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Development and Applications of a Prototypic SCALE Control Module for Automated Burnup Credit Analysis

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Executive Summary

Consideration of the depletion phenomena and isotopic uncertainties in burnup-credit criticality analysis places an increasing reliance on computational tools and significantly increases the overall complexity of the calculations. An automated analysis and data management capability is essential for practical implementation of large-scale burnup credit analyses that can be performed in a reasonable amount of time. STARBUCS is a new prototypic analysis sequence being developed for the SCALE code system to perform automated criticality calculations of spent fuel systems employing burnup credit. STARBUCS is designed to help analyze the dominant burnup credit phenomena including spatial burnup gradients and isotopic uncertainties. A search capability also allows STARBUCS to iterate to determine the spent fuel parameters (e.g., enrichment and burnup combinations) that result in a desired k_{eff} for a storage configuration. Although STARBUCS was developed to address the analysis needs for spent fuel transport and storage systems, it provides sufficient flexibility to allow virtually any configuration of spent fuel to be analyzed, such as storage pools and reprocessing operations. STARBUCS has been used extensively at Oak Ridge National Laboratory (ORNL) to study burnup credit phenomena in support of the NRC Research program.

1. Introduction

The Nuclear Regulatory Commission (NRC) Interim Staff Guidance 8 (ISG8), Rev. 1 [1], provides guidance on the application of actinide-only burnup credit in criticality safety analyses for pressurized water reactor (PWR) spent fuel in transportation and storage casks. In contrast to criticality safety analyses that employ a fresh-fuel assumption (i.e., conservatively assuming unirradiated fuel compositions), burnup credit requires the prediction of both fissile and absorbing nuclide inventories in spent nuclear fuel (SNF) and consideration of the many burnup-related phenomena, in addition to the criticality issues. Consideration of the burnup-simulation aspects in the criticality assessment of SNF places an increasing reliance on computational tools and methods, significantly increasing the overall complexity of the criticality analysis and necessitating consideration of many additional sources of uncertainty associated with fuel depletion phenomena.

To assist in performing and reviewing criticality safety assessments of transport and storage casks that apply burnup credit, a new prototypic SCALE control sequence, STARBUCS (Standardized Analysis of Reactivity for Burnup Credit using SCALE) has been created. STARBUCS automates the calculation of the spatially-varying isotopic compositions in a spent fuel assembly, and applies the compositions in a three-dimensional (3-D) Monte Carlo model of the system. STARBUCS automatically prepares input files for each of the codes in the analysis sequence, executes the codes through the SCALE system driver, and performs all flow control, module interface, and data management functions. The new STARBUCS sequence uses the well-established code modules currently available in the SCALE-4 code system [2].

2. Program Description

STARBUCS automates the criticality analysis of spent fuel configurations by coupling the depletion and criticality aspects of the analysis, thereby eliminating the need to manually process the spent fuel nuclide compositions into a format compatible with criticality safety codes. STARBUCS performs a depletion analysis calculation for each spatially-varying burnup region of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. The ORIGEN-ARP methodology serves as a faster alternative to the SAS2H depletion analysis sequence in SCALE, while maintaining calculational accuracy. The spent fuel compositions are then used to generate resonance self-shielded cross sections for each burnup-dependent fuel region using the SCALE Criticality Safety Analysis Sequence, CSAS. Finally, a KENO V.a criticality calculation is performed using the spatially-varying cross sections to determine the neutron multiplication factor for the system. The overall structure of STARBUCS, illustrating the modules executed in the calculational sequence, is shown in Figure 1.

