the k_{eff} of the flooded and reflected single unit, the edge-to-edge spacing of the packages is not sufficient to permit full reflection.

However, for responses such as those illustrated in curves D, E, and F, there is no need to increase spacing and recalculate the array k_{eff} because the maximum k_{eff} of the array will be that of the reflected single unit, or the k_{eff} of the optimally moderated array (i.e., the first local maxima of curves D, E, and F), whichever is larger. For curves A through F, the packages in the array are essentially isolated at full-density moderation and the corresponding k_{eff} will typically be the same (within statistical limits) as the flooded and reflected single-unit case.

Curve G represents an array where the optimum array moderator density has not been achieved even with full-density water, and the maximum k_{eff} has not been determined. For this situation, the applicant should increase the center-to-center spacing of the packages in the array and all cases should be recalculated. The center-to-center spacing must be sufficiently large for the curve to reach a plateau (like curve D) or to peak and then decrease (like curves E and F).

The treatment of array moderation can be easy or complex, depending on the placement of the materials of construction and their susceptibility to damage from hypothetical accident conditions. For all of these conditions and combinations of conditions, the applicant should carefully investigate the optimum degree of internal and interspersed moderation consistent with the chemical and physical form of the material and the packaging, and should demonstrate that subcriticality is maintained. The applicant should consider the numerous conditions for which the effects of moderation must be investigated, such as

1. moderation from packing materials that are inside the primary containment system,
2. moderation due to preferential flooding of different regions in the packages,
3. moderation from hydrogenous materials of construction (e.g., thermal insulation and neutron shielding), and
4. interspersed moderation in the region between the packages in an array.

In determining the TI of an array of packages under normal conditions of transport, the applicant should consider only the possible ranges of hydrogenous (or other) moderators present in the package [items (1) and (3) above and, if applicable, item (2) above]; interspersed moderation between packages [item (4) above] from conditions such as mist, rain, snow, or flooding need not be considered (per the specifications of 10 CFR § 71.59). In determining the TI of an array of damaged packages, the applicant should carefully consider all four of the above conditions, including how each form of moderation can change under hypothetical accident conditions. As an example, consider a package with thermally degradable insulation. The applicant should evaluate the array with the insulation for the normal conditions of transport. For the hypothetical accident conditions, the applicant should investigate moderation effects caused by changes in the insulation due to the thermal tests. The applicant should carefully evaluate the varying degrees of internal moderation in the containment.

6.3 RELATING ANALYSES TO TRANSPORT INDEX

The TI for criticality control should be determined by the applicant using the information from the array analyses on the number of packages that will remain subcritical (below the USL) under normal and hypothetical accident conditions. The USL should be determined using the criteria discussed in Sect. 5.4. Table 3 illustrates the tabular form that the applicant should use to summarize the results on the limiting number of packages shown to be subcritical in the analysis of the package arrays. The value N in the table can be defined so that

N = maximum number of packages per shipment for a nonexclusive use shipment, where $5 \leq N \leq \infty$.
2N = maximum number of packages per shipment for an exclusive use shipment, where $0.5 \leq N \leq \infty$.

Table 3 Requirements of 10 CFR § 71.59

Case	No. of fissile packages that must be subcritical
Undamaged	5N with nothing between packages
Damaged	2N with optimum interspersed moderation

With the information provided in Table 3, the applicant can determine the TI for criticality control using the expression

$$TI = 50 \div N \ .$$

7 SUMMARY

This report provides recommendations on the information that should be included in the criticality safety section of an application for approval of a transportation package. The emphasis has been on the design information, analysis models, and computational results and discussion that should be in the application. However, the applicant should recognize that the recommendations may not be exhaustive and that additional information or analyses may be needed for selected applications.

Section 2 of the report discusses the design information that the applicant should include in the criticality safety section of the application. Specification of the contents (e.g., form, type, mass, composition) considered in the application should be provided, including any anticipated variations and uncertainties.

Section 3 of the report reviews the description and figures that should be included in the application to adequately explain the calculational models. In preparing these models, the applicant should limit the use of fixed neutron absorbers to 75% of the composition, unless adequate (see Sect. 3.1.3) consideration is made for testing the presence and uniformity of the absorber. Fixed, burnable poisons should not be considered in spent fuel packages. And, until the NRC provides direction on use of spent fuel isotopics, it is recommended that unburned (fresh) fuel isotopics be assumed in applications for spent fuel packages. Water moderation and reflection specifications based on the normal and accident conditions of 10 CFR Part 71 must be considered in the development of the analysis models.

Sections 4–5 of the report recommend the information that should be considered by the applicant in selecting and using an appropriate analysis method (code and nuclear data) for determination of the neutron multiplication factor. Codes that adequately model the kinematics of neutron transport, including angular scattering, are needed to provide the best estimate of k_{eff}. The codes and data used in the application should be validated against critical experiments appropriate for the package conditions and contents. This validation provides a basis for development of a USL that considers bias and uncertainties (determined from the validation), the statistical nature of the analysis method, and a margin of subcriticality. The minimum margin of subcriticality accepted by the NRC for transportation packages is 0.05 Δk.

Section 6 of the report discusses the analyses that should be considered to demonstrate that the requirements of 10 CFR § 71.55 and 71.59 are met. This section provides practical information on how to proceed with the analyses, the single-package and array conditions that should be considered, and a process for determination of the TI for criticality control. Development and analysis of the array models should carefully consider the various conditions that could lead to an increased k_{eff} value. Optimum moderation of the packages according to the normal and accident conditions, package arrangement and spacing for optimum interaction between packages, and proper water reflection of the array should be considered.

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APPENDIX A

EXAMPLE OF CALCULATIONAL MODELS AND RESULTS

This appendix uses a simple example of a fictitious transport package to illustrate many of the recommendations provided in this report regarding the content of the criticality safety section of the application for a transport package. This example package and analysis have not been approved by the NRC, and there has been no assessment as to whether the package would meet all of the requirements for approval. The descriptions provided herein do not include all the information that would be necessary for an actual package evaluation; rather they provide an illustrative sampling of the type of information discussed in this report.

The following sections provide information as if it were imbedded as the criticality section of the application. However, since this is intended to be an illustrative example, only that information pertinent to developing the calculational models is included. The dimensional and material specifications provided are the minimum to support the calculations in this appendix and do not represent certified container loadings or configurations. Also, the descriptions, calculations, and justifications presented here may not be complete or acceptable to the NRC.

