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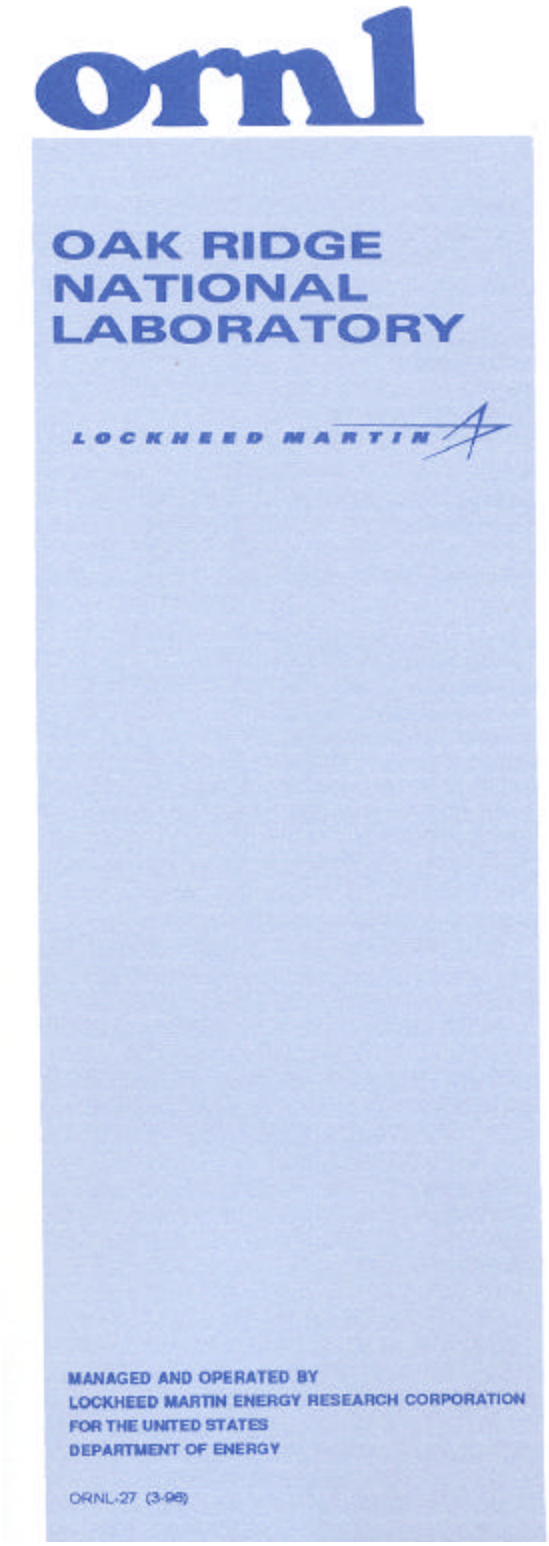

Parametric Analysis of PWR Spent Fuel Depletion Parameters for Long-Term-Disposal Criticality Safety

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Computational Physics and Engineering Division

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Parametric Analysis of PWR Spent Fuel Depletion Parameters for Long-Term-Disposal Criticality Safety

M. D. DeHart

ABSTRACT

Utilization of burnup credit in criticality safety analysis for long-term disposal of spent nuclear fuel allows improved design efficiency and reduced cost due to the large mass of fissile material that will be present in the repository. Burnup-credit calculations are based on depletion calculations that provide a conservative estimate of spent fuel contents (in terms of criticality potential), followed by criticality calculations to assess the value of the effective neutron multiplication factor (k_{eff}) for a spent fuel cask or a fuel configuration under a variety of probabilistically derived events. In order to ensure that the depletion calculation is conservative, it is necessary to both qualify and quantify assumptions that can be made in depletion models.

This report describes calculations performed at the Oak Ridge National Laboratory (ORNL) to assess the relative effects of depletion modeling assumptions on the predicted value of the neutron multiplication factor for an infinite lattice (k_{inf}) of pressurized-water-reactor (PWR) fuel. Calculations are performed assuming an infinite lattice of a Westinghouse 17 H 17 fuel pin design. It is anticipated that trends identified for such fuel will be generally applicable to specific cask designs; however, design-specific calculations are likely to be necessary in licensing that design. Furthermore, because of significant differences between pressurized- and boiling-water reactors (BWRs), results in this report are not applicable to the depletion analysis of BWR fuels.

1. INTRODUCTION

Historically, criticality analysis of spent fuel from light-water-reactor (LWR) operations has been based on the assumption that the fuel is fresh (i.e., comprised of its initial isotopic loading). This approach is extremely conservative, because it does not take into account the decrease in reactivity caused by the depletion of fissile nuclides and the simultaneous buildup of fission-product and higher-actinide neutron poisons during operation. This reactivity decrease is substantial in most fuel removed from a reactor; in fact, the fuel eventually must be removed because the net negative reactivity of actinide and fission product poisons makes continued reactor operation impossible.

Although the conservatism of the fresh-fuel assumption allows for a considerable safety margin, it limits the amount of spent fuel that can be stored within a fixed storage medium (e.g., cask, rack, or pool). Hence, there is an offsetting cost associated with the fresh-fuel assumption. Economic forces have driven a desire to find a balance between conservatism in criticality safety and more accurate representation of spent fuel contents. This approach, which is based on taking partial credit for the reactivity of spent fuel, is called "burnup credit." Beginning in the late 1980s, the U.S. Department of Energy began to investigate burnup credit as a safe, but more economic, alternative to the fresh-fuel assumption for the storage, transportation, and disposal of spent nuclear fuel.[1-9]

Significant work has been performed at ORNL in the study of phenomena related to spent fuel analysis.[10-22] Much of the early work focused on issues related to the transportation of pressurized-water-reactor (PWR) fuel, although some study of boiling-water-reactor (BWR) behavior has also been documented.[21–22] Current work described in this report builds on the

earlier work performed in the sensitivity analysis of PWR spent fuel[10] by (1) applying more realistic axial-burnup profiles in the analyses, and (2) performing parametric analyses using three-dimensional (3-D) KENO V.a calculations based on these burnup profiles, rather than the one-dimensional (1-D) analyses of ref. 10. The purpose of this report is to document a series of calculations performed to assess the effect of various simplifying assumptions on the predicted value of k_{inf} as a function of burnup, enrichment, and cooling time for PWR fuel. Parameters studied in this report are based on conditions expected for PWR operation. Although similar conditions (e.g., fuel temperatures) may exist in BWR or other reactor designs, it is not appropriate to apply results reported herein for other such designs.

2. PROCEDURE

Several different modeling parameters were examined in the course of this work: axial-burnup profile, operating history, specific power, temperature, and soluble boron concentration. Each of these parameters was studied over a range of enrichments, burnups, and cooling times. However, because it was not feasible to study each of the parameters as a function of all other parameters, separability was assumed to reduce the required number of calculations to a manageable figure. Thus each of the listed parameters was studied independently as a function of enrichment, burnup, and cooling time.

All calculations were performed using SCALE 4.3, running on a DEC AlphaStation 500. Depletion calculations were performed using the SCALE SAS2H control sequence, and criticality calculations were performed using the SCALE CSAS25 (KENO V.a) sequence. All calculations were performed using the SCALE 44-group (ENDF/B-V) library. A utility code named CASKET (Computational Analysis of the Sensitivity of k_{inf} for Examination of Trends) was developed to automate the process of model development for a variety of initial conditions and modeling assumptions. Different versions of CASKET were developed for different types of analyses. Source-code listings of all versions are available in the Appendix.

The fuel model consisted of a single pin in an infinite lattice, subdivided into 18 uniform-height axial zones. Axially varying burnup profiles were applied, and depletion calculations were performed for each axial level. The criticality model contained isotopic specifications for each axial zone. The study of axial-burnup profiles and the development of a simplified axial model are described in the following section. The results of the axial-profile study were used as a basis for the subsequent analysis of other parameters, as described in the ensuing sections.

2.1 AXIAL-BURNUP PROFILES

As fuel is burned in a PWR, the burnup of the fuel becomes distributed axially. The initial profile is uniform (assuming uniformly enriched fuel), but, after startup, fuel is burned faster near the center of the fuel than at the ends. The burnup profile generally attains a flattened cosine shape with time, though the exact profile will vary significantly with reactor design, operation history, the use of control rods or burnable poison rods, a non-uniform initial loading, or other effects. In order to conservatively represent the reactivity worth of spent fuel for any PWR design and operating history, it is necessary to define a "bounding" axial-burnup profile, or a set of burnup-dependent bounding profiles. The issue of determining a bounding profile has been studied for several years,[10,23] and is still an ongoing topic of debate. The establishment of a set of bounding profiles was not attempted in this work. Instead, bounding axial profiles were assumed to be the bounding profiles determined by Parish[23] from a database of operating PWR spent fuel burnup profiles. Parish determined a bounding profile for each of a set of burnup ranges, as listed in Table 1.

Table 1. Axial burnup ranges[a]

Average burnup (GWd/MTU)	Burnup range lower limit (GWd/MTU)	Burnup range upper limit (GWd/MTU)
3	0	6
8	6	10
12	10	14
16	14	18
20	18	22
24	22	26
28	26	30
32	30	34
36	34	38
40	38	42
44	42	46
48	46	48+

[a]Table taken from ref. 23.

Each of the profiles from ref. 23 consists of 18 uniform axial divisions. Therefore, to apply these profiles in depletion/criticality analyses, a fuel pin model with 18 uniform axial zones was assumed. Table 2 lists dimensions assumed for this fuel pin. These parameters are based on a Westinghouse 17 H 17 assembly design.

Table 2. Pin dimensions used in depletion and criticality models

Parameter	Dimension (cm)
Fuel diameter	0.9563
Clad inner diameter	0.9855
Clad outer diameter	1.1176
Pin pitch	1.4732
Fuel height	365.76
Axial zone height	20.32

Although the fuel was divided into 18 uniform axial zones, past experience[10] has shown that axial zones can be combined near the center of the fuel, because burnup changes little in this area. By combining two or more axial zones with a single averaged burnup, the number of depletion cases can be reduced from 18 to a smaller number, reducing computational costs. However, it is also known that a single axial zone poorly represents the axial distribution for burned fuel,[10] because the burnup profile is far from flat over the full height of the fuel after a given length of operation. Thus, it is necessary to determine an optimum balance between a single axial zone and the initial 18 axial zones.

To determine the number of axial zones required as a function of burnup, version 1 of the utility code CASKET was developed. This code has limiting axial profiles of ref. 23 built in; the profile is allowed to vary with burnup according to the burnup ranges given in Table 1. CASKET_I automated the process to perform k_{inf} calculations at the midpoint of each burnup range for a varying axial height zoning model. In other words, calculations were performed to

find the minimum acceptable axial-burnup approximation for each of the range-averaged burnups given in Table 1. Each burnup state therefore had its own associated burnup profile. It is assumed that due to the lower burnup at the fuel ends relative to the center of the fuel rod, axial zones near the center of the fuel can be averaged. However, the axial height of the region classified as the "center" is unknown. Therefore, a series of 10 calculations are performed, in which the height of the center region is varied. Figure 1 illustrates the 18-zone model (shape 1) and 9 approximate shapes (shapes 2 through 10) for a skewed cosine profile (selected for the purposes of illustration only).

The purpose of CASKET_I was to calculate the burnup at each axial location in each of the 10 axial distribution models for a given burnup step. CASKET_I then set up a SAS2H calculation to perform a depletion calculation to estimate the fuel content of each axial location in each model. Once nuclide number densities were obtained for all axial levels, KENO V.a was used to calculate the value of k_{inf} for an infinite lattice of fuel pins for each of the 10 axial models. This process was repeated for each of the 12 burnup levels listed earlier, using the bounding axial profile corresponding to each burnup level.

Figure 2 shows the results of k_{inf} calculations for each of the 10 axial-burnup distributions, for each of 12 burnup ranges. The statistical error associated with each calculated value of k_{inf} is less that the size of the data point markers (#0.0005). Note that for all burnup shapes over all burnup ranges, axial-shape 7 is sufficient to accurately capture the "end effect" of reduced-burnup fuel near the rod ends with very small error. Coincidentally, axial-shape 7 consists of 7 axial zones; three 1/18-length zones at each end of the fuel rod, surrounding a central region comprised of 2/3 of the fuel length over which the 18-zone bounding profile (as provided by Parish[23]) is averaged.

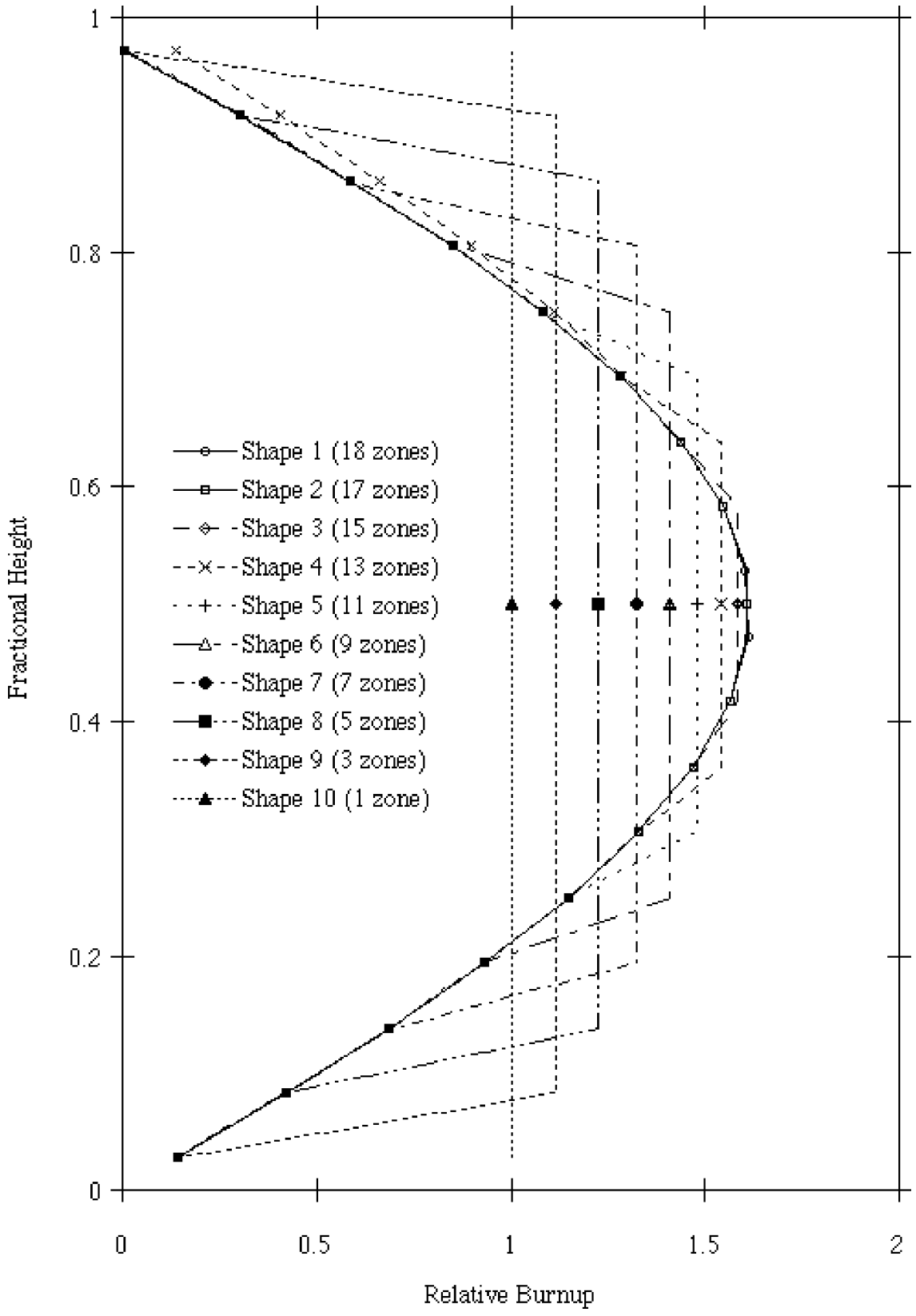

Fig. 1. Ten axial-burnup shapes assumed by CASKET.

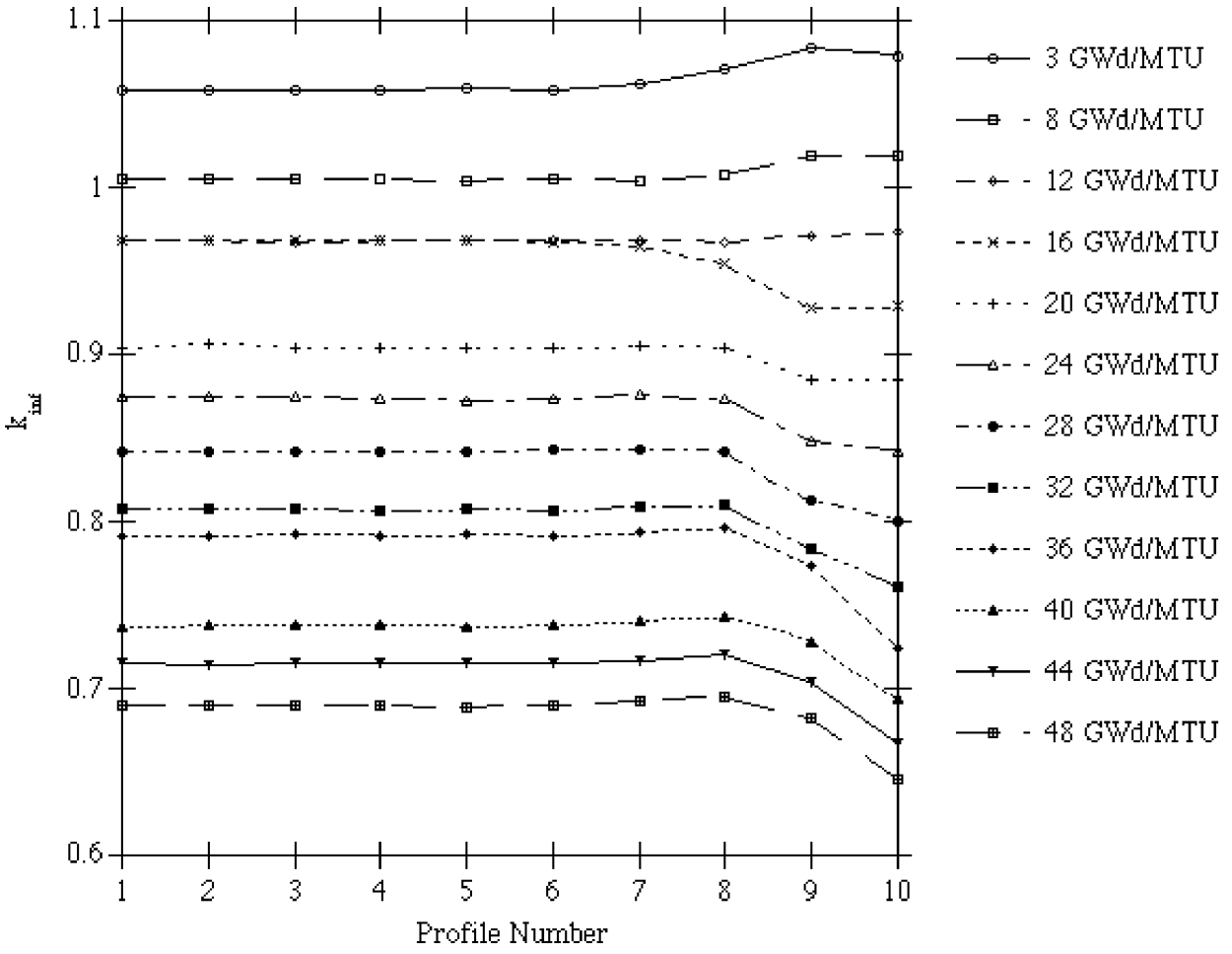

Fig. 2. Results of axial zoning studies for 3.0-wt % fuel burned at 25 MW/MTU.