3. Depletion Analysis Methods

Depletion analysis is performed using the ORIGEN-ARP methodology of SCALE. The ARP module uses algorithms that interpolate cross sections as a function of enrichment, burnup, and optionally, moderator density, to generate the problem- and time-dependent cross-section libraries for the ORIGEN-S burnup calculation. STARBUCS repeatedly executes ARP and ORIGEN-S, in sequence, until the compositions of all unique fuel regions have been calculated. The ARP cross-section libraries must be created in advance of the STARBUC analysis, or the user may select from ARP libraries distributed with the SCALE system (e.g., 8×8, 14×14, 15×15, 17×17). The primary motivation for using ARP is speed. A typical depletion calculation using SAS2H takes approximately 5 minutes of CPU time on a fast machine. For calculations involving many axial and/or radial spatial zones (e.g., > 10), the depletion analysis time for all zones can represent more the 2/3 of the total time required for a burnup credit calculation. An equivalent calculation using ARP takes about 5 seconds per spatial zone, which represents a reduction by more than a factor of 50. This can reduce the total time for a typical STARBUCS calculation by a factor of 3 or more.

The time savings is achieved by the ability of ARP to use pre-generated cross sections, tabulated as a function of enrichment, burnup, and moderator density. A depletion calculation using SAS2H generates the cross sections for the ORIGEN-S calculation “on the fly” using user-supplied fuel design and reactor operating conditions. The generation of problem-dependent

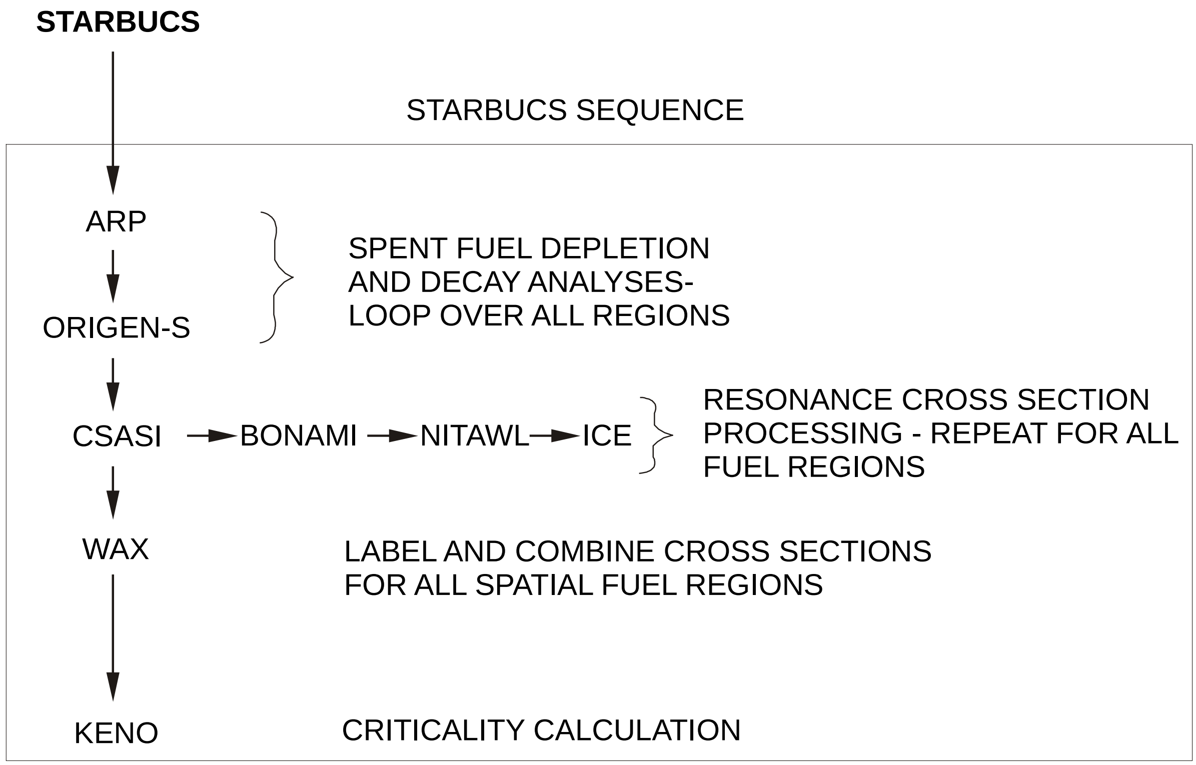

Figure 1. STARBUCS calculational sequence and flow.