A.1 GENERAL DESCRIPTION (Example)

The transport package uses a 55-gal steel drum overpack [22.5-in.(57.15-cm) inside diam by 40.5-in. (102.87-cm) inside height]. The drum body and bottom are fabricated from a 16-gauge [0.064-in. (0.16-cm)] low carbon steel sheet. The drum lid (head) is fabricated from a 14-gauge [0.080-in. (0.20-cm)] low-carbon steel sheet. Two approximately equally spaced, rolling hoops are swaged into the drum body. The removable head is closed by means of a bolt-locking ring.

The inner container (containment vessel) is the containment boundary. The inner container is fabricated from a 0.25-in. (0.64-cm)-thick carbon steel plate. The inner container [12.0-in. (30.48-cm) inside diam by 28.0-in. (71.12-cm) inside height] has a welded bottom plate and welded cover plate.

The 55-gal drum is filled between the drum wall and inner container with insulating fiber board that provides thermal insulation and vibration and shock isolation, and centers the inner container within the drum. The insulating fiber board provides a thickness between the inner container and drum of 5.0 in. (12.7 cm) radially and 5.0 in. (12.7 cm) axially (top and bottom).

The package shall be used to transport unirradiated uranium dioxide (UO_2) pellets of 0.325-in. (0.83-cm) nominal outside diameter. The contents are not to exceed 116.16 kg of UO_2 pellets at an enrichment in the ^{235}U isotope of 4.01%.

A.2 PACKAGE DESCRIPTION

Sections A.2.1 and A.2.2 describe the package contents and packaging, specifically the dimensions and material components that influence k_{eff}.

A.2.1 CONTENTS

The package shall be used to transport right cylindrical UO_2 pellets of 10.40 g/cm^3 oxide density. The pellets have a 0.325-in. (0.83-cm) nominal outside diameter and height and a maximum enrichment of 4.01 wt % ^{235}U. The uranium isotopic distribution is given in Table A.1.

Table A.1 Uranium isotopic distribution

Isotope	wt %
^{234}U	0.02
^{235}U	4.01
^{236}U	0.02
^{238}U	95.95

A.2.2 PACKAGING

The packaging consists of the inner container assembly (DWG-X12G64) comprising 316 stainless steel tubes that accommodate the fuel pellets, the inner container or containment vessel (DWG-D184K), plywood board, insulating fiber board, and the 55-gal drum (DWG-4201V).

A.2.2.1 Inner Container Assembly

Pellets and end plugs are contained in 27.75-in. (70.49-cm)-long stainless steel tubes of 0.350-in. (0.89-cm) inside and 0.366-in. (0.93-cm) outside diam. Each of the 316 tubes is filled with 80 pellets. The composition and atom densities of the 304-stainless steel tubes and other package materials are given in Table A.2. The tube ends are sealed with 0.350-in. (0.89-cm)-diam, 1.0-in. (2.54-cm)-long top and 0.75-in. (1.91-cm)-long bottom stainless steel plugs that are welded in place. The tube bottoms are welded into 0.75-in. (1.91-cm)-deep recesses on a 0.528-in. (1.34-cm)-square pitch of a 1.0-in. (2.54-cm)-thick, 12.0-in. (30.48-cm)-diam stainless steel bottom plate. The tube tops extend through 0.375-in. (0.95-cm)-diam holes to the top of a 1.0-in. (2.54-cm)-thick, 12.0-in. (30.48-cm)-diam stainless steel top plate. Rubber o-rings between the tubes and plate holes provide a tight tube-to-top-plate fit. The top plate is connected by four 26.0-in. (66.04-cm)-long, 0.667-in. (1.69-cm)-diam stainless steel support rods to the bottom plate. The structural evaluation has shown that the inner container assembly remains intact, and the pellets remain inside the tubes, under normal conditions of transport and hypothetical accident conditions.

A.2.2.2 Inner Container

The inner container is fabricated from 0.25-in. (0.635-cm)-thick carbon steel plate. The inner container [12.0-in. (30.48-cm)-inside diameter by 28.0-in. (71.12-cm) inside height] has a welded 0.25-in. (0.635-cm)-thick bottom plate with a welded 0.25-in. (0.635-cm)-thick cover plate.

Table A.2 Material specifications

Material	Density (g/cm^3)	Constituent	Atomic density (atoms/b-cm)
304 stainless steel	7.92	Fe	5.935e-2
		Cr	1.7428e-2
		Nu	7.7188e-3
		Mn	1.7363e-3
Insulating fiber board	0.24	H	8.914e-3
		C	5.348e-3
		O	4.457e-3
Plywood	0.45	H	1.671e-2
		C	1.003e-2
		O	8.357e-3
Water	0.9982	H	6.675e-2
		O	3.338e-2
Carbon steel	7.821	C	3.9250e-3
		Fe	8.3498e-2
Rubber	1.321	C	3.8414e-2
		H	5.1298e-2
		Ca	2.2627e-3
		S	4.2182e-4
		O	1.0988e-2
		Si	8.4972e-5

A.2.2.3 Drum

The transport package uses a 55-gal steel drum overpack [22.5-in. (57.15-cm) inside diameter by 40.5-in. (102.87-cm) inside height]. The drum body and bottom are fabricated from a 16-gauge [0.064-in. (0.163-cm)] low-carbon steel sheet. The drum lid (head) is fabricated from a 14-gauge [0.080-in. (0.20-cm)] low-carbon steel sheet. Two approximately equally spaced, rolling hoops are swaged into the drum body. The removable head is closed by means of a bolt-locking ring.

The 55-gal drum is filled between the drum wall and inner container with insulating fiber board that provides thermal insulation and vibration and shock isolation, and centers the inner container within the drum. The drum is loaded top-to-bottom with (1) a 5.0-in. (12.7-cm)-thick, 22.5-in. (57.15-cm)-diam insulating fiber board block, (2) a 1.0-in. (2.54-cm)-thick, 22.5-in. (57.15-cm)-diam plywood load bearing plate, (3) the inner container assembly, centered, and surrounded by a 22.5-in. (57.15-cm)-outer-diam, 12.5-in. (31.75-cm)-inner-diam, 13.75-in. (34.93-cm)-thick insulating fiber board ring, followed by a 1.0-in. (2.54-cm)-thick, 22.5-in. (57.15-cm)-outer-diam, 12.5-in. (31.75-cm)-inner-diam plywood support ring, followed by a 22.5-in. (57.15-cm)-outer-diam, 12.5-in. (31.75-cm)-inner-diam, 13.75-in. (34.93-cm)-thick insulating fiber board ring, (4) a 1.0-in. (2.54-cm)-thick, 22.5-in. (57.15-cm)-diam plywood load-bearing plate, and (5) a 5.0-in. (12.7-cm)-thick, 22.5-in. (57.15-cm)-diam insulating fiber board block.