The results of Fig. 2 are for calculations performed using 3.0-wt % enrichment as a basis for the fresh fuel starting point, and burnup at an average power level of 25 MW/MTU. CASKET_I calculated the irradiation time required to obtain the assembly-averaged burnup desired for each burnup case, and performed calculations using this exposure and axially weighted specific power for each axial zone. Calculations were based on an assumed constant-power continuous-burn cycle (with 10 SAS2H libraries within the single cycle), and a 5-year downtime after exposure. Since it is possible that an axial model is sensitive to the initial isotopic content of the fuel and the average power assumed, the above calculations were repeated

for 3.0-wt % fuel and an average power of 40 MW/MTU, and also for 4.5-wt % fuel, with powers of 25 and 40 MW/MTU. The results of calculations for 4.5-wt % fuel and 25 MW/MTU are shown in Fig. 3. Results obtained for both enrichments, but for higher power (40 MW/MTU), are very close to those obtained for 25 MW/MTU, and are not shown here. The two figures demonstrate that the 7-axial-zone model is adequate irrespective of initial enrichment and power level during depletion.

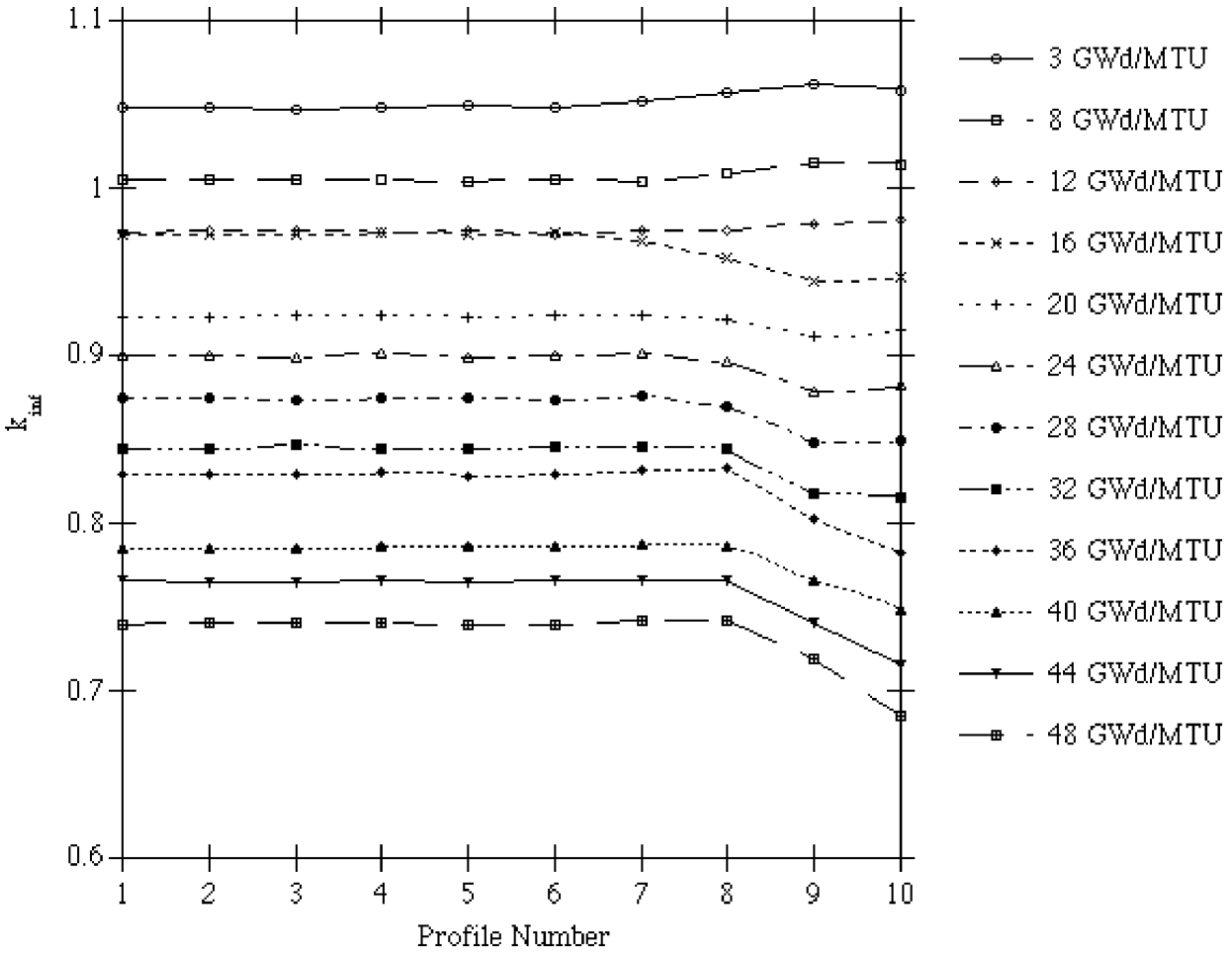

Fig. 3. Results of axial zoning studies for 4.5-wt % fuel burned at 25 MW/MTU.

As an aside, it is worth noting a few features of both figures:

1. One-zone (profile-10) models overestimate k_{inf} for burnups less than or equal to 12 GWd/MTU, but underestimate it for higher burnups by as much as 5%) k/k;
2. One-zone and three-zone models (profiles 10 and 9, respectively) are nearly identical for burnups up to 20 GWd/MTU for 3-wt % fuel, and up to 32 GWd/MTU for 4.5-wt % fuel;
3. The k_{inf} values for the 16-GWd/MTU case (and to a lesser extent the 36-GWd/MTU case) seem high relative to adjacent burnups. These two cases correspond to bounding profiles with the largest "end effect reactivities" (see Table VI of ref. 23). The shape of the various profiles are illustrated in Fig. 4; both the 16- and 36-GWd/MTU profiles show a higher relative central burnup and reduced burnup toward the upper end of the fuel. It is important to note that the limiting profile for each burnup range results from the most limiting profile found in the database for burnups within that range. The 16- and 36-GWd/MTU ranges happened to contain “outlier” assemblies with especially conservative profiles.

Based on the results above, all further sensitivity work in the remainder of this report will be based on the 7-axial-zone collapses of the Parish 18-zone bounding-profile database.

2.2 OPERATING HISTORY

As was demonstrated in earlier parametric analyses,[10] the reactivity worth of spent fuel with a given burnup is dependent on the path taken to reach that burnup. It was decided to simply try to repeat the method of ref. 10 using the current model and the 44-group cross-section library to determine if trends were similar to those observed in the previous study. However, rather than the single-zone 1-D pin calculations performed in the earlier work, these calculations were performed using multiple-axial zones in KENO V.a calculations to include any effects due

to axial burnup. Also, decay calculations were performed assuming both 5- and 20,000-year cooling times. Calculations were automated using CASKET_II, a modified version of the previous utility code. CASKET_II used SAS2H to generate cross-section libraries for each of six fuel cycles; the calculation was then rerun using these libraries and a standalone ORIGEN-S calculation to perform accurate long-term decay calculations (SAS2H is known to have inadequate timestep meshing for long decay times).

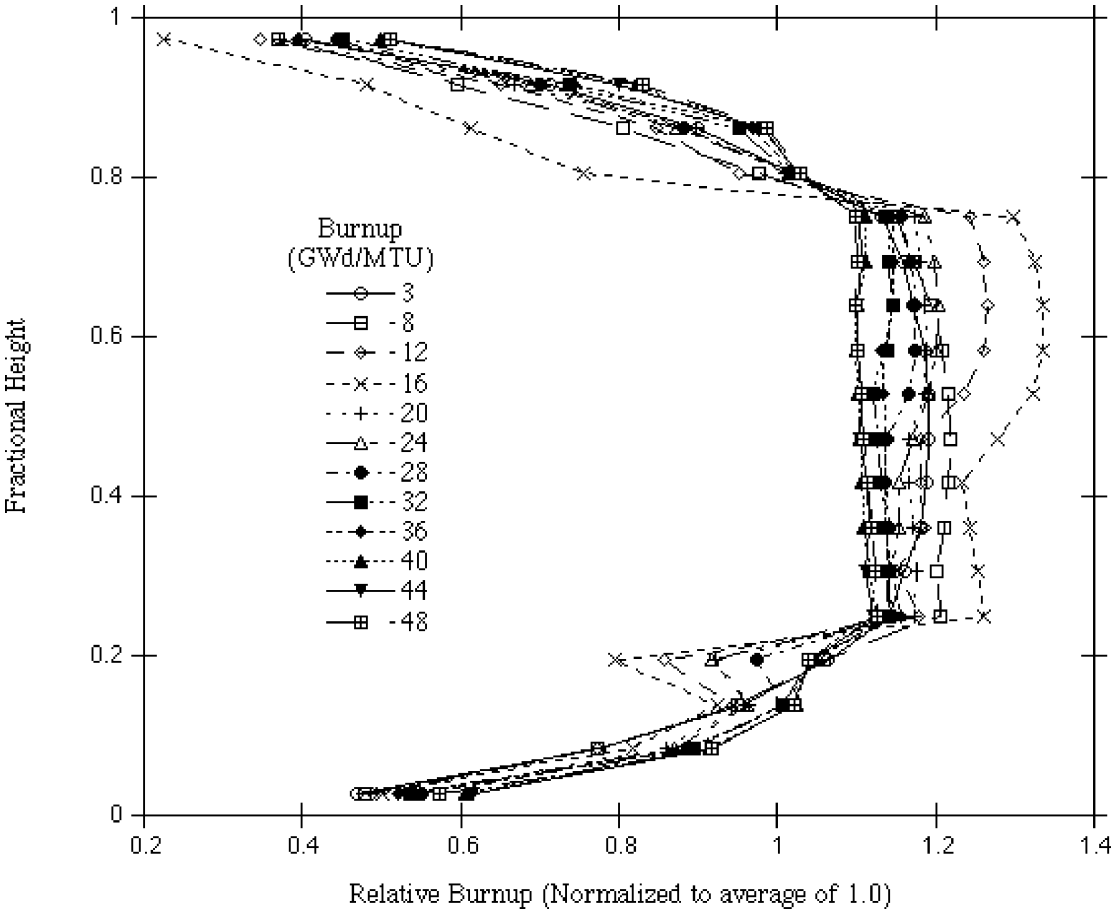

Fig. 4. Shape of bounding axial profiles used in this study.

The operating history models assumed in these calculations are shown in Fig. 5 (ref. 10). These candidate operating histories are in no way representative of all possible reactor histories.

However, the trends in these cycles are hoped to represent trends seen during typical reactor operation to allow the determination of the types of reactor operations that result in the most significant changes in spent fuel reactivity worth. Calculations were performed for variable enrichments and burnups for each of the operating histories. Cycle lengths were fixed to values shown in Fig. 5; specific powers were computed based on the specified final burnup and the irradiation time. Depletion calculations were performed for each of the 7 axial zones as defined earlier.

Results are shown in Fig. 6 for depletion/decay calculations based on a 5-year cooling period. Figure 7 shows results based on a 20,000-year cooling period. In both plots, results for each enrichment/burnup pair were normalized such that the average value of k_{inf} for all 11 cases was 1.0 This normalization allows direct comparison of results for each enrichment/burnup calculation to highlight trends as a function of operating history type. Additionally, although there is no functional relationship between the 11 cases, lines are drawn connecting each data point to help to visually identify trends. In both figures, error terms (1-F) are on the order of ±0.0005 for each calculation. For clarity, error bars are omitted; however, horizontal lines at 0.9990 and 1.0010 are included to show the range of 2F around the mean of 1.0. Variations outside this range (i.e., 1.0 ± 2 σ) are considered to be statistically significant with a 95% confidence level.

For the results calculated based on a 5-year cooling time (Fig. 6), most variations are close to the average, with no clear, well-defined trends. However, probable trends exist for operating histories 5, 6, 8, 9, and possibly 11. In terms of conservatism, the highest value of k_{inf} is calculated based on operating histories 6 and 9, but perhaps only for high-burnup fuel. These two cases are similar in the sense that both effectively had a lower specific power when averaged

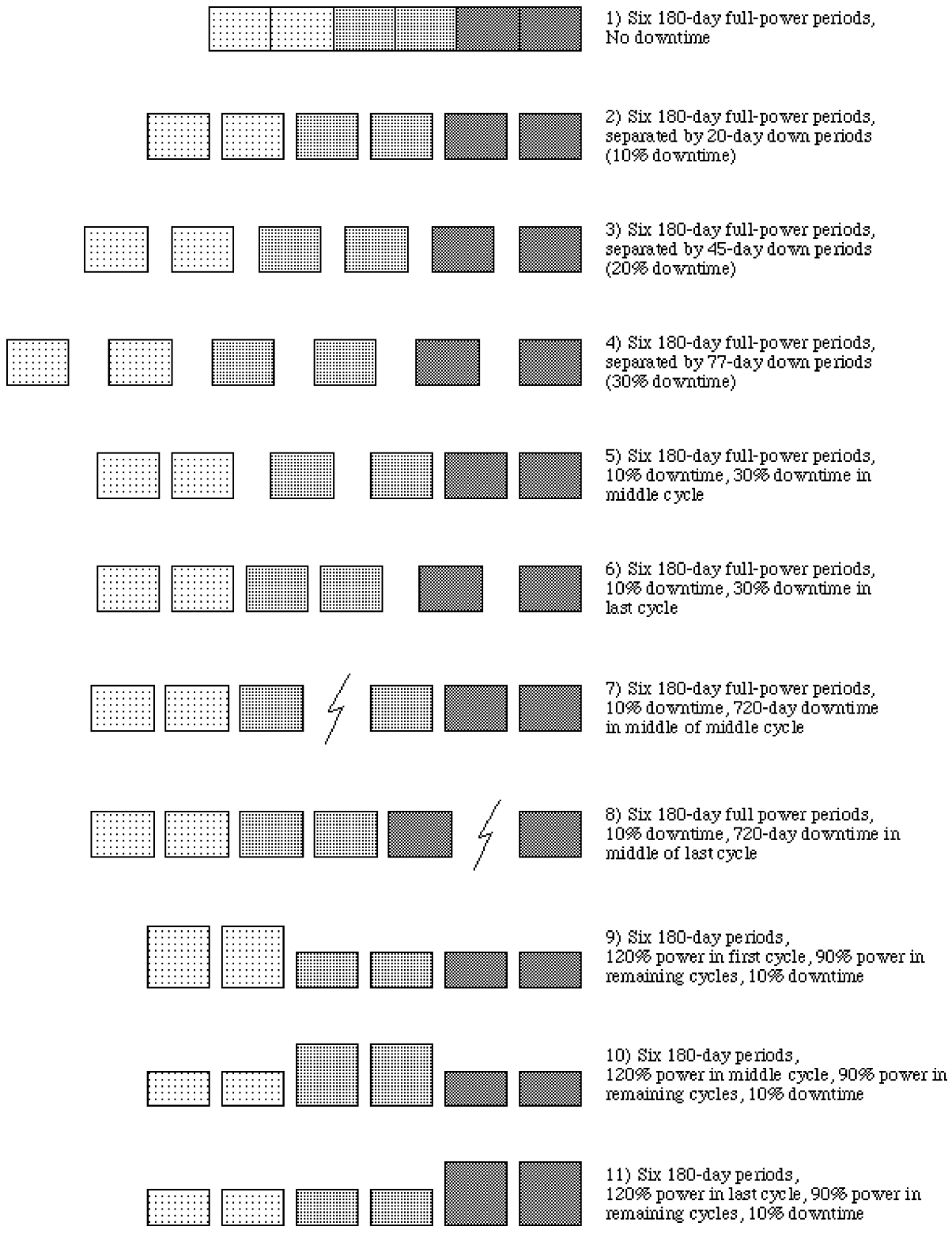

Fig. 5. Operating history profiles used for studying operating history effects.

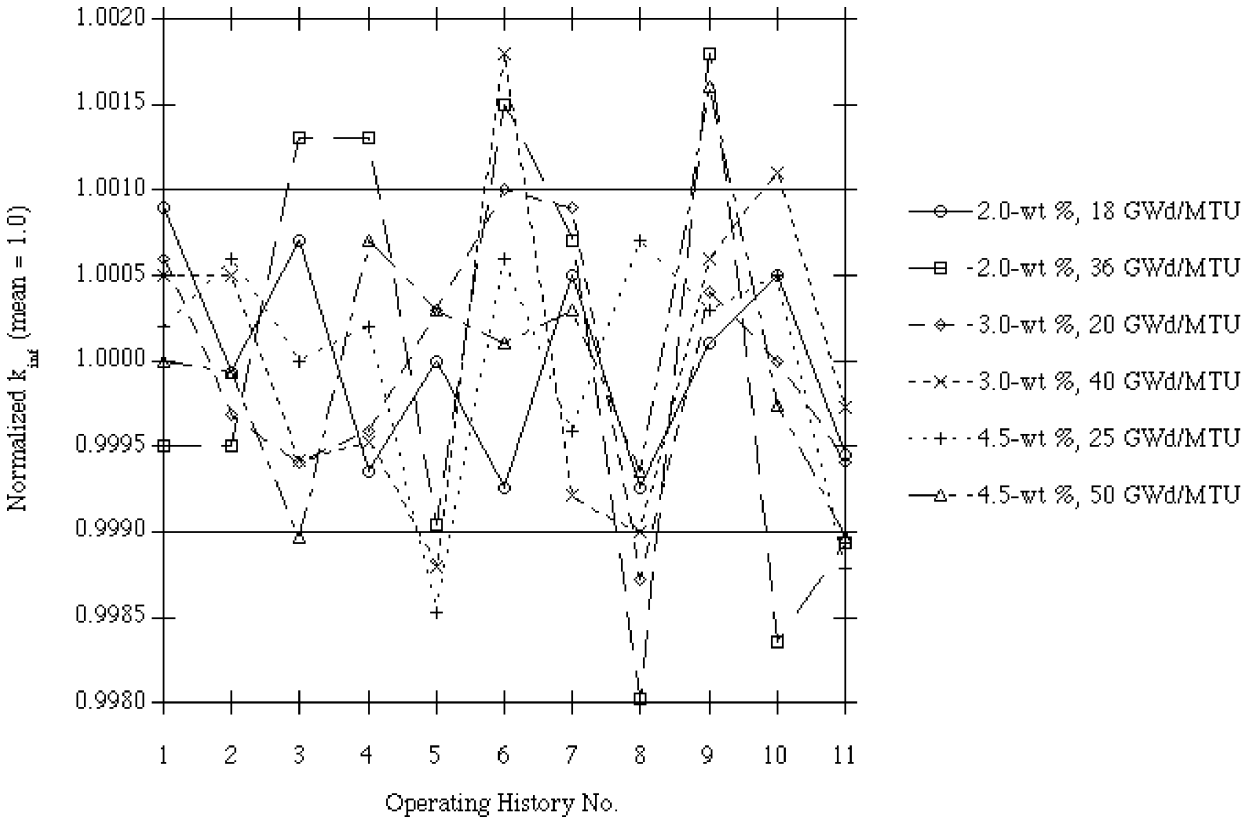

Fig. 6. Sensitivity of k_{inf} to operating history after a 5-year cooling period.

over the full-cycle length, relative to the other operating histories. The net effect of both operating histories is to extend the length of the final cycle. This procedure would allow time for the decay of the fission product ^{155}Eu to ^{155}Gd, which is then quickly burned out because of its large absorption cross section. In other words, a lower (effective) specific power results in a lower equilibrium concentration of ^{155}Eu during operation, thus less ^{155}Gd is produced post-shutdown, resulting in a more reactive fuel after 5 years of cooling time. ^{155}Eu is certainly not the only fission product that would contribute to fuel reactivity, but it is one of the most important nuclides because of the high worth of its ^{155}Gd daughter.