cross sections represents the majority of computing time in SAS2H. ARP interpolates from cross-section libraries created by SAS2H to generate the problem-dependent cross sections for the ORIGEN-S calculation. The ORIGEN-ARP methodology maintains the accuracy of SAS2H and reproduces results from SAS2H calculations in a small fraction of the time. The one limitation is that appropriate cross sections reflecting the fuel design and reactor operating conditions (other than moderator density) must be available in advance of the STARBUCS calculation.

4. Criticality Calculation

The spent fuel isotopics from the multiple depletion calculations are used to generate macroscopic fuel cross sections for each spatially-varying burnup region of the assembly using the SCALE Criticality Safety Analysis Sequence (CSAS). STARBUCS automatically generates input for a series of CSASI (BONAMI-NITAWL-ICE) calculations using the spent fuel compositions for each spatial region. The BONAMI and NITAWL modules perform resonance self shielding in the resolved and unresolved resonance groups. The ICE module creates a library of self-shielded macroscopic fuel cross sections for each region, significantly reducing the data management associated with tracking individual isotopic concentrations for each region, and reducing the size of the cross-section library.

The criticality calculation is performed using the 3-D KENO V.a Monte Carlo (optionally KENO-VI) code to determine the k_{eff} for the system. The criticality calculation uses the cross-section library created using the spent fuel concentrations from the depletion calculations. Unique material numbers are assigned to each spatially-varying burnup zone. All of the KENO geometry features and parameter options are available to the user, allowing virtually any configuration of spent fuel to be simulated, within the capabilities of the KENO codes.

5. STARBUCS Capabilities

The prototypic STARBUCS control module is designed to facilitate burnup credit criticality analysis by automating and linking the depletion analysis and criticality calculations. The input format has been designed around the existing depletion analysis and criticality safety sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel calculation is needed to perform a burnup credit calculation.

STARBUCS has been designed specifically to allow analysts and reviewers to assess the major burnup credit phenomena identified in the NRC Interim Staff Guidance 8 (ISG8). Specifically, STARBUCS allows the user to:

1. Input an arbitrary axial and/or horizontal assembly burnup gradient. The spatial burnup distribution may be controlled entirely by the user. Optionally, built-in “bounding” axial profiles may be selected by the user. A maximum of 100 axial and 10 horizontal zones may be defined.

2. Any or all of the spent fuel actinide or fission product isotopes may be included in the criticality calculation. The user may select from any of the more than 1000 nuclides in the ORIGEN-S libraries, provided cross sections are available for the KENO calculation. This allows the fission product margin to be readily evaluated. Optionally, the user may request all nuclides to be included to obtain “best-estimate” results.

3. The burnup calculations can specify any desired operating history. The user may specify the assembly-average specific fission power, cycle lengths, cycle down time, and post irradiation cooling time. This allows the user to readily evaluate power history and cooling time effects.

4. Isotopic correction factors may be input to adjust the calculated isotopic inventories to acount for known bias and/or uncertainties associated with the depletion calculations.

5. Virtually any arrangement of spent fuel may be simulated. STARBUCS is not restricted to spent fuel transport and storage cask analysis. Any KENO geometry model is permissible. For example, spent fuel arrays in a storage pool could be easily simulated.

6. An iterative search capability is currently being developed for STARBUCS. This option will allow multiple burnup credit calculations to be performed using a search parameter to determine the types of fuel acceptable for cask loading. This capability will automate the generation of cask loading curves.

6. Validation and Verification Studies

STARBUCS uses the existing, well-established modules of the SCALE system that have each been validated independently. The ORIGEN-ARP sequence has been validated in comparisons against SAS2H and measured isotopic assay data [3]. Similarly a large number of validation exercises involving KENO V.a have been published [4].