A.3 CRITICALITY SAFETY ANALYSIS MODELS

Section A.3.1.1 provides dimensioned sketches of a modeled package. The material specifications for regions of the sketches in Sect. A.3.1.1 are given in Sect. A.3.1.2. Section A.3.1 identifies differences between the models and actual package configurations. Section A.3.2 describes the contents models representing each of the different loading configurations. Models depicting the configuration of packaging and contents of a single package under normal and accident conditions are discussed in Sect. A.3.3. Section A.3.4 contains a discussion on the package array models.

A.3.1 GENERAL MODEL

A.3.1.1 Dimensions

Figure A.1 represents the vertical elevations of the package seen along the vertical centerline of the package. A cross section of the package along A-A of Fig. A.1 is displayed in Fig. A.2. The figures' dimensions were used in the calculations.

Note: Although not included in this example, a real application should not *a priori* use nominal dimensions, but instead should address dimensional tolerances of the package that tend to add conservatism to the models.

A.3.1.2 Materials

Figures A.1 and A.2 show cross sections of the single-package calculational model. Table A.3 identifies the regions, materials, material densities, and masses as used in the calculations, and the actual masses.

Note: Although not included in this example, a real application should not *a priori* use nominal material specifications, but instead should address maximum and minimum fissile, neutron-absorbing, moderating, and structural materials parameter values that produce conservative k_{eff} results within the allowable tolerances.