Using the above rationale, one would expect to see similar trends for operating history No. 8, with its 720-d downtime in the middle of the final cycle. However, Fig. 6 shows just the opposite effect — a sharp decrease in reactivity after a 5-year cooling period. As was suggested in ref. 2, the extended (roughly 2-year) downtime of history number 8 allows for a significant decay of ^{241}Pu, with its 14-year half-life. The subsequent operation would not allow ^{241}Pu to regain equilibrium levels, so the net effect of ^{241}Pu loss not only offsets but also exceeds the reactivity gain from lower ^{155}Gd concentrations. Again, other phenomena are present as well; this scenario is postulated as a likely partial contributor to the effect seen for long downtimes in the final cycle.

Finally, note that the trends seen in Fig. 6 are similar to, but not identical to, those observed in earlier work reported in ref. 10. The magnitude of the effect seen for the various operating histories in ref. 10 is less than that seen in the current work, especially for operating history Nos. 8 and 9. This difference is probably due to the 3-D effects of fission product distributions modeled in the current work, which were not evaluated in the previous work. The previous work was based on 1-D pin-cell calculations and therefore did not capture axial effects. In addition, the differences may have been further exacerbated by known weaknesses in the cross-section data for ^{155}Eu in the 27-group library used in the earlier work. The ^{155}Eu cross-section evaluation in that library resulted in an overprediction of ^{155}Gd inventories. This overprediction would be most significant in cases 6 and 9, as discussed earlier.

Results of calculations performed for identical operating histories, but with a 20,000-year cooling time, are shown in Fig. 7. These results indicate very little sensitivity to operating history, *except* for histories 8 and 11, which have a significant reactivity peak and reactivity dip, respectively. For conservatism in estimating k_{inf} for such long cooling times, operating history 8

is the most bounding. In this case, the effect of ^{155}Gd depletion subsequent to the extended downtime would not be masked by the loss of ^{241}Pu, since all of this plutonium isotope would have decayed away by 20,000 years.

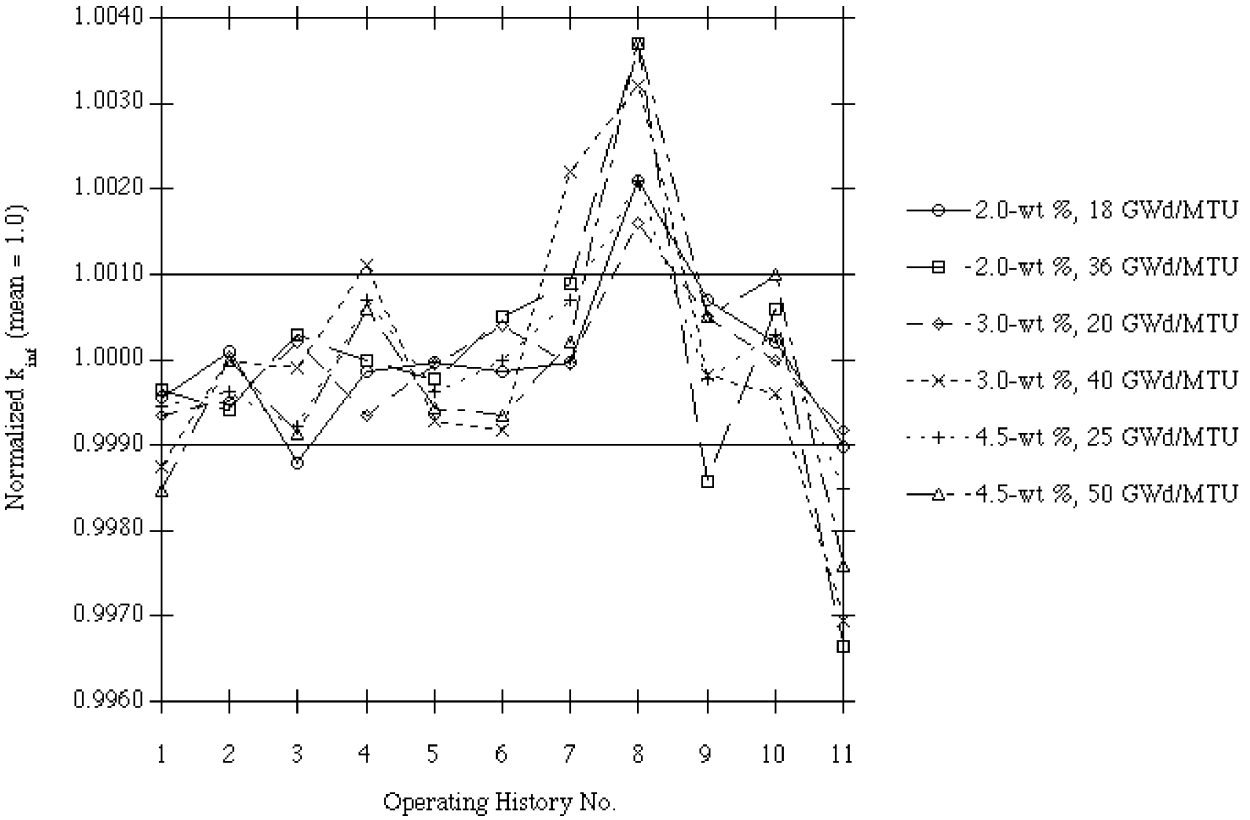

Fig. 7. Sensitivity of k_{inf} to operating history after a 20,000-year cooling period.

For all operating histories studied, the effect of operating history on the value of k_{inf} is well within a 0.3%)k/k band of the simple continuous burn of operating history No. 1, for 5-year-cooled fuel. For longer 20,000-year downtimes, the uncertainty increases to less than 0.5%)k/k. Because there is no single operating history that is clearly most conservative for all cooling times, it would perhaps be most efficient to assume a simplified operating history, such as constant power operation. A conservative margin must then be added to account for operating

history uncertainty. The work presented here *does not* seek to determine the magnitude of such a margin, as an insufficient number of operating history profiles have been studied. The values of 0.5% $\Delta k/k$ for 20,000-year-cooled fuel were observed for the limited set of histories studied and may or may not be 0.3% $\Delta k/k$ for 5-year-cooled fuel and conservative limits. However, it is important that the margin selected corresponds to the cooling time selected for a set of calculations, since this margin has a clear dependence on cooling time.

2.3 SPECIFIC POWER

To study the effect of specific power independently of changes in operating history, CASKET_III was created. For this study, a constant operating history was assumed, with no intercycle downtime, using six cycles and one library per cycle. Average specific powers were varied from 10 to 50 MW/MTU — a range that exceeds the range of most reactor operations. Since axially varying burnups were employed, specific powers were axially varied according to the seven-zone burnup-dependent axial distributions described earlier. Isotopics were computed for both 5- and 20,000-year cooling times and were input into KENO V.a infinite lattice calculations to determine k_{inf}. Results are shown in Fig. 8 for 5-year-cooled fuel, and in Fig. 9 for a 20,000-year cooling time. Again, since we are only interested in trends, all k_{inf} values for a given enrichment, cooling time, and burnup combination were normalized by the average value for all specific powers. Because the variation in the normalized value of k_{inf} over the entire range is on the order of 1 to 2 F in the k_{inf} calculations, it is difficult to infer any correlation between specific power and burnup or enrichment. It appears (especially for the 20,000-year-cooled case) that the slope of the lines decreases (meaning less sensitivity to specific power) with increasing burnup. Looking at all sets of results, however, it is clear that there is a tendency for conservatism (i.e., higher predicted values of k_{inf}) with decreasing specific power. It also appears

that the trend is stronger after a 20,000-year cooling than with a 5-year cooling. The average slope of the curves in !0.0001 per MW/MTU, for 5-year-cooled fuel, and !0.0003 per MW/MTU for 20,000-year-cooled fuel. Finally, the trends observed here are consistent with those determined in ref. 10 for calculations in which fission products are retained. Note, however, that the earlier work showed the opposite trend (i.e., increasing conservatism with increasing specific power) when fission products were not included.

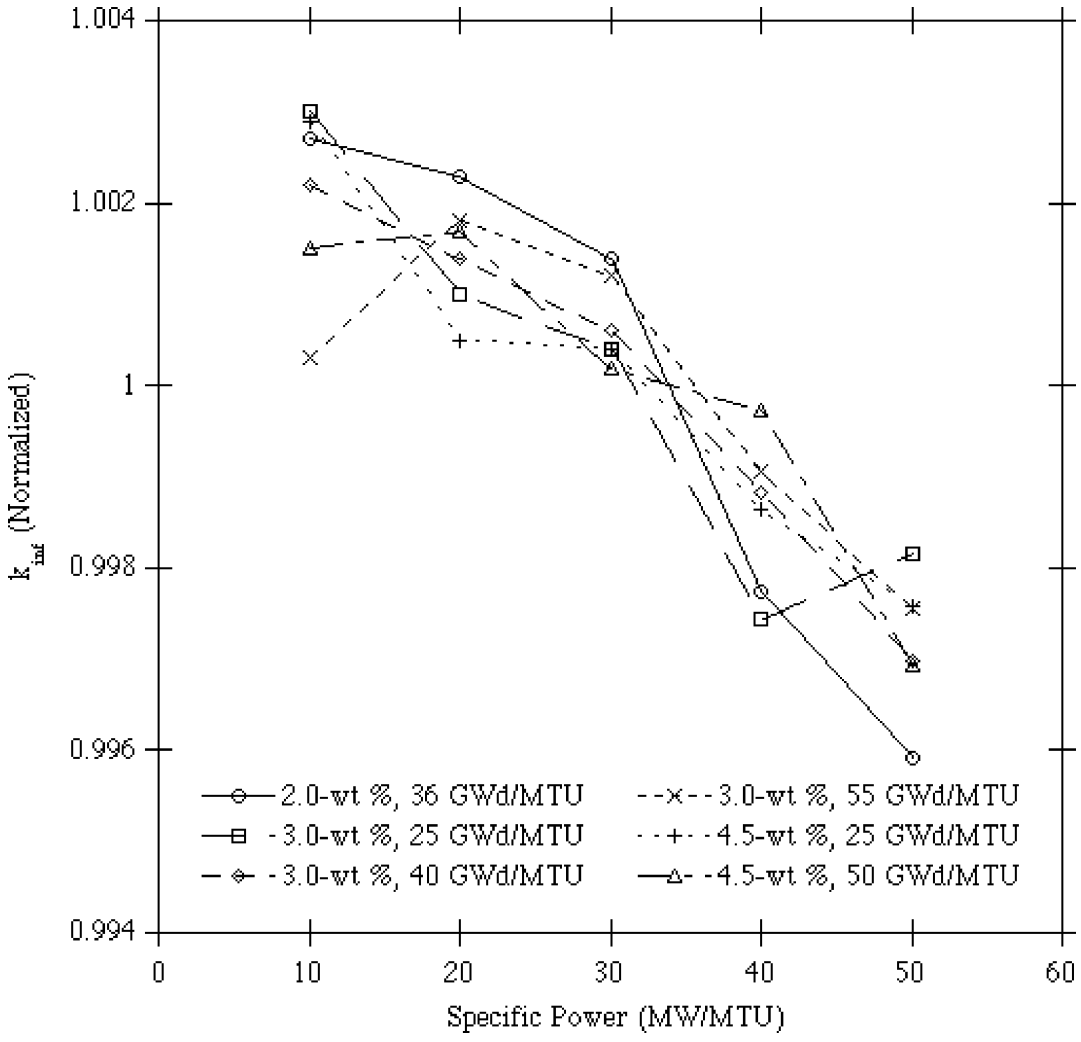

Fig. 8. Trends in k_{inf} as a function of specific power during depletion (5-year-cooled).

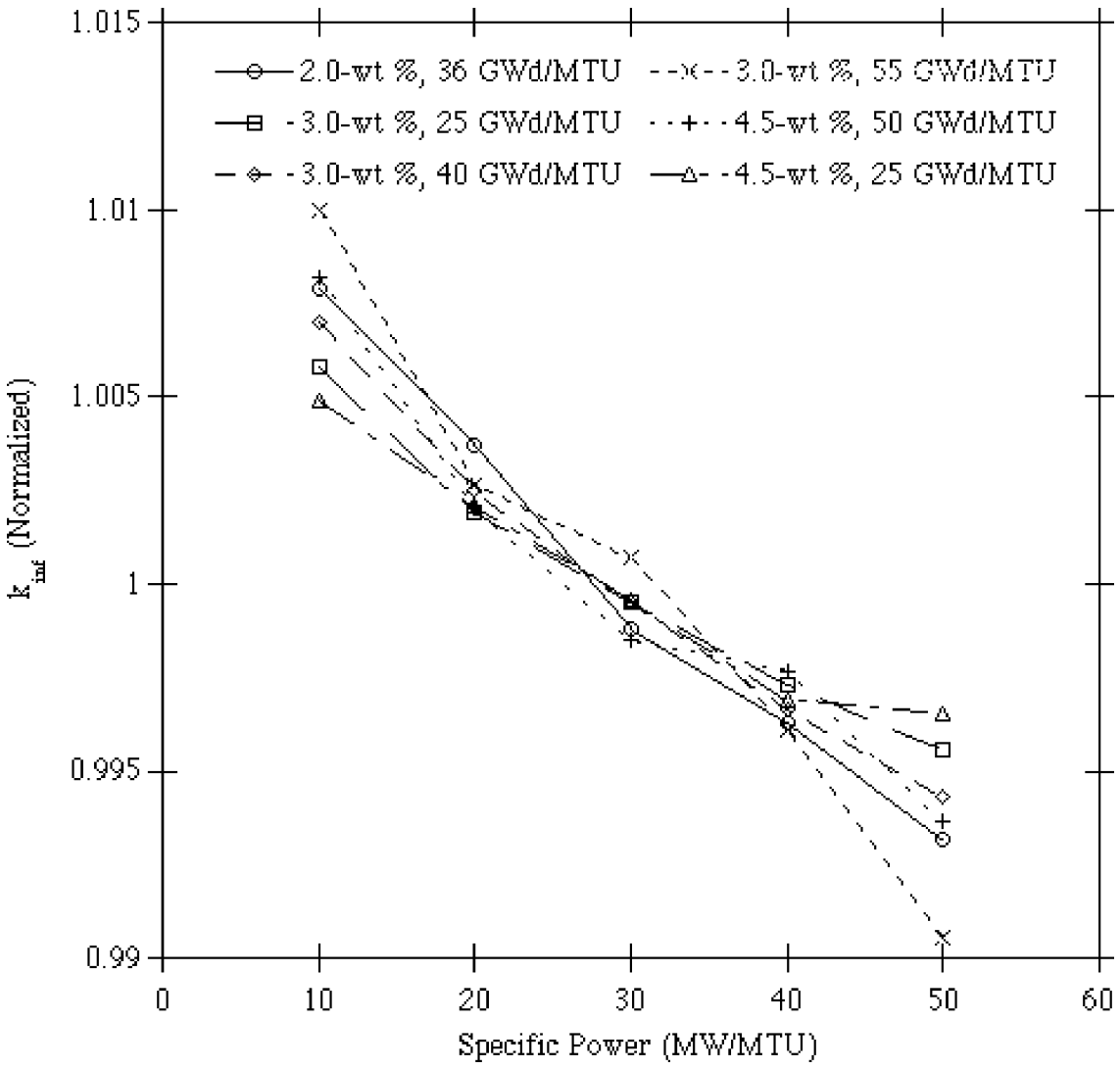

Fig. 9. Trends in k_{inf} as a function of specific power during depletion (20,000-year-cooled).

2.4 TEMPERATURE/BORON EFFECTS

Spectral hardening is known to occur with increased reactor temperature and with increased boron concentration. This phenomenon leads in turn to increased plutonium production from ^{238}U, reducing the burnup of ^{235}U, and increasing fuel reactivity for a given burnup. Earlier work[10] showed that increased fuel, moderator, or clad temperatures during

depletion calculations resulted in more conservative (higher) estimates of k_{inf}. The same trend was observed with increasing boron concentrations. CASKET_IV was created to perform automated calculations for a 7-axial-zone model and 5 uniform-burn periods with zero inter-cycle downtime to assess the trends in k_{inf} for each of these parameters in a 3-D infinite lattice simulation.

Variable temperature calculations were performed, assuming the nominal conditions listed in Table 3.

Table 3. Nominal depletion conditions

Fuel temperature	841 K
Clad temperature	628 K
Moderator temperature	558 K
Boron concentration	500 ppm

Fuel temperature sensitivity calculations were performed with each of these conditions fixed but with fuel temperatures varying from 700 to 1100 K. Fuel densities were not varied. Similarly, moderator temperature sensitivity calculations were performed, assuming the above conditions but with moderator temperatures allowed to vary between 500 and 600 K. However, moderator densities were calculated using a correlation that predicted the densities listed in Table 4.

Table 4. Moderator density function used in sensitivity calculations

Moderator temperature (K)	Moderator density (g/cm^3)
500	0.847
525	0.811
550	0.768
558	0.753
575	0.719
600	0.662

Sensitivity calculations were not performed based on clad temperatures, because clad materials have little effect on the reactivity of a system, and any temperature effects would be insignificant relative to the uncertainty of the KENO V.a calculation. Finally, boron concentration studies were performed at the above temperatures but with boron concentrations in the moderator allowed to vary from 0 to 1000 ppm soluble boron. (Since calculations were performed using a single library per cycle, each cycle was based on a single fixed boron concentration, rather than the time varying concentration employed by SAS2H when multiple libraries per cycle are used.)

2.4.1 Sensitivity to Boron Concentration

Figure 10 illustrates trends in k_{inf} calculated as a function of boron concentration for various enrichment and burnup combinations, for both 5- and 20,000-year cooling times. Again, k_{inf} values are normalized for each enrichment/burnup/cooling-time combination so that general trends can be studied. These results show that there is a definite positive trend in reactivity with increasing boron concentration. The slope of the trend increases with fissile depletion and does not appear to be sensitive to cooling time.