The application of KENO V.a to the analysis of configurations of spent fuel using isotopic concentrations calculated by ORIGEN-S has also been extensively validated using commercial reactor critical (CRC) benchmarks [5]. A recent CRC validation study involving LaSalle reactor state-points [6] was performed using isotopic concentrations from ORIGEN-S (SAS2H methodology) and used the CSASI and KENO V.a codes to perform the criticality calculation. These results, and others using similar techniques, indicate that the STARBUCS methodology is appropriate and accurate.

STARBUCS results have also been compared against independent codes and cross-section libraries. Specifically, burnup credit calculations were performed for a generic 32-assembly rail-type transport cask (GBC-32), loaded with Westinghouse 17×17 assemblies, in the context of a numerical benchmark [7] that can be used to assess the ability of different computational methods [8] to calculate the fission product margin for the configuration. Reference 7 provides results of analyses performed with the SAS2H (depletion) and CSAS25 (criticality) sequences of the SCALE 4.4a code package. Reference 8 presents results of analyses performed with HELIOS-1.6 (depletion) and KENO V.a (criticality) codes as well as HELIOS-1.6 (depletion) and MCNP4B (criticality) codes. A summary of the results is given in Table 1. Note that a subset of actinide nuclides was used for the burnup credit calculations (i.e., actinide-only burnup credit). The STARBUCS results agree to within Δk = 0.5% of the results using alternate codes and cross-section data.

Table 1. K_{eff} values with uniform axial burnup for the cask as a function of burnup. The results correspond to an initial fuel enrichment of 4.0 wt % ^{235}U and no cooling time (discharge).

Burnup (MWd/kgU)	K_{eff} [a] (HELIOS/KENO)	K_{eff} (SAS2/CSAS25)	K_{eff} (HELIOS/MCNP)	K_{eff} (STARBUCS)
0	1.1398 ± 0.0005	1.1398 ± 0.0007	1.1399 ± 0.0046	1.1397 ± 0.0005
20	1.0399 ± 0.0006	1.0425 ± 0.0006	1.0392 ± 0.0041	1.0392 ± 0.0006
60	0.8559 ± 0.0004	0.8675 ± 0.0006	0.8628 ± 0.0037	0.8626 ± 0.0005

[a] (depletion code / criticality code).

7. Search Feature

A search capability in STARBUCS is currently being developed. This feature will allow repeated burnup credit criticality calculations to be performed, using a least-squares analysis of the results to automatically adjusting a search parameter, such as burnup, until a desired k_{eff} is obtained within a desired tolerance. A prototype of this option has been implemented and used to generate cask loading curves, which define the acceptable enrichment and burnup combinations of spent fuel that may be loaded into a burnup credit cask.

Currently, a typical STARBUCS calculation (actinide only) requires approximately 1 hour on a very fast computer. Based on experience to date, roughly five iterations are needed to converge a parameter to a desired k_{eff} using the least squares approach. Assuming it takes at least ten points to adequately characterize a loading curve, more than 50 STARBUCS calculations representing more then 2 days of continuous computing time, would be needed. The need and advantage of implementing an automated search capability is apparent.

8. Application to Loading Curve Generation

Several loading curves are presented for the GBC-32 rail-type burnup credit cask, loaded with Westinghouse 17×17 OFA assemblies. A cross section of the GBC-32 cask model is shown in Figure 2.