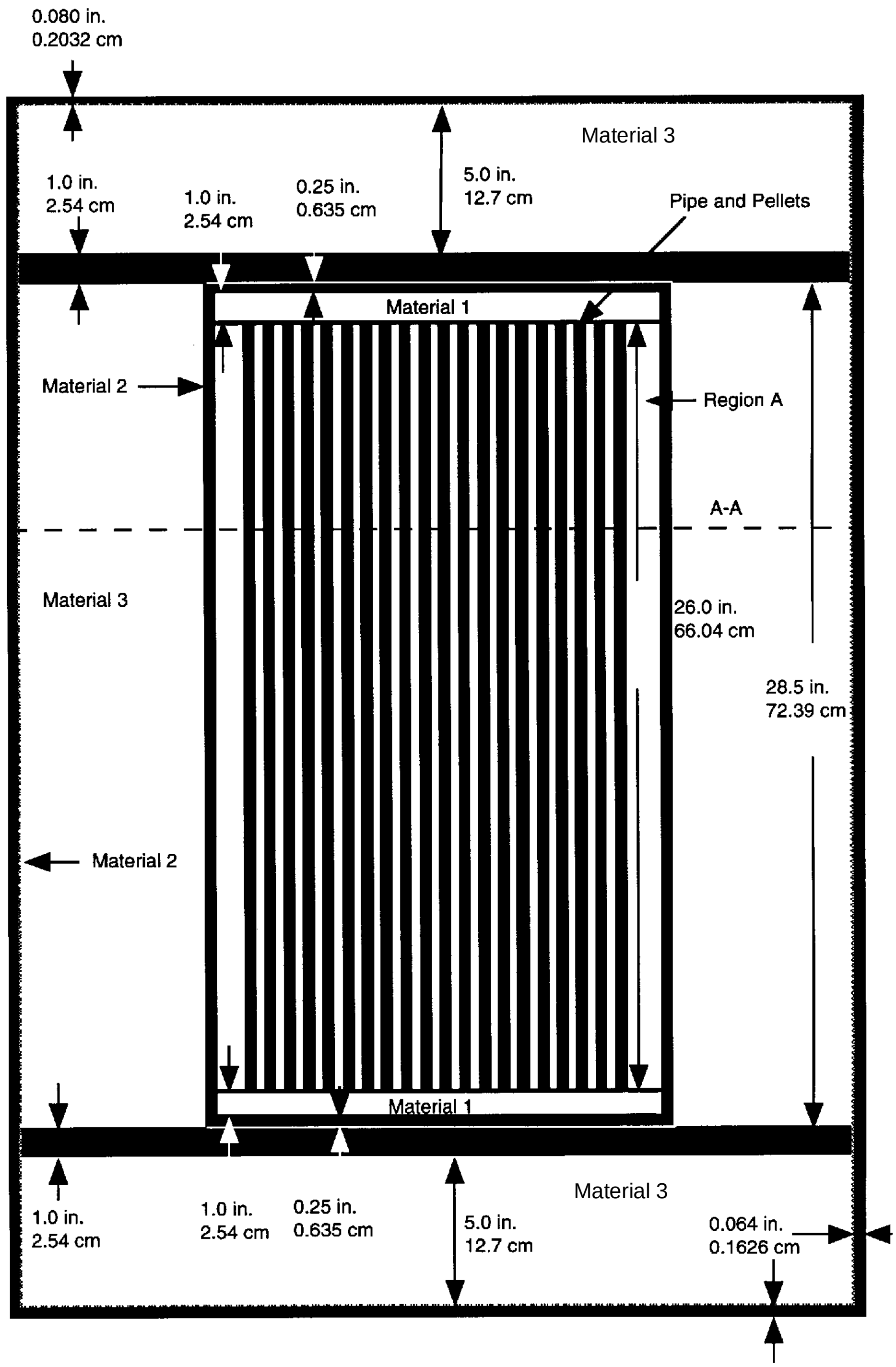

Figure A.1 Axial cross section of the single-package model

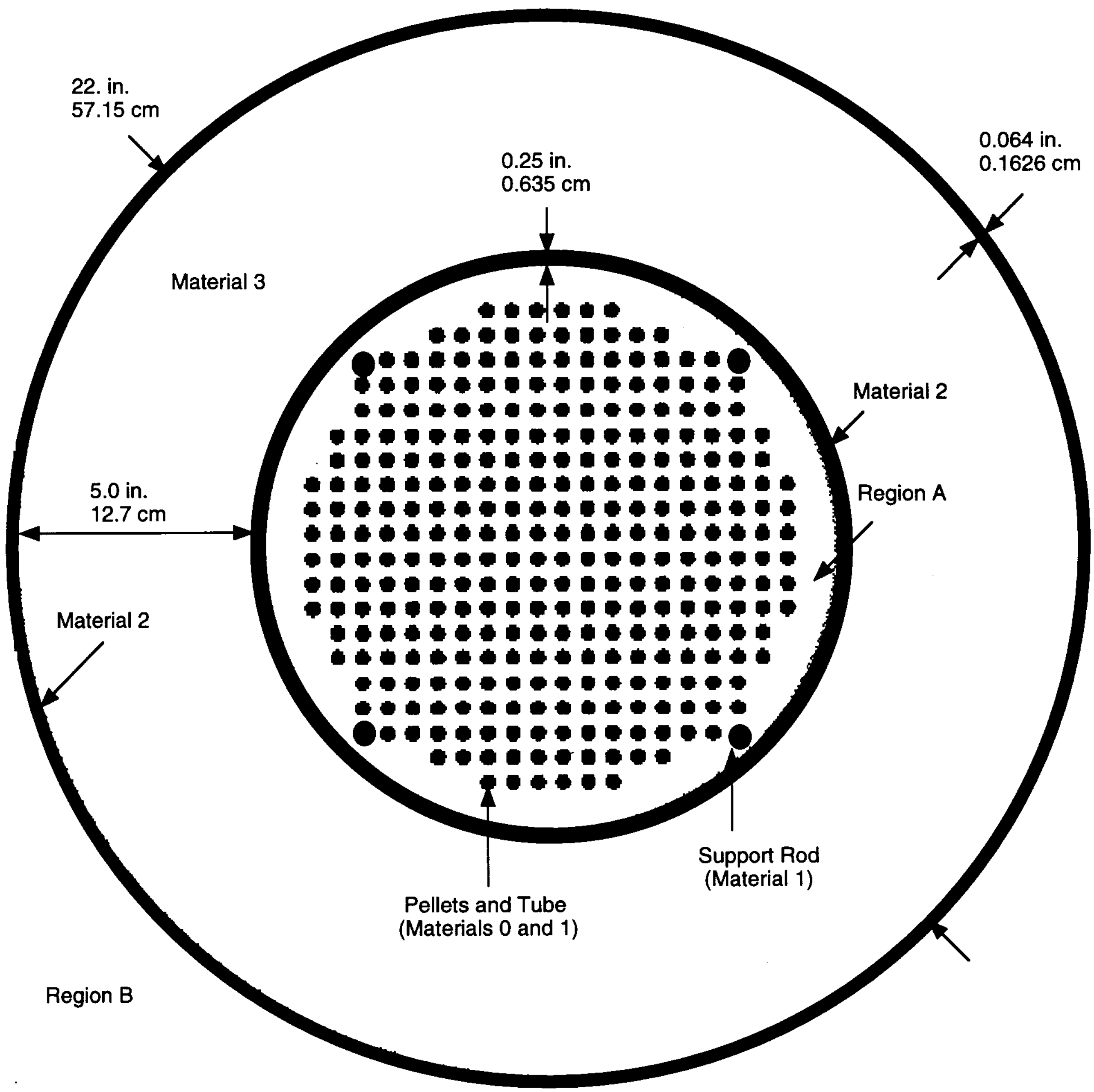

Figure A.2 Radial cross section of single-package model

Table A.3 Material specifications for Figs. A.1 and A.2

Material No.	Material	Density (g/cm^3)	Model mass (kg)	Actual mass (kg)
0	UO_2	10.40	116.19	116.16
1	SS-304	7.92 [a]	41.87	42.12
2	Carbon steel	7.8212 [a]	73.37	77.23
3	Insulating fiber board	0.24	46.42	44.29
4	Plywood	0.45	5.860	8.796

[a]SCALE Standard Composition Library values.

A.3.1.3 Models—Actual Package Differences

The single-package calculational model of the 55-gal drum differs from the actual drum in the treatment of the drum wall. In the model, the drum wall is a straight wall cylinder without the rolling hoops. The drum model does not have the top and bottom inset into the drum wall, bolts, locking rings, etc.

The rubber o-ring fittings around the tubes in the top plate of the inner container assembly were treated as stainless steel, the surrounding material. The change constitutes such a small change in stainless steel mass in the positive axial direction relative to the fuel region that the impact on k_{eff} would be negligible. To simplify the modeling, the center plywood support ring was modeled as insulating fiber board, the surrounding material. The exchange of materials would have a negligible effect on k_{eff} because the constituents of the two materials are identical and the thickness of the region is small relative to the radial surface of the containment vessel (i.e., ~4% of the surface available for radial neutron leakage).

A.3.2 CONTENTS MODEL

Figure A.2 shows the package contents (pellets in tubes) configured for both the single-package and package-array calculations. Each tube is physically restricted to a maximum loading of 80 pellets. Partial-loading (variable-mass) configurations are allowed, as are variations in pellet enrichment (up to 4.01 wt % ^{235}U). However, partial loadings must be from the inner tubes outward with only the last loaded tube containing less than 80 pellets (see Chapter 1). Because of this restriction and the fixed tube spacing, partial loadings do not require further analysis because they are bounded by the more reactive configuration of full loading. Chapter 2 of the application for approval has shown that the tube spacing remains at 1.34 cm (0.528 in.), and that the pellets remain inside the tubes, under normal conditions of transport and hypothetical accident conditions.

A.3.3 SINGLE PACKAGES

To meet the general requirements for fissile material packages, 10 CFR § 71.55, a package must be designed and its contents so limited that it would be subcritical under the most reactive configuration of the material, optimum moderation, and close reflection of the containment system by water on all sides or surrounding materials of the packaging. Models of both reflective conditions have been considered. The package was subjected to the tests specified in 10 CFR § 71.71, Normal Conditions of Transport, and, as reported in

Chapters 2 and 3, the geometric form of the package was not substantially altered, no water leakage into the containment occurred, and no substantial reduction in the effectiveness of the packaging was observed. In short, the damage incurred will not affect the technical evaluation, and the package contents under normal conditions of transport will be less reactive than the contents under the aforementioned general requirements, requiring no further analysis.