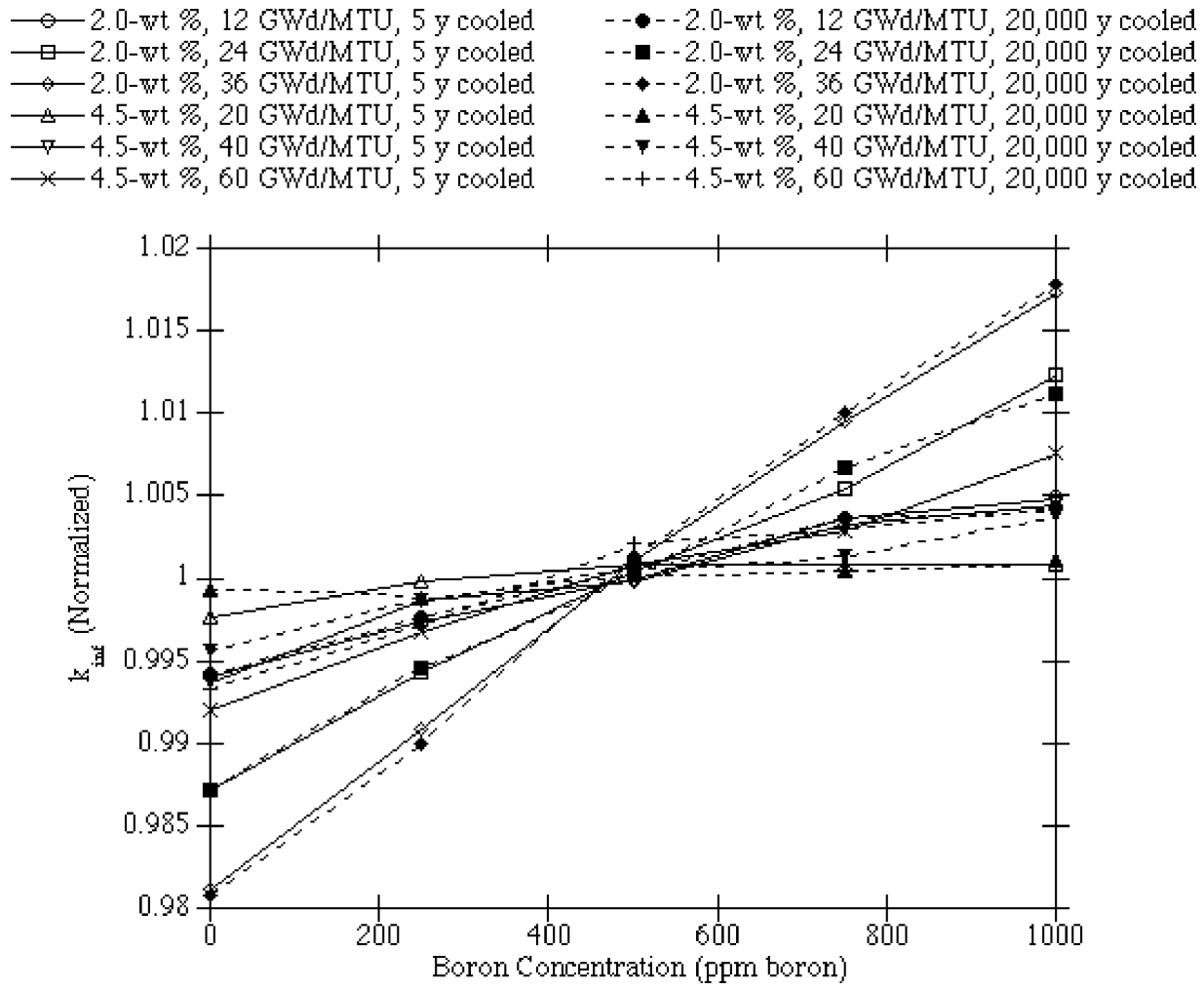

Fig. 10. Trends in k_{inf} as a function of moderator boron concentration during depletion calculations.

2.4.2 Sensitivity to Moderator Temperature

Figure 11 illustrates the trends calculated for k_{inf} as a function of moderator temperature. The figure is based on normalized k_{inf} values, as before. Since moderator (and soluble boron) density changes as a function of moderator temperature, the trends are a collateral effect of both increasing moderator temperature and decreasing moderator/boron density. Since resonance broadening is almost inconsequential in the moderator, any effect would be largely due to

moderator density effects. The trends observed in Fig. 11 are almost identical to those seen as a function of boron concentration: k_{inf} increases with increasing moderator temperature (decreasing density). Sensitivity increases with fissile depletion and is not noticeably affected by cooling time. Note that although increasing moderator temperature results in decreased boron concentration, which would in and of itself have a negative effect on k_{inf}, the net effect is positive.

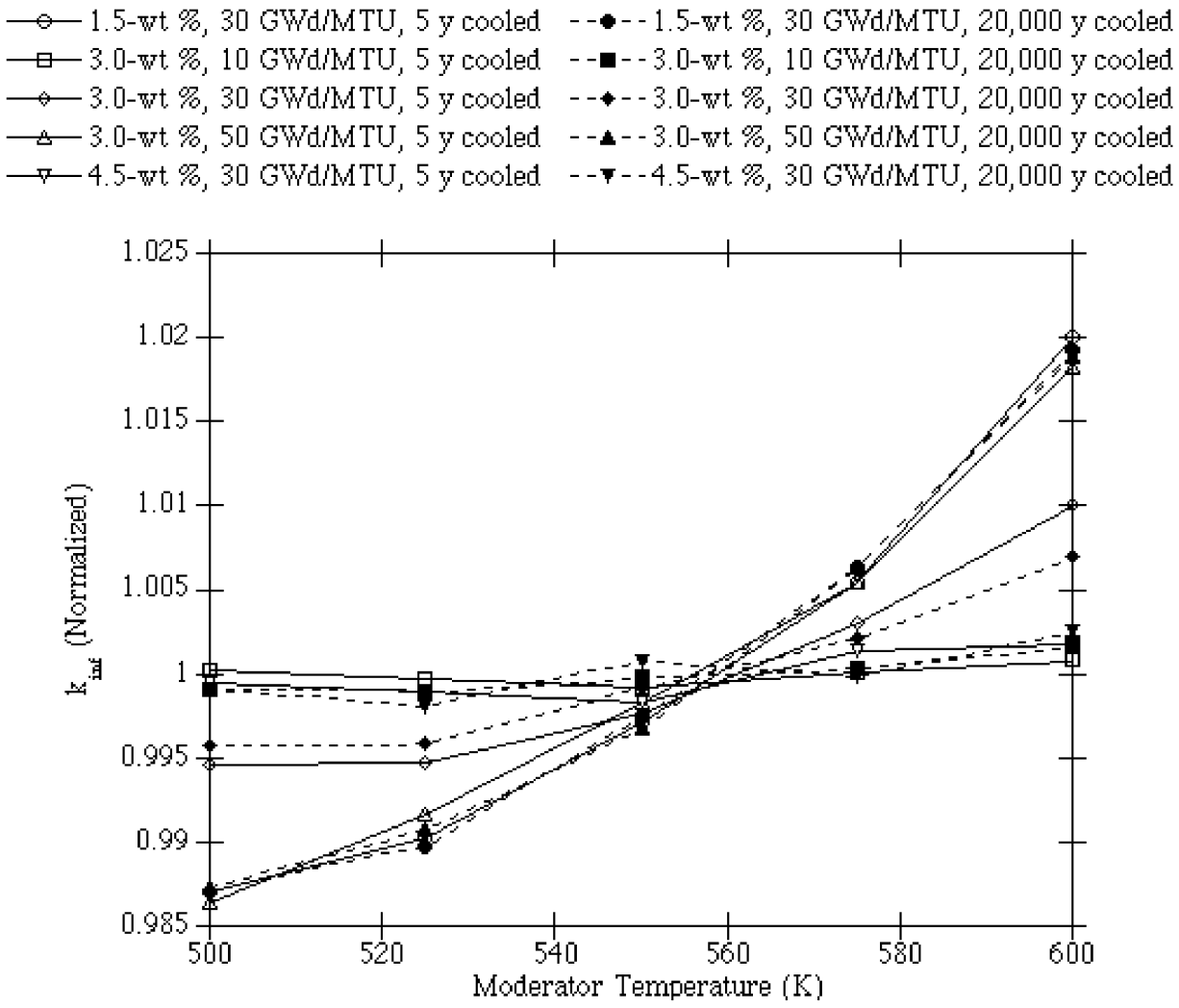

Fig. 11. Trends in k_{inf} as a function of moderator temperature during depletion calculations.

2.4.3 Sensitivity to Fuel Temperature

The final set of calculations were performed to determine the effect of fuel temperature on k_{inf}. Results are plotted in Fig. 12. Although fuel density does not change significantly with temperature in the range studied, resonance absorption by ^{238}U is enhanced by Doppler broadening with increasing fuel temperature. This enhanced absorption will result in increased plutonium production and increased reactivity for a given level of burnup. The trends seen in Fig. 12 are consistent with this phenomenon. Spent fuel reactivity clearly increases as the assumed fuel temperature during depletion is increased, although the sensitivity to temperature (in terms of $\partial k_{inf}/\partial T$) is smaller for fuel than for moderator. It does appear that sensitivity increases with increasing fissile depletion, but again trends are not as clear as for moderator temperature or boron concentration results. There is no apparent k_{inf} as a function of cooling time.

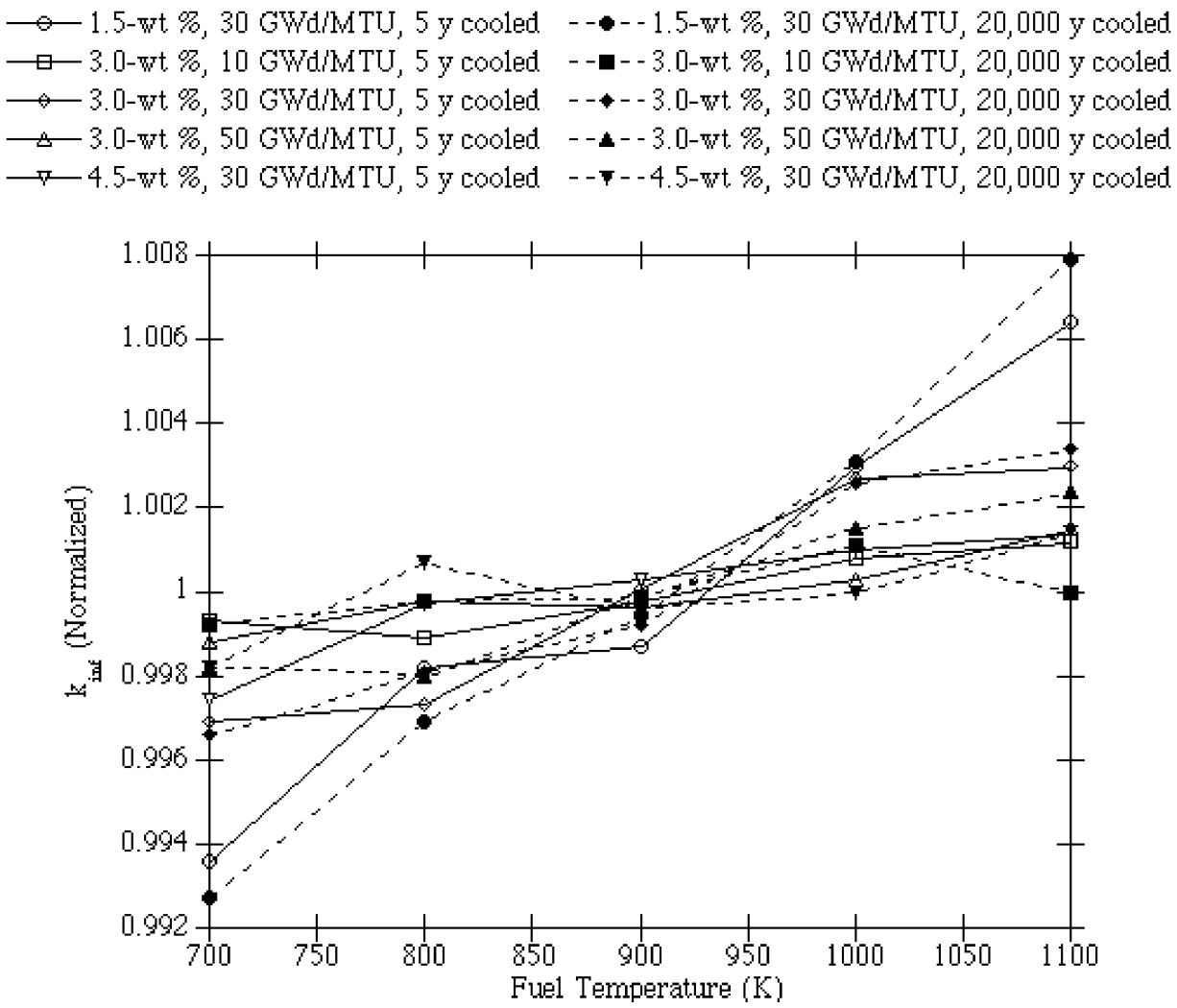

Fig. 12. Trends in k_{inf} as a function of fuel temperature during depletion calculations.

3. SUMMARY

The current study was based on SCALE version 4.3 and the SCALE 44-group ENDF/B-V library, using 3-D fuel models to capture effects of axial-burnup distribution. In contrast, an earlier ORNL parametric study of PWR fuel[10] was performed using SCALE 4.2 and its 27-group burnup library. The earlier parametric analyses were performed only for a 5-year-cooling time and were based on 1-D deterministic calculations. The results of this study have been found to be consistent with the results of the earlier analyses.

The axial zoning calculations confirmed the conclusions of the earlier work: most of the length of the fuel rod can be represented by the average burnup of that length; and axially discrete burnup representations are important only near the ends of the fuel. Calculations with as few as seven axial zones (three $1/18^{th}$-length zones at either end and one large central zone) were shown to converge to the same solution as an 18-uniform-zone model. The axial-zone models were shown to converge for a variety of initial enrichments and burnups. It may be possible to further combine two or all three of the zones near each end, although this combination was not studied in this work.

The effect of operating history on k_{inf} was demonstrated to be small, with a maximum effect on the order of 0.2% relative to the average for fuel cooled for 5 years. The maximum positive reactivity effect is driven by histories that operate at lower powers or longer downtimes late in life, allowing a preferential removal of fission products prior to shutdown. However, the operating histories presented here show that k_{inf} can be as much as 0.4% higher than the average for 20,000-year cooling. It is believed that this increase is due to the between-cycle decay of ^{241}Pu, with its 14.4-year half-life. Little of this isotope will have decayed after a 5-year cooling

period, but it will be completely gone after 20,000 years. Operating history results were for the most part consistent with the results of earlier work; differences seen are most likely due to the lack of an axial-burnup profile in the earlier calculations.

The remaining effects studied were specific power, fuel and moderator temperatures, and soluble boron concentrations. Results in each of these sets of analyses were consistent with those of earlier work. In each of these studies, the direction of the parameter that tends to harden the spectrum (i.e., lower specific power, higher temperature, and higher boron concentration) results in the most conservatism in the prediction of k_{inf}. The effect is always more pronounced with increased burnup and is a result of enhanced Pu production due to spectral hardening.

The purpose of this work has been to demonstrate the effects of variations in depletion modeling parameters on the calculated multiplication factor for spent fuel systems. From the trends observed in this work, it is possible to determine conservative bounds for various operating parameters by taking a limiting value from an operational database. For example, one might assume a moderator temperature based on the design maximum moderator temperature. However, it would be important to apply a reasonable upper bound for a given parameter, rather than a nonphysical limit, to avoid excess conservatism. Engineering judgement must be applied. Since bounding values are likely to be applied simultaneously and independently, additional conservatism will inherently be added because the parameters studied are not all independent. For instance, upper bounds on moderator temperature are not going to occur in a system running at a very low specific power, yet these represent bounding states when temperatures and specific power are treated conservatively and independently.

Finally, *it is important that the results reported herein be used to assess parametric trends, but not be used to assign a magnitude to expected conservatism for given parametric*

values. The magnitude of variation in system multiplication *may* be a function of the specific fuel and storage container design, and will require design-specific calculations.

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APPENDIX

A utility code nicknamed CASKET was developed for the analysis described in this report. CASKET was used to automate the calculational process to set up and run multiple SAS2H depletion calculations, extract required sets of isotopics, and use these isotopics in a final KENO-V.a criticality calculation driven by the SCALE CSAS25 sequence. Four different versions of the code were developed, for different aspects of this study. The nature of each version and the specific calculations in which each was used was described in the body of this report.

The following pages provide source listings of each of the four versions of CASKET.