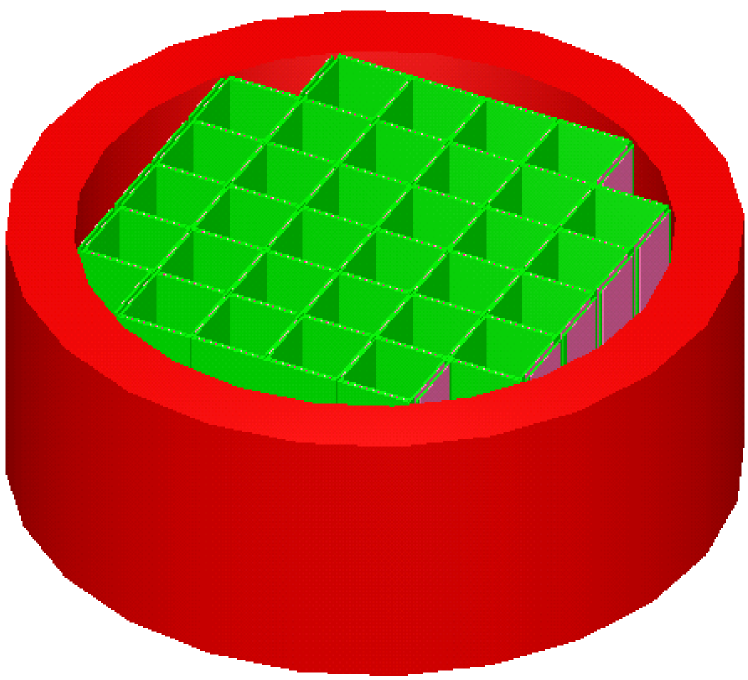

Figure 2. Cross-section view of the GBC-32 cask (unloaded)

Figure 3 compares the loading curves for the 17×17 assembly design assuming burnup credit for actinide-only, and major actinides plus fission products, assuming a 5 year cooling time. The actinide-only curves are presented both with and without bounding isotopic correction factors (ICFs) obtained from Ref. [9]. These loading curves are superimposed on the actual inventory of spent commercial PWR fuel up to 1999 to provide a qualitative indication of the amount of fuel that could be considered acceptable, or unacceptable for loading in a burnup credit cask for the different analysis assumptions. A burnup-dependent axial burnup profile was used for the calculations. The profiles correspond to the three bounding profiles suggested by Ref. [10] for PWR fuel with average-assembly discharge burnups less than 18 GWd/t, 18 to 30 GWd/t, and greater than 30 GWd/t. The discontinuities in the loading curves at 18 and 30 GWd/t are caused by the change in axial profile for the different burnup ranges. It is interesting to note that the vast majority of the current inventory of spent PWR fuel would be considered acceptable for loading in the GBC-32 cask with actinide-only burnup credit, provided that the bounding and highly conservative isotopic correction factors are not applied. This illustrates the importance of selecting realistic correction factors that are not overly conservative.

Figure 4 shows the loading curves 14×14, 15×15, 16×16, and 17×17 fuel assembly designs for a 5 year cooling time and actinide-only burnup credit. Spent fuel with enrichment and burnup combinations that lie below the curve would be considered unacceptable for loading, while fuel above the curve would be acceptable for loading. The importance of the fuel assembly type is comparable to the importance of actinide-only vs. actinide plus fission product assumptions. The 14×14 and 16×16 fuel assembly designs have very similar loading curves while the 15×15 and 17×17 fuel assembly designs display similar results. This is partially due to the fact that the 14×14 and 16×16 fuel assembly designs are smaller and have large water holes (four fuel lattice sites) while the 15×15 and 17×17 fuel designs are larger and have regular sized guide tubes (single lattice sites).

9. Summary

The complexity and computational requirements involved in burnup credit calculations necessitates automation of the calculations for the practical implementation of burnup credit. This is particularly true for loading curve calculations where continuous computing times of several days may be required. The STARBUCS prototype module has been developed at ORNL as a SCALE control module to automate and link the depletion and criticality aspects of the analysis, and provide a standardized analysis methodology. The STARBUCS module performs all code input generation, data management, code interface, and code execution functions. The high degree of automation eliminates the need for analyst intervention during the calculational sequence to manually process and transfer large quantities of intermediate results between codes, or prepare various utility codes to aid in this task, greatly reducing the potential for user error. Although STARBUCS is specifically designed to assist in the analysis and review of spent fuel cask criticality analyses, the module is sufficiently flexible to allow virtually any configuration of spent fuel to be assessed.