To address the requirement of 10 CFR § 71.55(e), a single package was analyzed with optimum internal moderation and a 30-cm water reflector on all sides. The damaged package experienced a 4.7% reduction in diameter due to impact testing (see Chapter 2, Structural Evaluation). The packaging diameter reduction is to be analyzed as a reduction in insulating fiber board and plywood thicknesses while conserving the carbon steel drum, insulating fiber board, and plywood masses. Limited material loss occurred as a result of fire testing (see Chapter 3, Thermal Evaluation). The outer 0.8 in. (2.03 cm) of insulating fiber board (axially and radially) and plywood (radially) exhibited charring and off-gassing during the fire test. The regions were modeled as residual carbon and water (immersion test). The water from the immersion test optimally moderates the inner containment. The minimal damage resulting from crush and puncture tests (see Chapter 2, Structural Evaluation) will not influence the reactivity of the packages.

A.3.4 PACKAGE ARRAYS

Cylindrical transport packages such as this example package may be shipped in a tightly packed triangular-pitch configuration (or may be shifted to that configuration because of hypothetical accident conditions). This arrangement may provide a more reactive configuration than a square-pitch arrangement because the triangular pitch provides absolute minimum center-to-center spacing of the fissile contents, the maximum density of fissile units, and thus the greatest potential for increased neutron interaction between fissile contents. To avoid the complex modeling required to analyze triangular-pitch arrays with the computational method used in this application, a square-pitch array model with a modified single-package model was developed to emulate the effects of a triangular-pitch package array. The single-package modification involved a reduction of the drum diameter by 7% to produce an array density in a square-pitch lattice equal to the array density of a triangular-pitch lattice of packages with the full-diameter package. If the mass of steel of the drum and the mass of the insulating fiber board are conserved, the neutron reaction rates within the array are essentially identical. To conserve the mass of steel in this example, the drum wall density was increased; and to conserve the mass of the insulating fiber board in this example, the insulating fiber board density was increased. The diameter reduction was applied only to regions of the "array package model," not the "contents model."

The justification for the 7% diameter reduction is seen in the following derivation. Consider three full-diameter packages in contact on triangular pitch and four reduced-diameter packages in contact on square pitch. The equivalent array density of each configuration is

$$\rho_t = \frac{3(m/6)}{\left(\frac{1}{2}\right)(d_t)\left(\frac{\sqrt{3}}{2}\right) \times (d_t)(h)} = \frac{m}{(d_t^2)(\sqrt{3}/2)\,(h)} \ ,$$

and

$$\rho_s = \frac{4(m/4)}{(d_s^2)(h)} = \frac{m}{(d_s^2)(h)} \ ,$$

where

the subscripts *t* and *s* indicate triangular and square pitch, respectively,
d is the package diameter,
h is the package height (same for both packages), and
m is the fissile material mass (same for both packages).

If ρ_t is set equal to ρ_s and d_s is calculated in terms of d_t, the diameter of a square pitch is 0.9306 that of the triangular pitch, to produce the equivalent array density. If a constant mass of materials is maintained outside the fissile unit (i.e., the thermal insulation and steel outer drum), the neutron reaction rates between fissile units remain constant. Because the drum is smaller in diameter, the mass of thermal insulation is conserved by increasing the density, and the mass of steel in the outer drum is conserved by increasing the steel density.

Two array model types are included in the evaluation. The first model type consists of an infinite array of close-packed, triangular-pitch, undamaged packages consistent with the normal conditions of transport. From 10 CFR § 71.59, standards for arrays of fissile material packages, undamaged package arrays are evaluated with void between the packages. The second model type consists of various size finite arrays of close-packed triangular-pitch, damaged packages. As required by 10 CFR § 71.59, the damaged packages are evaluated as if each package was subjected to the tests specified in 10 CFR § 71.73, Hypothetical Accident Conditions, with optimum interspersed hydrogenous moderation. Further, the finite array of packages must be reflected by 30 cm of water on all sides.

Various finite array sizes had to be investigated in order to ascertain the number of subcritical packages under hypothetical accident conditions. The condition of each damaged package in the array is that described in Sect. A.3.3 for the single package.

A.4 METHOD OF ANALYSIS

Sections A.4.1 and A.4.2 describe the sequences and modules of the SCALE-4.3 system used in the analysis of these computational models. Section A.4.3 identifies all major code input parameters. Section A.4.4 discusses the adequacy of the calculations.

All calculations were performed on CA02 and CA29, IBM RS/6000 workstations in the Computational Physics and Engineering Division at ORNL with SCALE version 4.3 (1/6/97 production date) and the 44-group ENDF/B-V cross-section library.

A.4.1 COMPUTER CODE SYSTEM

SCALE is a computational system consisting of a set of well-established codes and data libraries suitable for analyses of nuclear fuel facility and package designs in the areas of criticality safety, radiation shielding, source-term characterization, and heat transfer. The codes are compiled in a modular fashion and are called by control modules that provide automated sequences for standard system analyses in each area. The CSAS control module contains automated sequences that perform problem-dependent cross-section processing and three-dimensional (3-D) Monte Carlo calculations of neutron multiplication.

KENO V.a, a 3-D multigroup Monte Carlo criticality code, determines the effective multiplication factor (k_{eff}) from the problem-dependent cross-section data and the user-specified geometry data. Other calculated

KENO V.a quantities include average neutron lifetime and generation time, energy-dependent leakages, energy- and region-dependent absorptions, fissions, fluxes, and fission densities.

A.4.2 CROSS SECTIONS AND CROSS-SECTION PROCESSING

All neutronic control sequences use the SCALE Material Information Processor to calculate material number densities, prepare geometry data for resonance self-shielding and optional flux-weighting cell calculations, and create data input files for the cross-section processing codes. The BONAMI and NITAWL-II codes are then used to perform problem-specific (resonance- and temperature-corrected) cross-section processing. BONAMI applies the Bondarenko method of resonance self-shielding for nuclides that have Bondarenko data included in the cross-section library. NITAWL-II uses the Nordheim integral treatment to perform resonance self-shielding corrections for nuclides that have resonance parameters included with their cross-section data.