FORTRAN-90 SOURCE LISTING FOR CASKET_I.F90

```
program casket
!
!  CASKET - Computational Analysis of the Sensitivity of K-eff for
Examination of Trends
!
!  Version I - Used to determine number of axial zones needed for each burnup
!  range for a specific cask design.
!
  implicit none
  character*7 nuclide(29)
  character*9 filename
  real upperbound(0:12), boundprofile(12,18), burn(27),u234,u235,u236,u238
  real ave_burn,sum,enrichment,specific_power
  integer i, j, iburn, icollapse, iset, icase, izone, material, nuc,
profile(10,18)
  integer
istart,iend,next,last,idum,id(29),refid(29),nucid(29),skipped(12,10)
  real dum,den(27,29),keff(12,10),sigma(12,10)
  logical file_exists
  integer STEPS
  parameter (STEPS=10)
!
!   Bounding axial profiles, taken from "Bounding Axial Profile Analysis for
!   the Topical Report Database," by T. A. Parish and C. H. Chen, Nuclear
!   Engineering Dept., Texas A&M University, March 1997.
  data
(upperbound(i),i=0,12)/0.,6.,10.,14.,18.,22.,26.,30.,34.,38.,42.,46.,50./
  data ((boundprofile(i,j),j=1,18),i=12,1,-1)/  & ! note that j moves
backwards since first set is for highest B/U
    0.573, 0.917, 1.021, 1.040, 1.126, 1.123, 1.118, 1.113, 1.109, &  !48
    1.105, 1.101, 1.098, 1.101, 1.098, 1.028, 0.986, 0.831, 0.512, &  !48
    0.615, 0.918, 1.020, 1.045, 1.120, 1.112, 1.116, 1.114, 1.104, &  !44
    1.107, 1.101, 1.101, 1.107, 1.104, 1.025, 0.981, 0.800, 0.512, &  !44
    0.607, 0.914, 1.024, 1.041, 1.124, 1.117, 1.108, 1.107, 1.103, &  !40
    1.102, 1.099, 1.101, 1.111, 1.112, 1.029, 0.981, 0.823, 0.498, &  !40
    0.520, 0.888, 1.009, 1.046, 1.155, 1.143, 1.136, 1.137, 1.137, &  !36
    1.133, 1.130, 1.145, 1.145, 1.143, 1.025, 0.970, 0.743, 0.393, &  !36
    0.537, 0.895, 1.007, 1.045, 1.141, 1.140, 1.135, 1.130, 1.125, &  !32
    1.121, 1.138, 1.145, 1.142, 1.136, 1.020, 0.953, 0.738, 0.451, &  !32
    0.551, 0.886, 1.007, 0.974, 1.146, 1.138, 1.140, 1.135, 1.138, &  !28
    1.166, 1.173, 1.173, 1.169, 1.157, 1.022, 0.882, 0.701, 0.444, &  !28
    0.544, 0.869, 0.962, 0.918, 1.138, 1.140, 1.153, 1.153, 1.172, &  !24
    1.192, 1.201, 1.203, 1.199, 1.185, 1.014, 0.871, 0.689, 0.396, &  !24
    0.540, 0.860, 0.965, 0.921, 1.174, 1.176, 1.171, 1.166, 1.167, &  !20
    1.185, 1.188, 1.186, 1.182, 1.173, 1.008, 0.898, 0.669, 0.373, &  !20
    0.502, 0.817, 0.925, 0.796, 1.260, 1.254, 1.242, 1.234, 1.277, &  !16
    1.323, 1.336, 1.335, 1.325, 1.299, 0.756, 0.614, 0.481, 0.225, &  !16
    0.489, 0.772, 0.944, 0.857, 1.179, 1.151, 1.186, 1.181, 1.180, &  !12
    1.236, 1.261, 1.265, 1.261, 1.244, 0.951, 0.847, 0.650, 0.348, &  !12
    0.478, 0.773, 0.950, 1.059, 1.205, 1.201, 1.211, 1.215, 1.218, &  ! 8
    1.216, 1.209, 1.194, 1.170, 1.151, 0.976, 0.806, 0.596, 0.370, &  ! 8
    0.470, 0.775, 0.955, 1.064, 1.141, 1.162, 1.180, 1.189, 1.192, &  ! 3
    1.191, 1.185, 1.172, 1.158, 1.130, 1.021, 0.900, 0.714, 0.403 /   ! 3
  data ((profile(i,j),j=1,18),i=1,10)/ &
```

```
    1, 2, 3, 4, 5, 6, 7, 8, 9,10,11,12,13,14,15,16,17,18, &
    1, 2, 3, 4, 5, 6, 7, 8,19,19,11,12,13,14,15,16,17,18, &
    1, 2, 3, 4, 5, 6, 7,20,20,20,20,12,13,14,15,16,17,18, &
    1, 2, 3, 4, 5, 6,21,21,21,21,21,21,13,14,15,16,17,18, &
    1, 2, 3, 4, 5,22,22,22,22,22,22,22,22,14,15,16,17,18, &
    1, 2, 3, 4,23,23,23,23,23,23,23,23,23,23,15,16,17,18, &
    1, 2, 3,24,24,24,24,24,24,24,24,24,24,24,16,17,18, &
    1, 2,25,25,25,25,25,25,25,25,25,25,25,25,25,17,18, &
    1,26,26,26,26,26,26,26,26,26,26,26,26,26,26,26,18, &
   27,27,27,27,27,27,27,27,27,27,27,27,27,27,27,27,27 /
  data (nuclide(i),i=1,29)/ &
    '  u-233',' np-237',' pu-238',' pu-239',' pu-240',' pu-241',' pu-242', &
    ' am-241','am-242m',' am-243','  mo-95','  tc-99',' ru-101',' rh-103', &
    ' ag-109',' nd-143',' nd-145',' sm-147',' sm-149',' sm-150',' sm-151', &
    ' eu-151',' sm-152',' eu-153',' gd-155','  u-234','  u-235','  u-236', &
    '  u-238'/
  data (refid(i),i=1,29)/ 922330, 932370, 942380, 942390, 942400, 942410, &
          942420, 952410, 952421, 952430, 420950, 430990, 441010, 451030, &
          471090, 601430, 601450, 621470, 621490, 621500, 621510, 621520, &
          631510, 631530, 641550, 922340, 922350, 922360, 922380 /
  data (nucid(i),i=1,29)/ 92233, 93237, 94238, 94239, 94240, 94241, &
          94242, 95241, 95601, 95243, 42095, 43099, 44101, 45103, &
          47109, 60143, 60145, 62147, 62149, 62150, 62151, 62152, &
          63151, 63153, 64155, 92234, 92235, 92236, 92238 /
!
!  First renormalize boundprofile arrays to average of 1.0 for each burnup
range -
!  the tabulated values have some roundoff and are not exact.
!
   do iburn = 1,12
     sum = 0.0
     do izone = 1,18
       sum = sum + boundprofile(iburn,izone)
     end do
     sum = sum/18.0
     boundprofile(iburn,:) = boundprofile(iburn,:)/sum
   end do
!
!  Read problem specifications from keyboard input
!
    write(6,'(''Initial enrichment (wt %)? '')',advance='no')
    read(5,*)enrichment
    write(6,'(''Specific power (MW/MTU)? '')',advance='no')
    read(5,*)specific_power
    write(6,'(''Starting burnup shape (1-12)? '')',advance='no')
    read(5,*)istart
    write(6,'(''Ending burnup shape (1-12)? '')',advance='no')
    read(5,*)iend
!
!  Calculate fractional components of other U nuclides
!
    u234 = 0.007731*enrichment**1.0837
    u235 = enrichment
    u236 = 0.0046*enrichment
    u238 = 100.0-u235-u234-u236
!
!  Sweep through each of the 12 burnup ranges, analyzing each one separately
```

```
!  at the central B/U of each range
!
  do iburn = istart,iend
    ave_burn = 0.5*(upperbound(iburn-1)+upperbound(iburn))
!
!  For each burnup range, determine the fuel burnups that will be needed
!  to generate the different sets of isotopics to be used when the 18-zone
!  models are collapsed into smaller sets.  The 10 collapsing schemes
!  are represented schematically below:
!
!  1) 01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18
!  2) 01 02 03 04 05 06 07 08 19 19 11 12 13 14 15 16 17 18
!  3) 01 02 03 04 05 06 07 20 20 20 20 12 13 14 15 16 17 18
!  4) 01 02 03 04 05 06 21 21 21 21 21 21 13 14 15 16 17 18
!  5) 01 02 03 04 05 22 22 22 22 22 22 22 22 14 15 16 17 18
!  6) 01 02 03 04 23 23 23 23 23 23 23 23 23 44 15 16 17 18
!  7) 01 02 03 24 24 24 24 24 24 24 24 24 24 24 24 16 17 18
!  8) 01 02 25 25 25 25 25 25 25 25 25 25 25 25 25 25 17 18
!  9) 01 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 26 18
! 10) 27 27 27 27 27 27 27 27 27 27 27 27 27 27 27 27 27 27
!  where 19 = average(09, 10), 20 = average(08, 09, 10, 11)
!  ... 27 = average (01 -> 18)
!
    burn(1:18) = boundprofile(iburn,:)
    do icollapse = 19,27
      burn(icollapse) = 0.0
      do iset = 9-(icollapse-19),10+(icollapse-19)
        burn(icollapse) = burn(icollapse) + boundprofile(iburn,iset)
      end do
      burn(icollapse) = burn(icollapse)/((icollapse-18)*2)
    end do
!
!  set up and execute 27 sas2h cases to obtain isotopics for the 27
!  different burnups to be used.  The SAS2H cases are run to "ave_burn"
!  burnup at the user-specified specific power for the user-specified
!  initial enrichment.  The SAS2H calculation is a single constant-power
!  burn cycle with a 5-year cooling time with STEPS libraries/cycle
!
!#########################################################################
!    inquire(file='nucdata',exist=file_exists)                           !##
!    if(file_exists)then                                                 !##
!      open(10,file='nucdata',form='unformatted',status='old')           !##
!      read(10)den                                                       !##
!      close (10)                                                        !##
!      goto 123                                                          !##
!    endif                                                               !##
!#########################################################################
    do material = 1,27
!
!  Create sas2h input case for this average burnup step and for this material
!
      open(10,file='sas2h.in',status='unknown')

write(10,1000)STEPS,enrichment,specific_power,ave_burn,material,u234,u235,u23
6,u238
      do nuc = 1,25
        write(10,'(1x,a7,'' 1 0 1-20 841 end'')')nuclide(nuc)
```

```
      end do

write(10,1010)STEPS,specific_power*burn(material),ave_burn*1000/specific_powe
r
      close(10)
!
!  Submit this case
!
      call system('/scale4.3/cmds/scale43 sas2h.in sas2h.out')
!
!  Open unit 72 and read concentrations for desired nuclides
!
      open(10,file='ft72f001',status='old')
      do i = 1,1198 !skip first 1198 lines
        read(10,*)
      end do

read(10,1020)idum,dum,id(1),den(material,1),id(26),den(material,26),id(27),de
n(material,27) ! u-233, -234, -235
      read(10,1020)id(28),den(material,28),idum,dum,id(29),den(material,29)
! u-236, -238
      read(10,*)
      read(10,1020)idum,dum,id(2),den(material,2) !np-237
      read(10,*)
      read(10,1020)idum,dum,(id(i),den(material,i),i=3,5) !pu-238, pu-239,
pu-240
      read(10,1020)(id(i),den(material,i),i=6,7) !pu-241,pu-242
      read(10,*)

read(10,1020)(id(i),den(material,i),i=8,9),idum,dum,id(10),den(material,10)
!am-241, am-242m, am-243
      do i = 1,62 !skip next 62 lines
        read(10,*)
      end do
      read(10,1020)idum,dum,idum,dum,idum,dum,id(11),den(material,11) ! mo-95
      do i = 1,8
        read(10,*)
      end do
      read(10,1020)id(12),den(material,12) ! tc-99
      do i = 1,3
        read(10,*)
      end do
      read(10,1020)idum,dum,idum,dum,idum,dum,id(13),den(material,13) ! ru-
101
      do i = 1,4
        read(10,*)
      end do
      read(10,1020)idum,dum,id(14),den(material,14)  ! rh-103
      do i = 1,14
        read(10,*)
      end do
      read(10,1020)idum,dum,idum,dum,id(15),den(material,15) ! ag-109
      do i = 1,82
        read(10,*)
      end do
      read(10,1020)id(16),den(material,16) !nd-143
      do i = 1,3
```

```
        read(10,*)
      end do
      read(10,1020)idum,dum,id(17),den(material,17) !nd-145
      do i = 1,4
        read(10,*)
      end do
      read(10,1020)idum,dum,id(18),den(material,18) !sm-147
      do i = 1,3
        read(10,*)
      end do
      read(10,1020)idum,dum,idum,dum,id(19),den(material,19)  !sm-149
      read(10,*)
      read(10,1020)idum,dum,idum,dum,idum,dum,id(20),den(material,20) !sm-150
      read(10,*)
      read(10,1020)idum,dum,idum,dum,idum,dum,id(21),den(material,21) !sm-151
      read(10,1020)id(23),den(material,23) !eu-151
      read(10,*)
      read(10,1020)id(22),den(material,22) !sm-152
      read(10,*)
      read(10,1020)idum,dum,idum,dum,id(24),den(material,24) !eu-153
      do i = 1,4
        read(10,*)
      end do
      read(10,1020)idum,dum,id(25),den(material,25) !gd-155
      close(10,status='delete')
      do i = 1,29
        write(6,*)id(i),den(material,i)
        if(id(i).ne.refid(i))then
          write(6,*)'Error during burnup stage ',iburn,', material
#',material
          write(6,*)'Expecting nuclide id ',refid(i),' but read id ',id(i)
          stop
        endif
      end do
    end do ! material
!#########################################################################
!    open(10,file='nucdata',form='unformatted',status='new')              !##
!    write(10)den                                                         !##
!    close (10)                                                           !##
!123 continue
!#########################################################################
!
!  We now have the 27 different materials necessary to run the 10 different
axial
!  profile models for this burnup.  Create a csasn case to make a library
that
!  contains all 27 fuel materials with weighted cross-sections, plus clad and
!  moderator.
!
    open(10,file='csasn.in',status='unknown')
    write(10,1030)enrichment,specific_power,ave_burn
    do material = 1,27
      do nuc = 1,29
        write(10,'(1x,a7,1x,i2,'' 0 '',1pe10.4,'' 293
end'')')nuclide(nuc),material,den(material,nuc)
      end do
    end do
```

```
    write(10,1040)
    close (10)
    call system('/scale4.3/cmds/scale43 csasn.in csasn.out')
!############    call system('/scale4.3/cmds/scale43 csasn.in csasn.out')
!
!  We now have a working library with cross-sections for 27 fuel materials
plus clad and moderator
!  Create and run keno v.a calculations for each of the 10 axial models, and
extract k-eff and sigma
!  from each.
!
    last = 0
    open(10,file='keno.in',status='unknown')
    do  icase = 1,10
      write(10,1050)enrichment,specific_power,ave_burn,icase  ! header for
keno case
      do izone = 1,18
        next = profile(icase,izone)
        if(next.ne.last)then
          last = next
          write(10,'(''mix='',i2.2)')profile(icase,izone)
          do nuc = 1,29

write(10,'(i10,2x,1pe11.5)')nucid(nuc)+profile(icase,izone)*1000000,den(profi
le(icase,izone),nuc)
          end do
        end if
      end do !izone
      write(10,1060) ! finish up with mixtures for water and clad
      do izone = 1,18
        write(10,'('' cylinder   '',i2,'' 1  0.47815 '',f7.2,'' -
182.88'')')profile(icase,izone),-182.88+izone*20.32
      end do
      write(10,1070)
    end do !icase
    close (10)
    call system('/scale4.3/cmds/scale43 keno.in keno.out')
!
!  Grep the lines containing the final k-eff results into a file.  Then
!  Edit the file to get k-eff values, uncertainties, and no. of generations
!  skipped.
!
    call system('grep "generations skipped." keno.out > keno.results')
    open(10,file='keno.results',status='old')
    do i = 1,10

read(10,'(t34,f7.4,t48,f8.4,t73,i6)')keff(iburn,i),sigma(iburn,i),skipped(ibu
rn,i)
    end do
    close(10)
    write(filename,'("BUGroup",i2.2)')iburn
    open(10,file=filename,status='unknown')
    write(10,'("Axial Position,",10("Profile ",i2.2," k-eff=",f6.4,"+/-
",f6.4,:,","))')(j,keff(iburn,j),sigma(iburn,j),j=1,10)
    do i=1,18
      write(10,'(11(f7.3,:,","))')376.65/18*i -
376.65/36,(ave_burn*burn(profile(j,i)),j=1,10)
```

```
    end do
    close(10)
  end do ! iburn
stop
1000 format(  &
"=sas2h       parm='halt",i2.2,",skipshipdata'",/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U,
Material No. ',i2.2,/ &
'44group latticecell',/ &
'  uo2 1 den=10.045 1 841',/ &
'    92234 ',f6.4,' 92235 ',f6.4,' 92236 ',f6.4,' 92238 ',f7.4,' end',/ &
'  c 1 den=1.8-4 1 841 end',/ &
'  n 1 den=2.3-4 1 841 end',/ &
'  co-59 3 0 1-20 558 end',/ &
'  zr-94 1 0 1-20 841 end')
1010 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 2 1 620
end',/ &
'  h2o 3 den=0.7569 1 558 end',/ &
'  arbm-bormod 0.7569 1 1 0 0 5000 100 3 330.8e-6 558 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 1 3 1.1176 2 0.9855 0 end',/ &
'npin/assm=176 fuelnght=787.52 ncycles=1 nlib/cyc=',i2.2,/ &
'printlevel=4 lightel=9 inplevel=2 numztotal=5   end',/ &
'3  1.314  2  1.416  3  1.662  500  5.203  3  5.243 ',/ &
'power=',1pe9.3,' burn=',1pe9.3,' down=1826.25 end',/ &
'  o 119  cr  5.2  mn  0.29',/ &
'  fe 11. co 0.066 ni  8.7',/ &
'  zr 195 nb  0.63 sn  3.2',/ &
'end',/ &
'=shell',/ &
'cp $TMPDIR/ft72f001 $RTNDIR/',/ &
'end')
1020 format(4(i8, e12.4))
1030 format(  &
'=csasn          parm=(size=500000)',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U
(pin average)',/ &
'44group latticecell')
1040 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 28 1 293
end',/ &
'  h2o 29 1 293 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 27 29 1.1176 28 0.9855 0 end',/ &
'more data',/ &
'res=1 cylinder 0.47815  dan(1)=2.25244E-01',/ &
'res=2 cylinder 0.47815  dan(2)=2.25244E-01',/ &
'res=3 cylinder 0.47815  dan(3)=2.25244E-01',/ &
'res=4 cylinder 0.47815  dan(4)=2.25244E-01',/ &
'res=5 cylinder 0.47815  dan(5)=2.25244E-01',/ &
'res=6 cylinder 0.47815  dan(6)=2.25244E-01',/ &
'res=7 cylinder 0.47815  dan(7)=2.25244E-01',/ &
'res=8 cylinder 0.47815  dan(8)=2.25244E-01',/ &
'res=9 cylinder 0.47815  dan(9)=2.25244E-01',/ &
'res=10 cylinder 0.47815  dan(10)=2.25244E-01',/ &
'res=11 cylinder 0.47815  dan(11)=2.25244E-01',/ &
```

```
'res=12 cylinder 0.47815  dan(12)=2.25244E-01',/ &
'res=13 cylinder 0.47815  dan(13)=2.25244E-01',/ &
'res=14 cylinder 0.47815  dan(14)=2.25244E-01',/ &
'res=15 cylinder 0.47815  dan(15)=2.25244E-01',/ &
'res=16 cylinder 0.47815  dan(16)=2.25244E-01',/ &
'res=17 cylinder 0.47815  dan(17)=2.25244E-01',/ &
'res=18 cylinder 0.47815  dan(18)=2.25244E-01',/ &
'res=19 cylinder 0.47815  dan(19)=2.25244E-01',/ &
'res=20 cylinder 0.47815  dan(20)=2.25244E-01',/ &
'res=21 cylinder 0.47815  dan(21)=2.25244E-01',/ &
'res=22 cylinder 0.47815  dan(22)=2.25244E-01',/ &
'res=23 cylinder 0.47815  dan(23)=2.25244E-01',/ &
'res=24 cylinder 0.47815  dan(24)=2.25244E-01',/ &
'res=25 cylinder 0.47815  dan(25)=2.25244E-01',/ &
'res=26 cylinder 0.47815  dan(26)=2.25244E-01',/ &
'end more',/ &
'end')
1050 format( &
'=kenova',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU ave
B/U, Axial model #',i2.2,/ &
'read parm npg=1000 gen=1005 nsk=5 nub=yes',/ &
!'read parm npg=100 gen=105 nsk=5 nub=yes',/ &
'   lib=4 fdn=yes tme=300 end parm',/ &
'read boun all=mirror end boun',/ &
'read mixt')
1060 format( &
'mix=28',/ &
'  28040000  4.16270E-02',/ &
'  28026000  3.47236E-04',/ &
'  28050116  2.87770E-04',/ &
'  28050120  2.36120E-04',/ &
'mix=29',/ &
'  29001001  6.67692E-02',/ &
'  29008016  3.33846E-02',/ &
'end mixt',/ &
'read geom',/ &
'unit 1')
1070 format( &
' cylinder   0  1  0.49275  182.88  -182.88',/ &
' cylinder   28 1  0.55880  182.88  -182.88',/ &
' cuboid     29 1  2p0.73660  2p0.73660  192.88  -192.88',/ &
'end geom',/ &
'end data',/ &
'end')
end
```