It is anticipated that STARBUCS will be released as a standard control module in SCALE-5. The implementation of advanced options, such as the search capability, will depend largely on the level of interest and support.

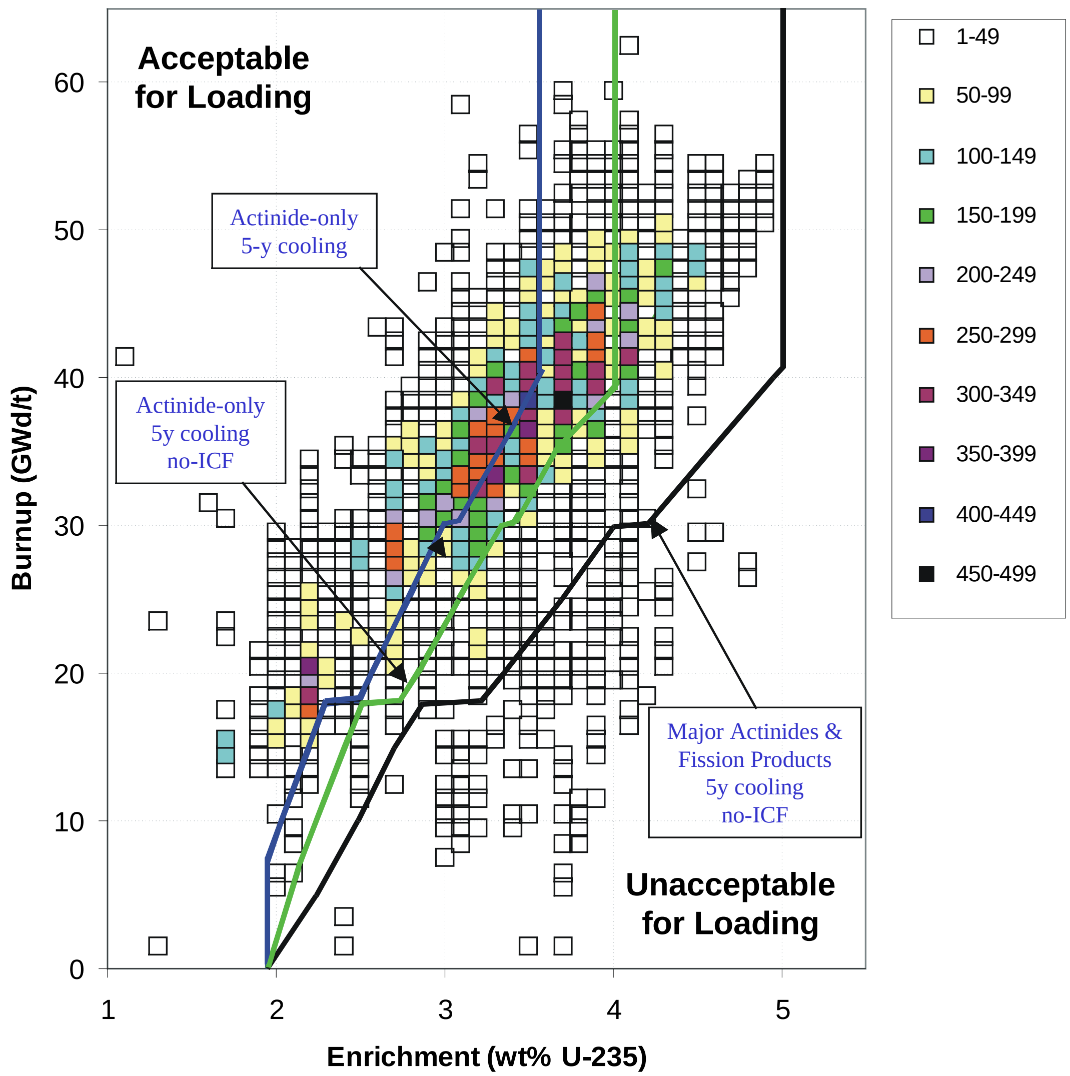

Figure 3. Illustrative loading curves for GBC-32 cask with 17×17 fuel assemblies calculated using the search capability in STARBUCS, plotted