The analyses discussed in this evaluation were performed using the broad-structure, 44-group neutron cross-section library. The 44-group library was chosen because the evaluated package contents have many similarities (e.g., form, enrichment) to light-water-reactor (LWR) fuel, and the 44-group library has demonstrated markedly improved performance in LWR-type fuel analyses over the ENDF/B-IV 27-group library. The reason: the 44-group neutron cross-section library was collapsed from the 238-group AMPX master-format neutron cross-section library contains data for all the nuclides available in ENDF/B-V, and the 44-group library was collapsed using a fuel cell spectrum based on a 17 × 17 Westinghouse pressurized-water-reactor (PWR) fuel assembly.

Additionally, the broad-group structure was designed to accommodate two windows in the oxygen cross-section spectrum, a window in the iron cross-section spectrum, the Maxwellian peak in the thermal range, and the 0.3-eV resonance in ^{239}Pu (which, because of low energy and lack of resonance data, cannot be modeled by the Nordheim integral treatment in NITAWL-II).

A.4.3 CODE INPUT

All problems were started with a flat initial neutron distribution over the system, in fissile material only. All problems were run for 305 generations of 400 neutrons per generation, skipping the first five generations, for a total of 120,000 histories. Mirror image reflection was applied to the orthogonal-plane boundaries of the single-package model to simulate infinite array-package models. A 12-in. (30.48-cm) water differential albedo with four incident angles was applied to the outer boundary of the single-package models and finite-array models to simulate tight, full-density water reflection. Biasing options were not applied.

Figures A.3(a) and A.3(b) are sample input files. The files correspond to cases **f-2_4** and **f-2_4a**, a 4 × 4 × 1 array of optimally moderated, damaged packages in square, with diameter correction factor of Sect. A.3.4, and triangular-pitch arrays.

A.4.4 CONVERGENCE OF CALCULATIONS

UO_2 mass data for each problem were checked against KENO V.a output. The input geometries were checked by examining the 2-D plots generated by KENO V.a. Problem convergence was determined by examining plots of k_{eff} by generation run and skipped, as well as the final k_{eff} edit tables. No trends were observed either in k_{eff} by generation run over the last half of total generations or, correspondingly, in k_{eff} by generation skipped over the first half of total generations. No sudden changes of greater than one standard deviation in k_{eff} by

```
=csas25
KENO-V.a, 4x4x1 array, optimally moderated damaged
'packages, square pitch, 4.7% and 7% diameter reduction
44g      latt
uo2 1 0.9489 293 92235 4.01 92234 0.02 92236 0.02 92238
             95.95 end
h2o   2 1.0      end
ss304 3 1.0      end
c  4 0 3.9250e-3 end
fe 4 0 8.3498e-2 end
h  5 0 1.293e-2  end
c  5 0 7.757e-3  end
o  5 0 6.464e-3  end
h  6 0 2.128e-2  end
c  6 0 1.277e-2  end
o  6 0 1.064e-2  end
c  7 0 4.550e-3  end
fe 7 0 9.679e-2  end
h  8 0 1.135e-2  end
c  8 0 6.809e-3  end
o  8 0 5.674e-3  end
c  9 0 7.757e-3  end
h2o   9 0.001    end
c 10 0 6.809e-3  end
h2o  10 0.001    end
h2o  12 1.0      end
end comp
squarepitch 1.34 0.8255 1 2 0.9296 3 0.889  12 end
read parm run=yes plt=no gen=305 npg=400 nsk=5 end parm
read geom
unit 1
cylinder 1 1 0.4128  2p33.02
cylinder 2 1 0.4445  2p33.02
cylinder 3 1 0.4648  2p33.02
cuboid   2 1 4p0.670 2p33.02
unit 2
cylinder 3 1 0.667   2p33.02
cuboid   2 1 4p0.670 2p33.02
unit 3
array 2 -4.02 0 -33.02
unit 4
array 3 -6.7  0 -33.02
unit 5
array 4 0 -4.02 -33.02
unit 6
array 5 0 -6.7  -33.02
unit 7
array 1 -10.72  -10.72   -33.02
cylinder 2 1 15.24   2p33.02
hole 6 10.72   0  0
hole 6 -12.06  0  0
hole 5 12.06   0  0
hole 5 -13.41  0  0
hole 4 0 10.72    0
hole 4 0 -12.06   0
hole 3 0 12.06    0
hole 3 0 -13.41   0
reflector 3  1 0 2r2.54   1
reflector 4  1 3r0.635    1
reflector 5  1 7.4165 2r0 1
reflector 9  1 2.032  2r0 1
reflector 6  1 0 2r2.54   1
reflector 8  1 0 2r10.668 1
reflector 10 1 0 2r2.032  1
reflector 7 1 0.1626 0.2032 0.1626 1
cuboid    0 1 4p25.4862 51.6383 -51.5977
global unit 8
array 6 3*0.0
end geom
read array
ara=1 nux=16 nuy=16 nuz=1 fill 2 14r1 2 224r1 2 14r1 2
end fill
ara=2 nux=6  nuy=1  nuz=1 fill 6r1  end fill
ara=3 nux=10 nuy=1  nuz=1 fill 10r1 end fill
ara=4 nux=1  nuy=6  nuz=1 fill 6r1  end fill
ara=5 nux=1  nuy=10 nuz=1 fill 10r1 end fill
ara=6 nux=4  nuy=4  nuz=1 fill 16r7 end fill
end array
read bnds all=h2o end bnds
end data
end
```