FORTRAN-90 SOURCE LISTING FOR CASKET_II.F90

```
program casket
!
!  CASKET - Computational Analysis of the Sensitivity of K-eff for
Examination of Trends
!
!  Version II - Used to study the effect of various operating histories on
the value of
!  k-eff for a specific cask design.
!
  implicit none
  character*7 nuclide(29)
  character*9 filename
  character*28 longfname
  real upperbound(0:12), boundprofile(12,18), burn(27),u234,u235,u236,u238
  real burnup,sum,enrichment,specific_power,cooltime,pwr,matpwr(27,6)
  integer i, j, icollapse, iset, icase, izone, material, nuc, ihist
  integer
istart,iend,next,last,idum,id(29),refid(29),nucid(29),skipped(12,10)
  real dum,den(27,29,2),keff(12,10),sigma(12,10)
  logical file_exists
  integer nstart,nend,ilite,iact,ifp,numnuc,icool,orgid(2000)
  real conc(2000,2),cycmult(6),cycdown(6)
!
!   Bounding axial profiles, taken from "Bounding Axial Profile Analysis for
!   the Topical Report Database," by T. A. Parish and C. H. Chen, Nuclear
!   Engineering Dept., Texas A&M University, March 1997.
  data
(upperbound(i),i=0,12)/0.,6.,10.,14.,18.,22.,26.,30.,34.,38.,42.,46.,50./
  data ((boundprofile(i,j),j=1,18),i=12,1,-1)/  & ! note that j moves
backwards since first set is for highest B/U
    0.573, 0.917, 1.021, 1.040, 1.126, 1.123, 1.118, 1.113, 1.109, &  !48
    1.105, 1.101, 1.098, 1.101, 1.098, 1.028, 0.986, 0.831, 0.512, &  !48
    0.615, 0.918, 1.020, 1.045, 1.120, 1.112, 1.116, 1.114, 1.104, &  !44
    1.107, 1.101, 1.101, 1.107, 1.104, 1.025, 0.981, 0.800, 0.512, &  !44
    0.607, 0.914, 1.024, 1.041, 1.124, 1.117, 1.108, 1.107, 1.103, &  !40
    1.102, 1.099, 1.101, 1.111, 1.112, 1.029, 0.981, 0.823, 0.498, &  !40
    0.520, 0.888, 1.009, 1.046, 1.155, 1.143, 1.136, 1.137, 1.137, &  !36
    1.133, 1.130, 1.145, 1.145, 1.143, 1.025, 0.970, 0.743, 0.393, &  !36
    0.537, 0.895, 1.007, 1.045, 1.141, 1.140, 1.135, 1.130, 1.125, &  !32
    1.121, 1.138, 1.145, 1.142, 1.136, 1.020, 0.953, 0.738, 0.451, &  !32
    0.551, 0.886, 1.007, 0.974, 1.146, 1.138, 1.140, 1.135, 1.138, &  !28
    1.166, 1.173, 1.173, 1.169, 1.157, 1.022, 0.882, 0.701, 0.444, &  !28
    0.544, 0.869, 0.962, 0.918, 1.138, 1.140, 1.153, 1.153, 1.172, &  !24
    1.192, 1.201, 1.203, 1.199, 1.185, 1.014, 0.871, 0.689, 0.396, &  !24
    0.540, 0.860, 0.965, 0.921, 1.174, 1.176, 1.171, 1.166, 1.167, &  !20
    1.185, 1.188, 1.186, 1.182, 1.173, 1.008, 0.898, 0.669, 0.373, &  !20
    0.502, 0.817, 0.925, 0.796, 1.260, 1.254, 1.242, 1.234, 1.277, &  !16
    1.323, 1.336, 1.335, 1.325, 1.299, 0.756, 0.614, 0.481, 0.225, &  !16
    0.489, 0.772, 0.944, 0.857, 1.179, 1.151, 1.186, 1.181, 1.180, &  !12
    1.236, 1.261, 1.265, 1.261, 1.244, 0.951, 0.847, 0.650, 0.348, &  !12
    0.478, 0.773, 0.950, 1.059, 1.205, 1.201, 1.211, 1.215, 1.218, &  ! 8
    1.216, 1.209, 1.194, 1.170, 1.151, 0.976, 0.806, 0.596, 0.370, &  ! 8
```

```
    0.470, 0.775, 0.955, 1.064, 1.141, 1.162, 1.180, 1.189, 1.192, &  ! 3
    1.191, 1.185, 1.172, 1.158, 1.130, 1.021, 0.900, 0.714, 0.403 /   ! 3
  data (nuclide(i),i=1,29)/ &
    '  u-233',' np-237',' pu-238',' pu-239',' pu-240',' pu-241',' pu-242', &
    ' am-241','am-242m',' am-243',' mo-95',' tc-99',' ru-101',' rh-103', &
    ' ag-109',' nd-143',' nd-145',' sm-147',' sm-149',' sm-150',' sm-151', &
    ' eu-151',' sm-152',' eu-153',' gd-155',' u-234',' u-235',' u-236', &
    '  u-238'/
  data (refid(i),i=1,29)/ 922330, 932370, 942380, 942390, 942400, 942410, &
          942420, 952410, 952421, 952430, 420950, 430990, 441010, 451030, &
          471090, 601430, 601450, 621470, 621490, 621500, 621510, 621520, &
          631510, 631530, 641550, 922340, 922350, 922360, 922380 /
  data (nucid(i),i=1,29)/ 92233, 93237, 94238, 94239, 94240, 94241, &
          94242, 95241, 95601, 95243, 42095, 43099, 44101, 45103, &
          47109, 60143, 60145, 62147, 62149, 62150, 62151, 62152, &
          63151, 63153, 64155, 92234, 92235, 92236, 92238 /
!
!  First renormalize boundprofile arrays to average of 1.0 for each burnup
range -
!  the tabulated values have some roundoff and are not exact.
!
   sum = 0.0
   do izone = 1,18
     sum = sum + boundprofile(12,izone)
   end do
   sum = sum/18.0
   boundprofile(12,:) = boundprofile(12,:)/sum
!
!  Read problem specifications from keyboard input
!
    write(6,'(''Initial enrichment (wt %)? '')',advance='no')
    read(5,*)enrichment
    write(6,'(''Burnup (GWd/MTU)? '')',advance='no')
    read(5,*)burnup
    istart = 0
    iend = 0
    do while (istart.lt.1 .or. istart.gt.11)
      write(6,'(''Starting operating history (1-11)? '')',advance='no')
      read(5,*)istart
    end do
    do while (iend.lt.1 .or. iend.gt.11)
      write(6,'(''Ending operating history (1-11)? '')',advance='no')
      read(5,*)iend
    end do
!
!  Calculate fractional components of other U nuclides
!
    u234 = 0.007731*enrichment**1.0837
    u235 = enrichment
    u236 = 0.0046*enrichment
    u238 = 100.0-u235-u234-u236
!
!  Sweep through each of the operating histories, analyzing each one
separately
!
  do ihist = istart,iend
!
```

```
!  Select the operating history parameters for this case
!
    select case (ihist)
    case (1:8)
      cycmult(:) = 1.0
    case (9)
      cycmult(1:2) = 1.2
      cycmult(3:6) = 0.9
    case (10)
      cycmult(1:2) = 0.9
      cycmult(3:4) = 1.2
      cycmult(5:6) = 0.9
    case (11)
      cycmult(1:4) = 0.9
      cycmult(5:6) = 1.2
    end select
    select case (ihist)
    case (1)
      cycdown(:) = 0.0
      cycdown(6) = 1826.25
    case (2,9:11)
      cycdown(:) = 20.0
      cycdown(6) = 1826.25
    case (3)
      cycdown(:) = 45.0
      cycdown(6) = 1826.25
    case (4)
      cycdown(:) = 77.0
      cycdown(6) = 1826.25
    case (5)
      cycdown(:) = 20.0
      cycdown(2:3) = 77.0
      cycdown(6) = 1826.25
    case (6)
      cycdown(:) = 20.0
      cycdown(4:5) = 77.0
      cycdown(6) = 1826.25
    case (7)
      cycdown(:) = 20.0
      cycdown(3) = 720.0
      cycdown(6) = 1826.25
    case (8)
      cycdown(:) = 20.0
      cycdown(5) = 720.0
      cycdown(6) = 1826.25
    end select
!
!  Use a seven-zone collapse of the original 18-zone Parish profile for this
!  burnup
!
!  1 2 3 19 19 19 19 19 19 19 19 19 19 19 19 16 17 18
!
!  Material 19 has a burnup equal to the average of zones 4-15 in the
!  corresponding Parish profile
!
    burn(1:18) = boundprofile(12,:)
    burn(19) = 0.0
```

```
    do iset = 4,15
      burn(19) = burn(19) + boundprofile(12,iset)
    end do
    burn(19) = burn(19)/12
!
!  set up and execute 7 sas2h/origen-s cases to obtain isotopics for the 7
!  different burnups to be used.  The SAS2H cases are run to "burnup"
!  burnup at the user-specified specific power for the user-specified
!  initial enrichment.  The SAS2H calculation uses operating history data
!  predefined for each of 11 histories, with 1 library/cycle.  This is
!  followed by an ORIGEN-S calculation to obtain isotopics at 5 and 20,000
!  years
!
    do material = 1,19
      if(material.gt.3 .and. material.lt.16)cycle
!
!  Create sas2h input case for this average burnup step and for this material
!
      open(10,file='sas2h.in',status='unknown')
      write(10,1000)enrichment,ihist,burnup,material,u234,u235,u236,u238
      do nuc = 1,25
        write(10,'(1x,a7,'' 1 0 1-20 841 end'')')nuclide(nuc)
      end do
      pwr = burnup*1000/1080.0*burn(material)
      write(10,1010)
      do i = 1,6
        matpwr(material,i) = pwr*cycmult(i)
        write(10,1009)pwr*cycmult(i),cycdown(i)
      end do
      write(10,1008)cycmult(1)/6.0,pwr*cycmult(1), &
        u234*1e4,u235*1e4,u236*1e4,u238*1e4,cycdown(1)/4.0,cycdown(1)
      do i = 2,5
        write(10,1011)i,i,180.0*(i-1),cycmult(i)/6.0,pwr*cycmult(i),180.0*(i-
1)+45.0,180.0*i,cycdown(i)/4.0,cycdown(i)
      end do
      write(10,1012) cycmult(6)/6.0,pwr*cycmult(6)
      close(10)
!
!  Submit this case
!
      call system('/scale4.3/cmds/scale43 sas2h.in sas2h.out')
!
!  Open unit 71 and read concentrations for desired nuclides
!
      open(71,file='ft71f001',status='old',form='unformatted')
      read(71)numnuc,ilite,iact,ifp
      read(71)(orgid(i),i=1,numnuc),(conc(i,1),i=1,numnuc)
      read(71)
      read(71)(orgid(i),i=1,numnuc),(conc(i,2),i=1,numnuc)
      close(71)
      den(material,:,:) = -1.0
      do i = 1,29
        select case (i)
        case (1:10,26:29) ! actinides
          nstart = ilite+1
          nend = ilite+iact
        case default ! fission products
```

```
          nstart = ilite+iact+1
          nend = numnuc
        end select
        do j = nstart,nend
          if(refid(i).eq.orgid(j))then
            den(material,i,:) = conc(j,1:2)
            exit
          endif
        end do
      end do
!
!  concentrations are in gram-atoms (moles).  Need to convert to a number
density.
!  This requires knowing the fuel volume.  The SAS2H model contains fuel pins
with
!  diameter 0.9563cm, length 893.8933cm, and a total of 176 pins.  This
translates
!  to a fuel volume of 1.13e5 cm**2.  Then make sure that all densities have
been
!  updated, and print an error message and stop if not.
!
      do i = 1,29
        do icool = 1,2
          if(den(material,i,icool).lt.1e-20)then
            den(material,i,icool) = 0.0
          else
            den(material,i,icool) = den(material,i,icool)*6.0221367e-1/1.13e5
          endif
          if(den(material,i,icool).lt.0.0)then
            write(6,*)'Error during operating history ',ihist,', material
#',material,', cooling period ',icool
            write(6,*)'Failed to find number density for nuclide id ',id(i)
            stop
          endif
        end do
      end do
    end do ! material
!
!  We now have the 7 different materials necessary to run this operating
history
!  Create a csasn case to make a library that contains all 7 fuel materials
!  with weighted cross-sections, plus clad and moderator, for cooling times
of
!  5 and 20,000 years.
!
    do icool = 1,2
      write(filename,'("csasn",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1030)enrichment,specific_power,burnup
      do material = 1,19
        if(material.gt.3.and.material.lt.16)cycle
        do nuc = 1,29
          write(10,'(1x,a7,1x,i2,'' 0 '',1pe10.4,'' 293
end'')')nuclide(nuc),material,den(material,nuc,1)
        end do
      end do
      write(10,1040)
```

```
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  We now have a working library with cross-sections for 7 fuel materials
plus clad and moderator
!  Create and run keno v.a calculations for each of the 2 cooling times, and
extract k-eff and sigma
!  from each.
!
      last = 0
      write(filename,'("keno_",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1050)enrichment,specific_power,burnup,ihist  ! header for keno
case
      do izone = 1,19
        if(izone.gt.3 .and. izone.lt.16) cycle
        write(10,'("''",6(1x,f7.4))')(matpwr(izone,i),i=1,6)
      end do
      do izone = 1,19
        if(izone.gt.3 .and. izone.lt.16) cycle
        write(10,'(''mix='',i2.2)')izone
        do nuc = 1,29

write(10,'(i10,2x,1pe11.5)')nucid(nuc)+izone*1000000,den(izone,nuc,icool)
        end do
      end do !izone
      write(10,1060) ! finish up with mixtures for water and clad
      write(10,1065)1,-162.56
      write(10,1065)2,-142.24
      write(10,1065)3,-121.92
      write(10,1065)19,-101.60
      write(10,1065)16,142.24
      write(10,1065)17,162.56
      write(10,1065)18,182.88
      write(10,1070)
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  Grep the lines containing the final k-eff results into a file.  Then
!  Edit the file to get k-eff values, uncertainties, and no. of generations
!  skipped.
!
      call system('grep "generations skipped." '//filename(1:6)//'.out >
keno.results')
      open(10,file='keno.results',status='old')

read(10,'(t34,f7.4,t48,f8.4,t73,i6)')keff(ihist,icool),sigma(ihist,icool),ski
pped(ihist,icool)
      close(10)
    end do ! icool
    write(longfname,'("ophist",f3.1,"%_",f4.1,"GWd_hist",i2.2,"-
",i2.2)')enrichment,burnup,istart,iend
    open(10,file=longfname,status='unknown')
    do i = istart,ihist-1
      read(10,*)
```

```
    end do

write(10,'(i2.2,2(1x,1pe12.5,1x,1pe12.5,1x,i4))')ihist,(keff(ihist,icool),sig
ma(ihist,icool),skipped(ihist,icool),icool=1,2)
    close(10)
  end do ! ihist
stop
1000 format(  &
"=sas2h       parm='skipshipdata'",/ &
'casket_II, ',f4.2,' wt% enrich., ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U, Mat.
# ',i2.2,/ &
'44group latticecell',/ &
'  uo2 1 den=10.045 1 841',/ &
'    92234 ',f6.4,' 92235 ',f6.4,' 92236 ',f6.4,' 92238 ',f7.4,' end',/ &
'  c 1 den=1.8-4 1 841 end',/ &
'  n 1 den=2.3-4 1 841 end',/ &
'  co-59 3 0 1-20 558 end',/ &
'  zr-94 1 0 1-20 841 end')
1010 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 2 1 620
end',/ &
'  h2o 3 den=0.7569 1 558 end',/ &
'  arbm-bormod 0.7569 1 1 0 0 5000 100 3 330.8e-6 558 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 1 3 1.1176 2 0.9855 0 end',/ &
'npin/assm=176 fuelnght=893.8933 ncycles=6 nlib/cyc=1',/ &
'printlevel=4 lightel=9 inplevel=2 numztotal=5   end',/ &
'3  1.314  2  1.416  3  1.662  500  5.203  3  5.243 ')
1009 format('power=',1pe9.3,' burn=180.0 down=',e9.3,' end')
1008 format('  o 119  cr  5.2  mn  0.29',/ &
'  fe 11. co 0.066 ni  8.7',/ &
'  zr 195 nb  0.63 sn  3.2',/ &
'end',0p,/ &
'=origen',/ &
'0$$ e t',/ &
'Library position 1/6',/ &
'3$$ 33 0 1 a16 2 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 0 a13 13 4 2 a17 4 1 e',/ &
'57** a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,0p,/ &
'60** 2i45 180',/ &
'66$$ 0 a5 2 a9 2 e',/ &
'73$$ 922340 922350 922360 922380 80000 240000 250000 260000',/ &
'     270000 280000 400000 410000 500000',/ &
'74** ',f5.1,1x,f7.1,1x,f5.1,1x,f8.1,' 119000 5200 290 11000',/ &
'      66 8700 195000 630 3200',/ &
'75$$ 4r2 9r4 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1011 format('Library Position ',i1,'/6', / &
'3$$ 33 0 ',i1,' e 2t',/ &
'4t',/ &
```

```
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
'57** ',f8.3,' a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1012 format('Library Position 6/6', / &
'3$$ 33 0 6 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
'57** 900 a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i945 1080',/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 12 a5 11 1 a10 4 a14 5 3 a17 4 1 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'20,000 year cooling period',/ &
'1 MTU',/ &
'60** 0.33 1.0 3.3 5.0 10 33 100 333 1000 3333 10000 20000',/ &
'65$$ a4 0 a25 1 a46 1 e 6t',/ &
'56$$ 0 0 a10 4 e t',/ &    ! write to unit 71 for 4th decay period (5 y)
'56$$ 0 0 a10 12 e t',/ &   ! write to unit 71 for 12th decay period (20,000
y)
'56$$ f0 t',/ &
'end',/ &
'=shell',/ &
'cp $TMPDIR/ft71f001 $RTNDIR/ft71f001',/ &
'cp $TMPDIR/ft72f001 $RTNDIR/ft72f001',/ &
'end')
1020 format(4(i8, e12.4))
1030 format(  &
'=csasn          parm=(size=500000)',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U
(pin average)',/ &
'44group latticecell')
1040 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 28 1 293
end',/ &
'  h2o 29 1 293 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 19 29 1.1176 28 0.9855 0 end',/ &
'more data',/ &
'res=1 cylinder 0.47815  dan(1)=2.25244E-01',/ &
'res=2 cylinder 0.47815  dan(2)=2.25244E-01',/ &
'res=3 cylinder 0.47815  dan(3)=2.25244E-01',/ &
'res=16 cylinder 0.47815  dan(16)=2.25244E-01',/ &
'res=17 cylinder 0.47815  dan(17)=2.25244E-01',/ &
'res=18 cylinder 0.47815  dan(18)=2.25244E-01',/ &
'end more',/ &
'end')
1050 format( &
```

```
'=kenova',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU ave
B/U, Axial model #',i2.2,/ &
'read parm npg=1000 gen=1005 nsk=5 nub=yes',/ &
!'read parm npg=100 gen=105 nsk=5 nub=yes',/ &
'   lib=4 fdn=yes tme=300 end parm',/ &
'read boun all=mirror end boun',/ &
'read mixt')
1060 format( &
'mix=28',/ &
'  28040000  4.16270E-02',/ &
'  28026000  3.47236E-04',/ &
'  28050116  2.87770E-04',/ &
'  28050120  2.36120E-04',/ &
'mix=29',/ &
'  29001001  6.67692E-02',/ &
'  29008016  3.33846E-02',/ &
'end mixt',/ &
'read geom',/ &
'unit 1')
1065 format(' cylinder   ',i2,' 1  0.47815 ',f7.2,' -182.88')
1070 format( &
' cylinder   0  1  0.49275  182.88  -182.88',/ &
' cylinder   28 1  0.55880  182.88  -182.88',/ &
' cuboid     29 1  2p0.73660  2p0.73660  192.88  -192.88',/ &
'end geom',/ &
'end data',/ &
'end')
end
```