over the inventory of discharged PWR fuel up to 1999 (numbers in legend indicate the number of assemblies).

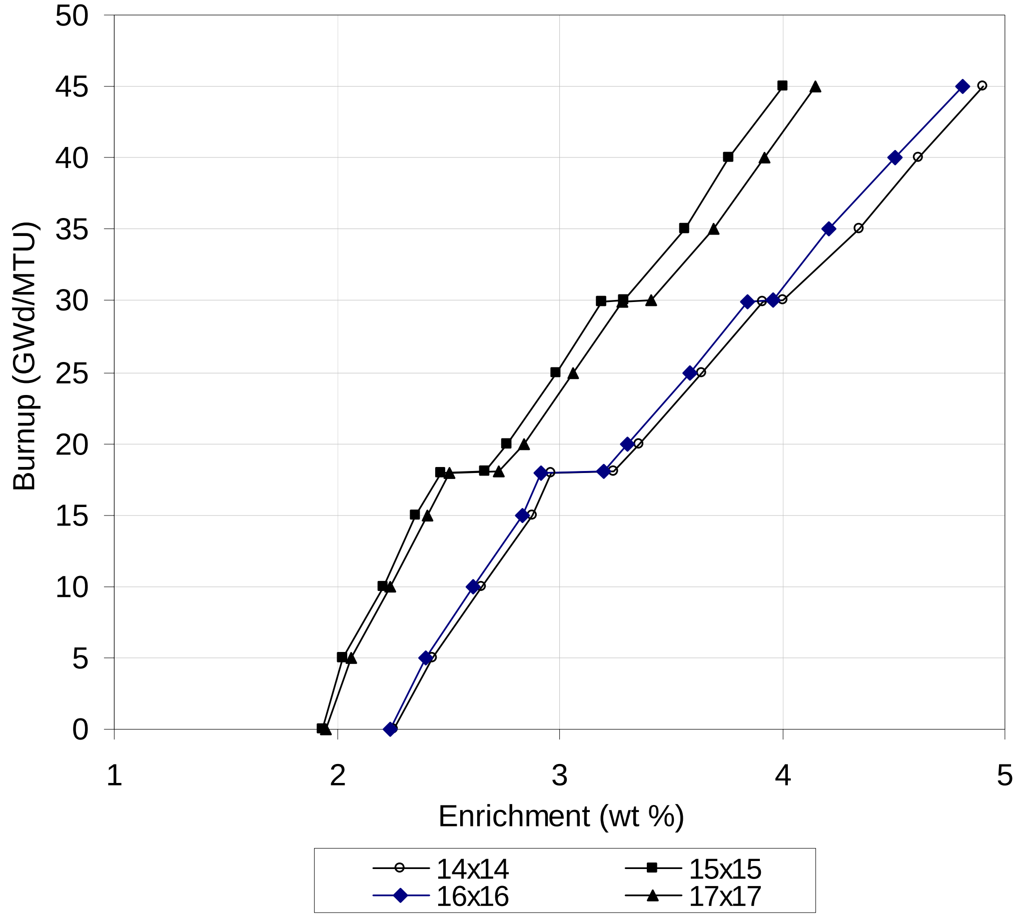

Figure 4. Illustrative loading curve for actinide-only burnup credit nuclides in 14×14, 15×15, 16×16, and 17×17 fuel assemblies in the GBC-32 cask, calculated using the search capability in STARBUCS.

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