Figure A.3a Sample input file **f-2_4**

```
=csas26
KENO-VI, 4x4x1 array, optimally moderated damaged
'packages, triangular pitch, 4.7% diam. reduction
44g      latt
uo2 1 0.9489 293 92235 4.01 92234 0.02 92236 0.02 92238
95.95 end
h2o 2 1.0 end
ss304 3 1.0 end
c  4 0 3.9250e-3 end
fe 4 0 8.3498e-2 end
h  5 0 1.029e-2  end
c  5 0 6.173e-3  end
o  5 0 5.144e-3  end
h  6 0 1.841e-2  end
c  6 0 1.105e-2  end
o  6 0 9.207e-3  end
c  7 0 4.167e-3  end
fe 7 0 8.864e-2  end
h  8 0 9.821e-3  end
c  8 0 5.892e-3  end
o  8 0 4.910e-3  end
c  9 0 6.173e-3  end
h2o 9  0.001     end
c 10 0 5.892e-3  end
h2o 10 0.001     end
h2o 11 1.0       end
end comp
squarepitch 1.34 0.8255 1 2 0.9296 3 0.889  11 end
read parm run=yes plt=no gen=305 npg=400 nsk=5 end parm
read geom
unit 1
cylinder 10 0.4128  2p33.02
cylinder 20 0.4445  2p33.02
cylinder 30 0.4648  2p33.02
cuboid   40 4p0.670 2p33.02
media 1 1 10
media 2 1 20 -10
media 3 1 30 -20 -10
media 2 1 40 -30 -20 -10
boundary 40
unit 2
cylinder 10 0.667   2p33.02
cuboid   20 4p0.670 2p33.02
media 3 1 10
media 2 1 20 -10
boundary 20
unit 3
cuboid   10 4p0.670 2p33.02
media 2 1 10
boundary 10
unit 4
cylinder 10 15.24 2p33.02
array 1 10 place 12 12 1 -0.67 -0.67 0
cylinder 20  15.24   2p35.56
cylinder 30  15.875  2p36.195
cylinder 40  25.1922 2p36.195
cylinder 50  27.2242 2p36.195
cylinder 60  27.2242 2p38.735
cylinder 70  27.2242 2p49.403
cylinder 80  27.2242 2p51.435
cylinder 90  27.3868 51.6382 -51.5976
hexprism 100 27.3869 51.6383 -51.5977
media 3  1 20  -10
media 4  1 30  -20
media 5  1 40  -30
media 9  1 50  -40
media 6  1 60  -50
media 8  1 70  -60
media 10 1 80  -70
media 7  1 90  -80
media 0  1 100 -90
boundary 100
unit 5
hexprism 10 27.3869 51.6383 -51.5977
media 2 1 10
boundary 10
global unit 6
cylinder 10 189.74  51.6383 -51.5977
array 2 10 place 5 5 1 -27.3869 -27.3869 0
cylinder 20 225. 2p82.
media 2 1 20 -10
boundary 20
end geom
read array
ara=1 nux=24 nuy=24 nuz=1 fill 48r3 9r3 6r1 9r3 7r3 10r1
7r3 4r3 2 14r1 2 4r3 4r3 16r1 4r3 1q24 3r3 18r1 3r3 1q24
2r3 20r1 2r3 5q24 3r3 18r1 3r3 1q24 4r3 16r1 4r3 1q24
4r3 2 14r1 2 4r3 7r3 10r1 7r3 9r3 6r1 9r3 48r3 end fill
ara=2 typ=tri nux=10 nuy=10 nuz=1 fill 30r5 4r5 4r4 2r5
3r5 4r4 3r5 3r5 4r4 3r5 2r5 4r4 4r5 30r5 end fill
end array
end data
end
```

Figure A.3b Sample input file **f-2_4a** generation run or skipped, resulting from an abnormal k_{eff} generation, were found. Frequency distribution bar graphs appear to approximate normal distribution with single peaks and no significant outlying values.

A.5 VALIDATION OF CALCULATION METHOD

For the purpose of this example, a negative value of 0.01 will be assumed for the bias and uncertainty ($\Delta k_u - \bar{\beta}$) associated with using SCALE-4.3 and the 44-group cross-section library. This is consistent with published information on validation of this computational method using low-enriched lattice criticals.[10,12] Note: The applicant should demonstrate the justification for the bias and uncertainty in the application for approval.

Using the general equation for the USL from Sect. 5.4 and the requirements of 10 CFR 71, it can be found that for the calculations to be considered subcritical, the following condition should be satisfied:

$$k_{eff} + 2\sigma \le 0.95 - \Delta k_u + \bar{\beta} \ ,$$
$$k_{eff} + 2\sigma \le 0.94 \ .$$

A.6 CRITICALITY CALCULATIONS AND RESULTS

This evaluation demonstrates the subcriticality of a single package (Sect. A.6.1) and an array of packages (Sect. A.6.2) during normal conditions of transport and hypothetical accident conditions. The determined TI for criticality control of a damaged and undamaged shipment is given in Sect. A.6.3.

A.6.1 SINGLE PACKAGE

Calculations show that a single package remains subcritical under general requirements for fissile material packages under normal conditions of transport and under hypothetical accident conditions. To meet the general requirements for fissile material packages, 10 CFR § 71.55, a package must be designed and its contents so limited that it would be subcritical under the most reactive configuration of the material, optimum moderation, and close reflection of the containment system by water on all sides or surrounding materials of the packaging. Case **s-0** of Table A.4 represents the optimally moderated inner containment reflected on all sides by 30 cm of water. For case **s-1**, the container reflection is provided by the surrounding materials of the packaging and 30 cm of water. In both cases, the gap region between the tubes and pellets are completely flooded with full-density water, as is the void region in the inner container (Region A of Fig. A.2). Full-density water is optimum in both regions because the fissile content of the package is slightly undermoderated at a tube pitch of 1.34 cm (see Fig. A.4). The highest single-package k_{eff} of 0.8942 ± 0.0019 is considered subcritical (i.e., $0.8942 + 2 \cdot 0.0019 = 0.8980 < 0.94$).

Case **s-2** in Table A.4 is the result for a single damaged package with internal water flooding and 30 cm of water reflection on all sides. As with the undamaged cases, the reported k_{eff} is less than the established USL of 0.94. The results for a reflected, damaged containment system would have been identical to the undamaged case (case **s-0**) because the configurations of the containment system or contents did not change under hypothetical accident conditions.

All calculations (damaged and undamaged) were performed at the maximum allowable ^{235}U enrichment (4.01 wt %) to ensure maximum reactivity and eliminate the need for calculations at lower possible enrichments.