FORTRAN-90 SOURCE LISTING FOR CASKET_III.F90

```
program casket
!
!  CASKET - Computational Analysis of the Sensitivity of K-eff for
Examination of Trends
!
!  Version III - Used to study the effect of specific powers on the value of
!  k-eff for a specific cask design.
!
  implicit none
  character*7 nuclide(29)
  character*9 filename
  character*19 longfname
  real upperbound(0:12), boundprofile(12,18), burn(27),u234,u235,u236,u238
  real burnup,sum,enrichment,specific_power,cooltime,pwr,burntime
  integer i, j, icollapse, iset, icase, izone, material, nuc, ispecpwr
  integer
istart,iend,next,last,idum,id(29),refid(29),nucid(29),skipped(12,10)
  real dum,den(27,29,2),keff(12,10),sigma(12,10)
  logical file_exists
  logical, parameter :: DEBUG=.true.
  integer nstart,nend,ilite,iact,ifp,numnuc,icool,orgid(2000)
  real conc(2000,2)
!
!   Bounding axial profiles, taken from "Bounding Axial Profile Analysis for
!   the Topical Report Database," by T. A. Parish and C. H. Chen, Nuclear
!   Engineering Dept., Texas A&M University, March 1997.
  data
(upperbound(i),i=0,12)/0.,6.,10.,14.,18.,22.,26.,30.,34.,38.,42.,46.,50./
  data ((boundprofile(i,j),j=1,18),i=12,1,-1)/  & ! note that j moves
backwards since first set is for highest B/U
    0.573, 0.917, 1.021, 1.040, 1.126, 1.123, 1.118, 1.113, 1.109, &  !48
    1.105, 1.101, 1.098, 1.101, 1.098, 1.028, 0.986, 0.831, 0.512, &  !48
    0.615, 0.918, 1.020, 1.045, 1.120, 1.112, 1.116, 1.114, 1.104, &  !44
    1.107, 1.101, 1.101, 1.107, 1.104, 1.025, 0.981, 0.800, 0.512, &  !44
    0.607, 0.914, 1.024, 1.041, 1.124, 1.117, 1.108, 1.107, 1.103, &  !40
    1.102, 1.099, 1.101, 1.111, 1.112, 1.029, 0.981, 0.823, 0.498, &  !40
    0.520, 0.888, 1.009, 1.046, 1.155, 1.143, 1.136, 1.137, 1.137, &  !36
    1.133, 1.130, 1.145, 1.145, 1.143, 1.025, 0.970, 0.743, 0.393, &  !36
    0.537, 0.895, 1.007, 1.045, 1.141, 1.140, 1.135, 1.130, 1.125, &  !32
    1.121, 1.138, 1.145, 1.142, 1.136, 1.020, 0.953, 0.738, 0.451, &  !32
    0.551, 0.886, 1.007, 0.974, 1.146, 1.138, 1.140, 1.135, 1.138, &  !28
    1.166, 1.173, 1.173, 1.169, 1.157, 1.022, 0.882, 0.701, 0.444, &  !28
    0.544, 0.869, 0.962, 0.918, 1.138, 1.140, 1.153, 1.153, 1.172, &  !24
    1.192, 1.201, 1.203, 1.199, 1.185, 1.014, 0.871, 0.689, 0.396, &  !24
    0.540, 0.860, 0.965, 0.921, 1.174, 1.176, 1.171, 1.166, 1.167, &  !20
    1.185, 1.188, 1.186, 1.182, 1.173, 1.008, 0.898, 0.669, 0.373, &  !20
    0.502, 0.817, 0.925, 0.796, 1.260, 1.254, 1.242, 1.234, 1.277, &  !16
    1.323, 1.336, 1.335, 1.325, 1.299, 0.756, 0.614, 0.481, 0.225, &  !16
    0.489, 0.772, 0.944, 0.857, 1.179, 1.151, 1.186, 1.181, 1.180, &  !12
    1.236, 1.261, 1.265, 1.261, 1.244, 0.951, 0.847, 0.650, 0.348, &  !12
    0.478, 0.773, 0.950, 1.059, 1.205, 1.201, 1.211, 1.215, 1.218, &  ! 8
    1.216, 1.209, 1.194, 1.170, 1.151, 0.976, 0.806, 0.596, 0.370, &  ! 8
```

```
    0.470, 0.775, 0.955, 1.064, 1.141, 1.162, 1.180, 1.189, 1.192, &  ! 3
    1.191, 1.185, 1.172, 1.158, 1.130, 1.021, 0.900, 0.714, 0.403 /   ! 3
  data (nuclide(i),i=1,29)/ &
    '  u-233',' np-237',' pu-238',' pu-239',' pu-240',' pu-241',' pu-242', &
    ' am-241','am-242m',' am-243','  mo-95','  tc-99',' ru-101',' rh-103', &
    ' ag-109',' nd-143',' nd-145',' sm-147',' sm-149',' sm-150',' sm-151', &
    ' eu-151',' sm-152',' eu-153',' gd-155','  u-234','  u-235','  u-236', &
    '  u-238'/
  data (refid(i),i=1,29)/ 922330, 932370, 942380, 942390, 942400, 942410, &
          942420, 952410, 952421, 952430, 420950, 430990, 441010, 451030, &
          471090, 601430, 601450, 621470, 621490, 621500, 621510, 621520, &
          631510, 631530, 641550, 922340, 922350, 922360, 922380 /
  data (nucid(i),i=1,29)/ 92233, 93237, 94238, 94239, 94240, 94241, &
          94242, 95241, 95601, 95243, 42095, 43099, 44101, 45103, &
          47109, 60143, 60145, 62147, 62149, 62150, 62151, 62152, &
          63151, 63153, 64155, 92234, 92235, 92236, 92238 /
!
!  First renormalize boundprofile arrays to average of 1.0 for each burnup
range -
!  the tabulated values have some roundoff and are not exact.
!
   sum = 0.0
   do izone = 1,18
     sum = sum + boundprofile(12,izone)
   end do
   sum = sum/18.0
   boundprofile(12,:) = boundprofile(12,:)/sum
!
!  Read problem specifications from keyboard input
!
    write(6,'(''Initial enrichment (wt %)? '')',advance='no')
    read(5,*)enrichment
    write(6,'(''Burnup (GWd/MTU)? '')',advance='no')
    read(5,*)burnup
    if(DEBUG) open(11,file='debug.out')
!
!  Calculate fractional components of other U nuclides
!
    u234 = 0.007731*enrichment**1.0837
    u235 = enrichment
    u236 = 0.0046*enrichment
    u238 = 100.0-u235-u234-u236
!
!  Sweep through each of five specific power cases
!
  do ispecpwr = 10,50,10
!
!  Use a seven-zone collapse of the original 18-zone Parish profile for this
!  burnup
!
!  1 2 3 19 19 19 19 19 19 19 19 19 19 19 19 16 17 18
!
!  Material 19 has a burnup equal to the average of zones 4-15 in the
!  corresponding Parish profile
!
    burn(1:18) = boundprofile(12,:)
    burn(19) = 0.0
```

```
    do iset = 4,15
      burn(19) = burn(19) + boundprofile(12,iset)
    end do
    burn(19) = burn(19)/12
!
!  set up and execute 7 sas2h/origen-s cases to obtain isotopics for the 7
!  different burnups to be used.  The SAS2H cases are run to "burnup"
!  burnup at the current specific power for the user-specified
!  initial enrichment.  The SAS2H calculation uses operating history data
!  assuming constant power operation with zero down time.  This is
!  followed by an ORIGEN-S calculation to obtain isotopics at 5 and 20,000
!  years
!
    do material = 1,19
      if(material.gt.3 .and. material.lt.16)cycle
!
!  Create sas2h input case for this average burnup step and for this material
!
      open(10,file='sas2h.in',status='unknown')
      write(10,1000)enrichment,ispecpwr,burnup,material,u234,u235,u236,u238
      do nuc = 1,25
        write(10,'(1x,a7,'' 1 0 1-20 841 end'')')nuclide(nuc)
      end do
      burntime = burnup*1000/ispecpwr/6.0
      pwr = ispecpwr*burn(material)
      write(10,1010)
      if(DEBUG)write(11,1009)pwr,burntime,float(ispecpwr)
      do i = 1,6
        write(10,1009)pwr,burntime,0.0
      end do
      write(10,1008)1.0/6.0,pwr, burntime/4.0,burntime, &
        u234*1e4,u235*1e4,u236*1e4,u238*1e4,0.0,0.0
      do i = 2,5
        write(10,1011)i,i,burntime*(i-1),1.0/6.0,pwr,burntime*(i-
1)+burntime/4.0,burntime*i,0.0,0.0
      end do
      write(10,1012)
5*burntime,1.0/6.0,pwr,5*burntime+burntime/4.0,burntime*6
      close(10)
!
!  Submit this case
!
      call system('/scale4.3/cmds/scale43 sas2h.in sas2h.out')
!
!  Open unit 71 and read concentrations for desired nuclides
!
      open(71,file='ft71f001',status='old',form='unformatted')
      read(71)numnuc,ilite,iact,ifp
      read(71)(orgid(i),i=1,numnuc),(conc(i,1),i=1,numnuc)
      read(71)
      read(71)(orgid(i),i=1,numnuc),(conc(i,2),i=1,numnuc)
      close(71)
      den(material,:,:) = -1.0
      do i = 1,29
        select case (i)
        case (1:10,26:29) ! actinides
          nstart = ilite+1
```

```
          nend = ilite+iact
        case default ! fission products
          nstart = ilite+iact+1
          nend = numnuc
        end select
        do j = nstart,nend
          if(refid(i).eq.orgid(j))then
            den(material,i,:) = conc(j,1:2)
            exit
          endif
        end do
      end do
!
!  concentrations are in gram-atoms (moles).  Need to convert to a number
density.
!  This requires knowing the fuel volume.  The SAS2H model contains fuel pins
with
!  diameter 0.9563cm, length 893.8933cm, and a total of 176 pins.  This
translates
!  to a fuel volume of 1.13e5 cm**2.  Then make sure that all densities have
been
!  updated, and print an error message and stop if not.
!
      do i = 1,29
        do icool = 1,2
          if(den(material,i,icool).lt.1e-20)then
            den(material,i,icool) = 0.0
          else
            den(material,i,icool) = den(material,i,icool)*6.0221367e-1/1.13e5
          endif
          if(den(material,i,icool).lt.0.0)then
            write(6,*)'Error during operating history ',ispecpwr,', material
#',material,', cooling period ',icool
            write(6,*)'Failed to find number density for nuclide id ',id(i)
            stop
          endif
        end do
      end do
    end do ! material
!
!  We now have the 7 different materials necessary to run this operating
history
!  Create a csasn case to make a library that contains all 7 fuel materials
!  with weighted cross-sections, plus clad and moderator, for cooling times
of
!  5 and 20,000 years.
!
    do icool = 1,2
      write(filename,'("csasn",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1030)enrichment,specific_power,burnup
      do material = 1,19
        if(material.gt.3.and.material.lt.16)cycle
        do nuc = 1,29
          write(10,'(1x,a7,1x,i2,'' 0 '',1pe10.4,'' 293
end'')')nuclide(nuc),material,den(material,nuc,1)
        end do
```

```
      end do
      write(10,1040)
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  We now have a working library with cross-sections for 7 fuel materials
plus clad and moderator
!  Create and run keno v.a calculations for each of the 2 cooling times, and
extract k-eff and sigma
!  from each.
!
      last = 0
      write(filename,'("keno_",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1050)enrichment,specific_power,burnup,ispecpwr  ! header for
keno case
      do izone = 1,19
        if(izone.gt.3 .and. izone.lt.16) cycle
        write(10,'(''mix='',i2.2)')izone
        do nuc = 1,29

write(10,'(i10,2x,1pe11.5)')nucid(nuc)+izone*1000000,den(izone,nuc,icool)
        end do
      end do !izone
      write(10,1060) ! finish up with mixtures for water and clad
      write(10,1065)1,-162.56
      write(10,1065)2,-142.24
      write(10,1065)3,-121.92
      write(10,1065)19,-101.60
      write(10,1065)16,142.24
      write(10,1065)17,162.56
      write(10,1065)18,182.88
      write(10,1070)
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  Grep the lines containing the final k-eff results into a file.  Then
!  Edit the file to get k-eff values, uncertainties, and no. of generations
!  skipped.
!
      call system('grep "generations skipped." '//filename(1:6)//'.out >
keno.results')
      open(10,file='keno.results',status='old')

read(10,'(t34,f7.4,t48,f8.4,t73,i6)')keff(ispecpwr,icool),sigma(ispecpwr,icoo
l),skipped(ispecpwr,icool)
      close(10)
    end do ! icool
    write(longfname,'("specpwr",f3.1,"%_",f4.1,"GWd")')enrichment,burnup
    open(10,file=longfname,status='unknown')
    do i = 1,ispecpwr/10-1
      read(10,*)
    end do
```

```
write(10,'(i2.2,2(1x,1pe12.5,1x,1pe12.5,1x,i4))')ispecpwr,(keff(ispecpwr,icoo
l),sigma(ispecpwr,icool),skipped(ispecpwr,icool),icool=1,2)
    close(10)
  end do ! ispecpwr
stop
1000 format(  &
"=sas2h       parm='skipshipdata'",/ &
'casket_II, ',f4.2,' wt% enrich., ',i2,' MW/MTU, ',f5.2,' GWd/MTU B/U, Mat. #
',i2.2,/ &
'44group latticecell',/ &
'  uo2 1 den=10.045 1 841',/ &
'    92234 ',f6.4,' 92235 ',f6.4,' 92236 ',f6.4,' 92238 ',f7.4,' end',/ &
'  c 1 den=1.8-4 1 841 end',/ &
'  n 1 den=2.3-4 1 841 end',/ &
'  co-59 3 0 1-20 558 end',/ &
'  zr-94 1 0 1-20 841 end')
1010 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 2 1 620
end',/ &
'  h2o 3 den=0.7569 1 558 end',/ &
'  arbm-bormod 0.7569 1 1 0 0 5000 100 3 330.8e-6 558 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 1 3 1.1176 2 0.9855 0 end',/ &
'npin/assm=176 fuelnght=893.8933 ncycles=6 nlib/cyc=1',/ &
'printlevel=4 lightel=9 inplevel=2 numztotal=5   end',/ &
'3  1.314  2  1.416  3  1.662  500  5.203  3  5.243 ')
1009 format('power=',1pe9.3,' burn=',1pe9.3,' down=',e9.3,' end')
1008 format('  o 119  cr  5.2  mn  0.29',/ &
'  fe 11. co 0.066 ni  8.7',/ &
'  zr 195 nb  0.63 sn  3.2',/ &
'end',0p,/ &
'=origen',/ &
'0$$ e t',/ &
'Library position 1/6',/ &
'3$$ 33 0 1 a16 2 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 0 a13 13 4 2 a17 4 1 e',/ &
'57** a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,0p,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e',/ &
'73$$ 922340 922350 922360 922380 80000 240000 250000 260000',/ &
'     270000 280000 400000 410000 500000',/ &
'74** ',f5.1,1x,f7.1,1x,f5.1,1x,f8.1,' 119000 5200 290 11000',/ &
'      66 8700 195000 630 3200',/ &
'75$$ 4r2 9r4 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1011 format('Library Position ',i1,'/6', / &
'3$$ 33 0 ',i1,' e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
```

```
'57** ',f8.3,' a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1012 format('Library Position 6/6', / &
'3$$ 33 0 6 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
'57** ',f8.3,' a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 12 a5 11 1 a10 4 a14 5 3 a17 4 1 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'20,000 year cooling period',/ &
'1 MTU',/ &
'60** 0.33 1.0 3.3 5.0 10 33 100 333 1000 3333 10000 20000',/ &
'65$$ a4 0 a25 1 a46 1 e 6t',/ &
'56$$ 0 0 a10 4 e t',/ &    ! write to unit 71 for 4th decay period (5 y)
'56$$ 0 0 a10 12 e t',/ &   ! write to unit 71 for 12th decay period (20,000
y)
'56$$ f0 t',/ &
'end',/ &
'=shell',/ &
'cp $TMPDIR/ft71f001 $RTNDIR/ft71f001',/ &
'cp $TMPDIR/ft72f001 $RTNDIR/ft72f001',/ &
'end')
1020 format(4(i8, e12.4))
1030 format(  &
'=csasn          parm=(size=500000)',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U
(pin average)',/ &
'44group latticecell')
1040 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 50120 0.73 28 1 293
end',/ &
'  h2o 29 1 293 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 19 29 1.1176 28 0.9855 0 end',/ &
'more data',/ &
'res=1 cylinder 0.47815  dan(1)=2.25244E-01',/ &
'res=2 cylinder 0.47815  dan(2)=2.25244E-01',/ &
'res=3 cylinder 0.47815  dan(3)=2.25244E-01',/ &
'res=16 cylinder 0.47815  dan(16)=2.25244E-01',/ &
'res=17 cylinder 0.47815  dan(17)=2.25244E-01',/ &
'res=18 cylinder 0.47815  dan(18)=2.25244E-01',/ &
'end more',/ &
'end')
1050 format( &
'=kenova',/ &
```

```
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU ave
B/U, Axial model #',i2.2,/ &
'read parm npg=1000 gen=1005 nsk=5 nub=yes',/ &
!'read parm npg=100 gen=105 nsk=5 nub=yes',/ &
'   lib=4 fdn=yes tme=300 end parm',/ &
'read boun all=mirror end boun',/ &
'read mixt')
1060 format( &
'mix=28',/ &
'  28040000  4.16270E-02',/ &
'  28026000  3.47236E-04',/ &
'  28050116  2.87770E-04',/ &
'  28050120  2.36120E-04',/ &
'mix=29',/ &
'  29001001  6.67692E-02',/ &
'  29008016  3.33846E-02',/ &
'end mixt',/ &
'read geom',/ &
'unit 1')
1065 format(' cylinder   ',i2,' 1  0.47815 ',f7.2,' -182.88')
1070 format( &
' cylinder   0  1  0.49275  182.88  -182.88',/ &
' cylinder   28 1  0.55880  182.88  -182.88',/ &
' cuboid     29 1  2p0.73660  2p0.73660  192.88  -192.88',/ &
'end geom',/ &
'end data',/ &
'end')
end
```