Table A.4 Single-package calculations

Case	Description	$k_{eff} \pm \sigma$
s-0	Optimally moderated, reflected undamaged containment	0.8942 ± 0.0019
s-1	Optimally moderated, reflected undamaged package	0.8798 ± 0.0019
s-2	Optimally moderated, reflected damaged package	0.8820 ± 0.0018

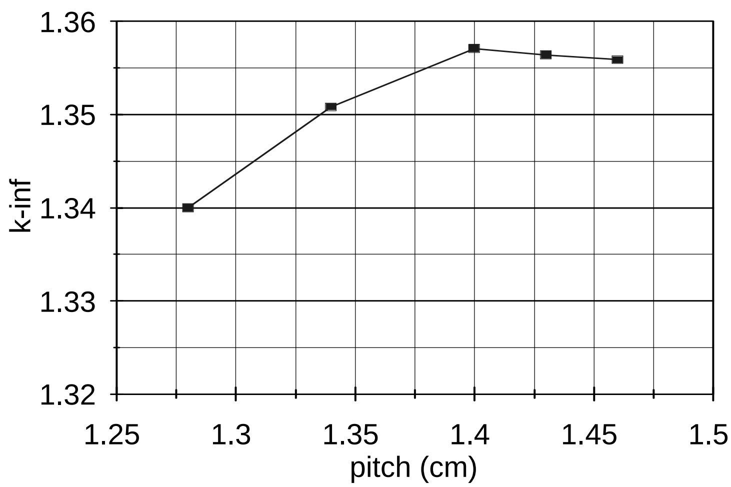

Figure A.4 k_∞ vs pitch for 4.01 wt % ^{235}U UO_2 pellets

A.6.2 PACKAGE ARRAYS

The calculational results of Table A.5 show that an infinite array of packages is adequately subcritical under normal conditions of transport. Case **i-1**, an infinite, triangular-pitch array of dry packages under normal conditions, calculates at a k_{eff} of 0.5343 ± 0.0012. An infinite array of packages under hypothetical accident conditions, however, is not subcritical. Case **i-2_7** represents an infinite array of close-packed, triangular-pitch (diameter reduction factor), flooded packages with optimum moderated contents, a 4.7% reduction in diameter, effects due to charring and off-gassing, and optimum interspersed moderation. The k_{eff} for case **i-2_7** is 0.9755 ± 0.0021, which exceeds the subcritical limit (i.e., $0.9755 + 2\cdot0.0021 = 0.9797 > 0.94$). Since the infinite array under hypothetical accident conditions calculates above the USL, finite array calculations are necessary.

Cases **i-3_1** through **i-3_3** are variants of **i-2_7** that investigate flooding of the insulating fiber board charred region. The optimally moderated package array **i-3_2** has full-density water inside the package containment, has 0.001 g H_2O/cm^3 in the charred region of the packaging, and has void between packages.

Table A.5 Results for triangular-pitch array calculations

Case	Interspersed H_2O density (g/cm^3)	Description	$k_{eff} \pm \sigma$
i-1	0	Infinite array, normal conditions of transport	0.5343 ± 0.0012
f-1	–	1×1×1 array, hypothetical accident conditions	0.8820 ± 0.0018
i-2_1	0.9982	Infinite, hypothetical accident conditions	0.9238 ± 0.0021
i-2_2	0.95	Infinite, hypothetical accident conditions	0.9237 ± 0.0021
i-2_3	0.5	Infinite, hypothetical accident conditions	0.9297 ± 0.0023
i-2_4	0.1	Infinite, hypothetical accident conditions	0.9618 ± 0.0025
i-2_5	0.01	Infinite, hypothetical accident conditions	0.9716 ± 0.0024
i-2_6	0.001	Infinite, hypothetical accident conditions	0.9718 ± 0.0024
i-2_7	0[a]	Infinite, hypothetical accident conditions	0.9755 ± 0.0021
i-3_1	0	Infinite, hypothetical accident conditions, 0 g H_2O/cm^3 charred region	0.9755 ± 0.0021
i-3_2	0	Infinite, hypothetical accident conditions, 0.01[b] H_2O/cm^3 charred region	0.9772 ± 0.0027
i-3_3	0	Infinite, hypothetical accident conditions, 0.01 g H_2O/cm^3 charred region	0.9759 ± 0.0022
f-2_1	0	2×2×1 array, hypothetical accident conditions	0.9103 ± 0.0018
f-2_2	0	2×2×2 array, hypothetical accident conditions	0.9158 ± 0.0018
f-2_3	0	3×3×1 array, hypothetical accident conditions	0.9270 ± 0.0017
f-2_4	0	4×4×1 array, hypothetical accident conditions	0.9369 ± 0.0019
f-2_4a	0	4×4×1 array, hypothetical accident conditions	0.9335 ± 0.0028[c]
f-2_5	0	3×3×2 array, hypothetical accident conditions	0.9306 ± 0.0017
f-2_6	0	5×5×1 array, hypothetical accident conditions	0.9284 ± 0.0019
f-2_7	0	3×3×3 array, hypothetical accident conditions	0.9405 ± 0.0023
f-2_8	0	4×4×2 array, hypothetical accident conditions	0.9359 ± 0.0017

[a]Determined to be near optimum interstitial moderation via CSAS4 search**.**
[b]Determined to be new optimum moderation via CSAS4 search
[c]KENO-VI calculation.

Cases **f-2_1** through **f-2_8** are variants of case **i-3_2** and represent finite arrays of close-packed, triangular-pitch packages (diameter reduction factor) that have optimally moderated contents, a reduced diameter by 4.7%, charred insulating fiber board, varying interstitial moderation, and 30 cm of full-density water reflection tightly fit on the array boundary. The finite array of $4 \times 4 \times 2$ (case **f-2_8**) packages is considered just subcritical because $0.9359 + 2 \cdot 0.0017 = 0.9393$ falls below the USL of 0.94.

Case **f-2_4a** is equivalent to case **f-2_4a** except that **f-2_4a** was modeled with KENO-VI, which allows explicit modeling of triangular-pitch arrays and does not require the use of the drum diameter reduction factor of Sect. A.3.4. The calculational results of **f-2_4** and **f-2_4a** are statistically the same, attesting to the correctness of the diameter reduction factor.

A.6.3 TRANSPORTATION INDEX

The TI for criticality control is determined by the number of packages that remain below the USL. For normal conditions of transport, an infinite array of packages is subcritical. However, under hypothetical accident conditions, only up to 32 damaged packages would remain subcritical. Thus a maximum of 16 packages may be shipped for a nonexclusive shipment, and the TI = 3.

Note: The example presented in this appendix is for illustrative purposes only. The fictitious transport package used in this example has not been approved by the NRC, and no assessment has been made as to whether the package would meet the requirements for NRC approval. Also, the descriptions, calculations, and justifications presented in this example have not been fully reviewed by the NRC, and may not be complete or acceptable to the NRC.

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11. ABSTRACT ***(200 words or less)***

This report provides recommendations on preparing the criticality safety section of an application for approval of a transportation package containing fissile material. The analytical approach to the evaluation is emphasized rather than the performance standards that the package must meet. Where performance standards are addressed, this report incorporates the requirements of 10 CFR Part 71.

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