FORTRAN-90 SOURCE LISTING FOR CASKET_IV.F90

```
program casket
!
!  CASKET - Computational Analysis of the Sensitivity of K-eff for
Examination of Trends
!
!  Version IV - Used to study the effect of material temperatures and boron
concentrations on the value of
!  k-eff for a specific cask design.
!
  implicit none
  character*7 nuclide(30)
  character*9 filename
  character*27 longfname
  real upperbound(0:12), boundprofile(12,18), burn(27),u234,u235,u236,u238
  real burnup,sum,enrichment,specific_power,cooltime,pwr,burntime
  integer i, j, icollapse, iset, icase, izone, material, nuc, option, nskip
  integer
istart,iend,next,last,idum,id(30),refid(30),nucid(30),skipped(12,10)
  real dum,den(27,30,2),keff(12,10),sigma(12,10),specpwr
  integer
bors,bore,tmods,tmode,tfuels,tfuele,tclads,tclade,delb,deltf,deltm,deltc
  integer iboron,imodt,ifuelt,icladt,istep
  real tfuel,tclad,tmod,denmod,concb
  logical file_exists
  logical, parameter :: DEBUG=.true.
  integer nstart,nend,ilite,iact,ifp,numnuc,icool,orgid(2000)
  real conc(2000,2)
!
!   Bounding axial profiles, taken from "Bounding Axial Profile Analysis for
!   the Topical Report Database," by T. A. Parish and C. H. Chen, Nuclear
!   Engineering Dept., Texas A&M University, March 1997.
  data
bors,bore,tmods,tmode,tfuels,tfuele,tclads,tclade/500,500,558,558,841,841,628
,628/
  data delb,deltm,deltf,deltc/1,1,1,1/
  data
(upperbound(i),i=0,12)/0.,6.,10.,14.,18.,22.,26.,30.,34.,38.,42.,46.,50./
  data ((boundprofile(i,j),j=1,18),i=12,1,-1)/  & ! note that j moves
backwards since first set is for highest B/U
    0.573, 0.917, 1.021, 1.040, 1.126, 1.123, 1.118, 1.113, 1.109, &  !48
    1.105, 1.101, 1.098, 1.101, 1.098, 1.028, 0.986, 0.831, 0.512, &  !48
    0.615, 0.918, 1.020, 1.045, 1.120, 1.112, 1.116, 1.114, 1.104, &  !44
    1.107, 1.101, 1.101, 1.107, 1.104, 1.025, 0.981, 0.800, 0.512, &  !44
    0.607, 0.914, 1.024, 1.041, 1.124, 1.117, 1.108, 1.107, 1.103, &  !40
    1.102, 1.099, 1.101, 1.111, 1.112, 1.029, 0.981, 0.823, 0.498, &  !40
    0.520, 0.888, 1.009, 1.046, 1.155, 1.143, 1.136, 1.137, 1.137, &  !36
    1.133, 1.130, 1.145, 1.145, 1.143, 1.025, 0.970, 0.743, 0.393, &  !36
    0.537, 0.895, 1.007, 1.045, 1.141, 1.140, 1.135, 1.130, 1.125, &  !32
    1.121, 1.138, 1.145, 1.142, 1.136, 1.020, 0.953, 0.738, 0.451, &  !32
    0.551, 0.886, 1.007, 0.974, 1.146, 1.138, 1.140, 1.135, 1.138, &  !28
    1.166, 1.173, 1.173, 1.169, 1.157, 1.022, 0.882, 0.701, 0.444, &  !28
    0.544, 0.869, 0.962, 0.918, 1.138, 1.140, 1.153, 1.153, 1.172, &  !24
```

```
    1.192, 1.201, 1.203, 1.199, 1.185, 1.014, 0.871, 0.689, 0.396, &  !24
    0.540, 0.860, 0.965, 0.921, 1.174, 1.176, 1.171, 1.166, 1.167, &  !20
    1.185, 1.188, 1.186, 1.182, 1.173, 1.008, 0.898, 0.669, 0.373, &  !20
    0.502, 0.817, 0.925, 0.796, 1.260, 1.254, 1.242, 1.234, 1.277, &  !16
    1.323, 1.336, 1.335, 1.325, 1.299, 0.756, 0.614, 0.481, 0.225, &  !16
    0.489, 0.772, 0.944, 0.857, 1.179, 1.151, 1.186, 1.181, 1.180, &  !12
    1.236, 1.261, 1.265, 1.261, 1.244, 0.951, 0.847, 0.650, 0.348, &  !12
    0.478, 0.773, 0.950, 1.059, 1.205, 1.201, 1.211, 1.215, 1.218, &  ! 8
    1.216, 1.209, 1.194, 1.170, 1.151, 0.976, 0.806, 0.596, 0.370, &  ! 8
    0.470, 0.775, 0.955, 1.064, 1.141, 1.162, 1.180, 1.189, 1.192, &  ! 3
    1.191, 1.185, 1.172, 1.158, 1.130, 1.021, 0.900, 0.714, 0.403 /   ! 3
  data (nuclide(i),i=1,30)/ &
    '  u-233',' np-237',' pu-238',' pu-239',' pu-240',' pu-241',' pu-242', &
    ' am-241','am-242m',' am-243','  mo-95','  tc-99',' ru-101',' rh-103', &
    ' ag-109',' nd-143',' nd-145',' sm-147',' sm-149',' sm-150',' sm-151', &
    ' eu-151',' sm-152',' eu-153',' gd-155','  u-234','  u-235','  u-236', &
    '  u-238','      o'/
  data (refid(i),i=1,30)/ 922330, 932370, 942380, 942390, 942400, 942410, &
          942420, 952410, 952421, 952430, 420950, 430990, 441010, 451030, &
          471090, 601430, 601450, 621470, 621490, 621500, 621510, 621520, &
          631510, 631530, 641550, 922340, 922350, 922360, 922380,  80160 /
  data (nucid(i),i=1,30)/ 92233, 93237, 94238, 94239, 94240, 94241, &
          94242, 95241, 95601, 95243, 42095, 43099, 44101, 45103, &
          47109, 60143, 60145, 62147, 62149, 62150, 62151, 62152, &
          63151, 63153, 64155, 92234, 92235, 92236, 92238, 8016 /
!
!  First renormalize boundprofile arrays to average of 1.0 for each burnup
range -
!  the tabulated values have some roundoff and are not exact.
!
   sum = 0.0
   do izone = 1,18
     sum = sum + boundprofile(12,izone)
   end do
   sum = sum/18.0
   boundprofile(12,:) = boundprofile(12,:)/sum
!
!  Read problem specifications from keyboard input
!
    write(6,'(''Initial enrichment (wt %)? '')',advance='no')
    read(5,*)enrichment
    write(6,'(''Burnup (GWd/MTU)? '')',advance='no')
    read(5,*)burnup
    if(burnup.lt.0.0)then
      burnup = -burnup
      write(6,'("Number of cases in existing file? ")',advance='no')
      read(5,*)nskip
    endif
    write(6,'(''Select the option to study:'')')
    write(6,'(''  (1) Boron concentration'')')
    write(6,'(''  (2) Fuel Temperature'')')
    write(6,'(''  (3) Clad Temperature'')')
    write(6,'(''  (4) Moderator Temperature'')')
    write(6,'(''  => '')',advance='no')
    read(5,*)option
    select case (option)
    case (1)
```

```
      write(6,'("Starting boron concentration (ppm)? ")',advance='no')
      read(5,*)bors
      write(6,'("Final boron concentration (ppm)? ")',advance='no')
      read(5,*)bore
      write(6,'("Increment? ")',advance='no')
      read(5,*)delb
    case (2)
      write(6,'("Starting fuel temperature (K)? ")',advance='no')
      read(5,*)tfuels
      write(6,'("Final fuel temperature (K)? ")',advance='no')
      read(5,*)tfuele
      write(6,'("Increment? ")',advance='no')
      read(5,*)deltf
    case (3)
      write(6,'("Starting clad temperature (K)? ")',advance='no')
      read(5,*)tclads
      write(6,'("Final clad temperature (K)? ")',advance='no')
      read(5,*)tclade
      write(6,'("Increment? ")',advance='no')
      read(5,*)deltc
    case (4)
      write(6,'("Starting moderator temperature (K)? ")',advance='no')
      read(5,*)tmods
      write(6,'("Final moderator temperature (K)? ")',advance='no')
      read(5,*)tmode
      write(6,'("Increment? ")',advance='no')
      read(5,*)deltm
    end select

    if(DEBUG) open(11,file='debug.out')
!
!  Calculate fractional components of other U nuclides
!
    u234 = 0.007731*enrichment**1.0837
    u235 = enrichment
    u236 = 0.0046*enrichment
    u238 = 100.0-u235-u234-u236
!
!  Sweep through each of the cases using the specified start, end, and
increment
!
  istep = 0
  do iboron = bors,bore,delb
  do ifuelt = tfuels,tfuele,deltf
  do icladt = tclads,tclade,deltc
  do imodt = tmods,tmode,deltm
    concb = iboron/1.0e6
    if (concb.eq.0.0)concb = 1.0e-8
    tfuel = ifuelt
    tclad = icladt
    tmod  = imodt
    denmod = 1.3734-0.0026305*tmod+6.902e-6*tmod*tmod-7.4905e-
9*tmod*tmod*tmod
    istep = istep + 1
!
!  Use a seven-zone collapse of the original 18-zone Parish profile for this
!  burnup
```

```
!
!  1 2 3 19 19 19 19 19 19 19 19 19 19 19 19 16 17 18
!
!  Material 19 has a burnup equal to the average of zones 4-15 in the
!  corresponding Parish profile
!
    burn(1:18) = boundprofile(12,:)
    burn(19) = 0.0
    do iset = 4,15
      burn(19) = burn(19) + boundprofile(12,iset)
    end do
    burn(19) = burn(19)/12
!
!  set up and execute 7 sas2h/origen-s cases to obtain isotopics for the 7
!  different burnups to be used.  The SAS2H cases are run to "burnup"
!  burnup at the current specific power for the user-specified
!  initial enrichment.  The SAS2H calculation uses operating history data
!  assuming constant power operation with zero down time.  This is
!  followed by an ORIGEN-S calculation to obtain isotopics at 5 and 20,000
!  years
!
    do material = 1,19
      if(material.gt.3 .and. material.lt.16)cycle
!
!  Create sas2h input case for this average burnup step and for this material
!
      specpwr = 37.5
      open(10,file='sas2h.in',status='unknown')

write(10,1000)enrichment,specpwr,burnup,material,tfuel,u234,u235,u236,u238,tf
uel,tfuel,tmod,tfuel
      do nuc = 1,25
        write(10,'(1x,a7," 1 0 1-20 ",f6.1," end")')nuclide(nuc),tfuel
      end do
      burntime = burnup*1000/specpwr/6.0
      pwr = specpwr*burn(material)
      write(10,1010)tclad,denmod,tmod,denmod,concb,tmod
      if(DEBUG)write(11,1009)pwr,burntime,specpwr
      do i = 1,6
        write(10,1009)pwr,burntime,0.0
      end do
      write(10,1008)1.0/6.0,pwr, burntime/4.0,burntime, &
        u234*1e4,u235*1e4,u236*1e4,u238*1e4,0.0,0.0
      do i = 2,5
        write(10,1011)i,i,burntime*(i-1),1.0/6.0,pwr,burntime*(i-
1)+burntime/4.0,burntime*i,0.0,0.0
      end do
      write(10,1012)
5*burntime,1.0/6.0,pwr,5*burntime+burntime/4.0,burntime*6
      close(10)
!
!  Submit this case
!
      call system('/scale4.3/cmds/scale43 sas2h.in sas2h.out')
!
!  Open unit 71 and read concentrations for desired nuclides
!
```

```
      open(71,file='ft71f001',status='old',form='unformatted')
      read(71)numnuc,ilite,iact,ifp
      read(71)(orgid(i),i=1,numnuc),(conc(i,1),i=1,numnuc)
      read(71)
      read(71)(orgid(i),i=1,numnuc),(conc(i,2),i=1,numnuc)
      close(71)
      den(material,:,:) = -1.0
      do i = 1,30
        select case (i)
        case (30) ! light elements (oxygen)
          nstart = 1
          nend = ilite
        case (1:10,26:29) ! actinides
          nstart = ilite+1
          nend = ilite+iact
        case default ! fission products
          nstart = ilite+iact+1
          nend = numnuc
        end select
        do j = nstart,nend
          if(refid(i).eq.orgid(j))then
            den(material,i,:) = conc(j,1:2)
            exit
          endif
        end do
      end do
!
!  concentrations are in gram-atoms (moles).  Need to convert to a number
density.
!  This requires knowing the fuel volume.  The SAS2H model contains fuel pins
with
!  diameter 0.9563cm, length 893.8933cm, and a total of 176 pins.  This
translates
!  to a fuel volume of 1.13e5 cm**2.  Then make sure that all densities have
been
!  updated, and print an error message and stop if not.
!
      do i = 1,30
        do icool = 1,2
          if(den(material,i,icool).lt.1e-20)then
            den(material,i,icool) = 0.0
          else
            den(material,i,icool) = den(material,i,icool)*6.0221367e-1/1.13e5
          endif
          if(den(material,i,icool).lt.0.0)then
            write(6,*)'Error during step ',istep,', material #',material,',
cooling period ',icool
            write(6,*)'Failed to find number density for nuclide id ',id(i)
            stop
          endif
        end do
      end do
    end do ! material
!
!  We now have the 7 different materials necessary to run this operating
history
!  Create a csasn case to make a library that contains all 7 fuel materials
```

```
!  with weighted cross-sections, plus clad and moderator, for cooling times
of
!  5 and 20,000 years.
!
    do icool = 1,2
      write(filename,'("csasn",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1030)enrichment,specific_power,burnup
      do material = 1,19
        if(material.gt.3.and.material.lt.16)cycle
        do nuc = 1,30
          write(10,'(1x,a7,1x,i2,'' 0 '',1pe10.4,'' 293
end'')')nuclide(nuc),material,den(material,nuc,1)
        end do
      end do
      write(10,1040)
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  We now have a working library with cross-sections for 7 fuel materials
plus clad and moderator
!  Create and run keno v.a calculations for each of the 2 cooling times, and
extract k-eff and sigma
!  from each.
!
      last = 0
      write(filename,'("keno_",i1,".in")')icool
      open(10,file=filename,status='unknown')
      write(10,1050)enrichment,specific_power,burnup,specpwr  ! header for
keno case
      do izone = 1,19
        if(izone.gt.3 .and. izone.lt.16) cycle
        write(10,'(''mix='',i2.2)')izone
        do nuc = 1,30

write(10,'(i10,2x,1pe11.5)')nucid(nuc)+izone*1000000,den(izone,nuc,icool)
        end do
      end do !izone
      write(10,1060) ! finish up with mixtures for water and clad
      write(10,1065)1,-162.56
      write(10,1065)2,-142.24
      write(10,1065)3,-121.92
      write(10,1065)19,-101.60
      write(10,1065)16,142.24
      write(10,1065)17,162.56
      write(10,1065)18,182.88
      write(10,1070)
      close (10)
      call system('/scale4.3/cmds/scale43 '//filename//'
'//filename(1:6)//'.out')
!
!  Grep the lines containing the final k-eff results into a file.  Then
!  Edit the file to get k-eff values, uncertainties, and no. of generations
!  skipped.
!
```

```
      call system('grep "generations skipped." '//filename(1:6)//'.out >
keno.results')
      open(10,file='keno.results',status='old')

read(10,'(t34,f7.4,t48,f8.4,t73,i6)')keff(istep,icool),sigma(istep,icool),ski
pped(istep,icool)
      close(10)
    end do ! icool

write(longfname,'("casket",f3.1,"%_",f4.1,"GWd_Option_",i1)')enrichment,burnu
p,option
    open(10,file=longfname,status='unknown')
    do i = 1,istep-1+nskip
      read(10,*)
    end do

write(10,'(5(1x,i4.4),2(1x,1pe12.5,1x,1pe12.5,1x,i4))')istep,iboron,ifuelt,ic
ladt,imodt,(keff(istep,icool), &
         sigma(istep,icool),skipped(istep,icool),icool=1,2)
    close(10)
  end do ! imodt
  end do ! icladt
  end do ! ifuelt
  end do ! iboron
stop
1000 format(  &
"=sas2h       parm='skipshipdata'",/ &
'casket_II, ',f4.2,' wt% enrich., ',f4.1,' MW/MTU, ',f5.2,' GWd/MTU B/U, Mat.
# ',i2.2,/ &
'44group latticecell',/ &
'  uo2 1 den=10.045 1 ',f6.1,1x,/ &
'    92234 ',f6.4,' 92235 ',f6.4,' 92236 ',f6.4,' 92238 ',f7.4,' end',/ &
'  c 1 den=1.8-4 1 ',f6.1,' end',/ &
'  n 1 den=2.3-4 1 ',f6.1,' end',/ &
'  co-59 3 0 1-20 ',f6.1,' end',/ &
'  zr-94 1 0 1-20 ',f6.1,' end')
1010 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 ',/, &
'           50120 0.73 2 1 ',f6.1,' end',/ &
'  h2o 3 den=',f5.3,' 1 ',f6.1,' end',/ &
'  arbm-bormod ',f5.3,' 1 1 0 0 5000 100 3 ',e10.3,1x,f6.1,' end',/, &
'end comp',/ &
'squarepitch 1.4732 0.9563 1 3 1.1176 2 0.9855 0 end',/ &
'npin/assm=176 fuelnght=893.8933 ncycles=6 nlib/cyc=1',/ &
'printlevel=4 lightel=9 inplevel=2 numztotal=5   end',/ &
'3  1.314  2  1.416  3  1.662  500  5.203  3  5.243 ')
1009 format('power=',1pe9.3,' burn=',1pe9.3,' down=',e9.3,' end')
1008 format('  o 119  cr  5.2  mn  0.29',/ &
'  fe 11. co 0.066 ni  8.7',/ &
'  zr 195 nb  0.63 sn  3.2',/ &
'end',0p,/ &
'=origen',/ &
'0$$ e t',/ &
'Library position 1/6',/ &
'3$$ 33 0 1 a16 2 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 0 a13 13 4 2 a17 4 1 e',/ &
```

```
'57** a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,0p,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e',/ &
'73$$ 922340 922350 922360 922380 80000 240000 250000 260000',/ &
'     270000 280000 400000 410000 500000',/ &
'74** ',f5.1,1x,f7.1,1x,f5.1,1x,f8.1,' 119000 5200 290 11000',/ &
'      66 8700 195000 630 3200',/ &
'75$$ 4r2 9r4 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1011 format('Library Position ',i1,'/6', / &
'3$$ 33 0 ',i1,' e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
'57** ',f8.3,' a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 4 a5 3 3 a10 4 a14 4 0 a17 4 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'65$$ a4 0 a25 1 a46 1 e 6t')

1012 format('Library Position 6/6', / &
'3$$ 33 0 6 e 2t',/ &
'4t',/ &
'56$$ 4 4 a5 0 1 a10 4 a14 4 2 a17 4 1 e',/ &
'57** ',f8.3,' a3 1e-2 ',f6.4,' e 5t',/ &
'1 MTU',/ &
'58** 4r',1pe9.4e1,/ &
'60** 2i',e9.4e1,1x,e9.4e1,/ &
'66$$ 0 a5 2 a9 2 e 6t',/ &
'56$$ 0 12 a5 11 1 a10 4 a14 5 3 a17 4 1 e',/ &
'57** 0 a3 1e-2 e 5t',/ &
'20,000 year cooling period',/ &
'1 MTU',/ &
'60** 0.33 1.0 3.3 5.0 10 33 100 333 1000 3333 10000 20000',/ &
'65$$ a4 0 a25 1 a46 1 e 6t',/ &
'56$$ 0 0 a10 4 e t',/ &    ! write to unit 71 for 4th decay period (5 y)
'56$$ 0 0 a10 12 e t',/ &   ! write to unit 71 for 12th decay period (20,000
y)
'56$$ f0 t',/ &
'end',/ &
'=shell',/ &
'cp $TMPDIR/ft71f001 $RTNDIR/ft71f001',/ &
'cp $TMPDIR/ft72f001 $RTNDIR/ft72f001',/ &
'end')
1020 format(4(i8, e12.4))
1030 format(  &
'=csasn          parm=(size=500000)',/ &
```

```
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU B/U
(pin average)',/ &
'44group latticecell')
1040 format( &
'  arbmzirc 6.44 4 0 0 1 40000 97.91 26000 0.5 50116 0.86 ',/, &
'           50120 0.73 28 1 293 end',/ &
'  h2o 29 den=1.0 1 293 end',/ &
'end comp',/ &
'squarepitch 1.4732 0.9563 19 29 1.1176 28 0.9855 0 end',/ &
'more data',/ &
'res=1 cylinder 0.47815  dan(1)=2.25244E-01',/ &
'res=2 cylinder 0.47815  dan(2)=2.25244E-01',/ &
'res=3 cylinder 0.47815  dan(3)=2.25244E-01',/ &
'res=16 cylinder 0.47815  dan(16)=2.25244E-01',/ &
'res=17 cylinder 0.47815  dan(17)=2.25244E-01',/ &
'res=18 cylinder 0.47815  dan(18)=2.25244E-01',/ &
'end more',/ &
'end')
1050 format( &
'=kenova',/ &
'casket_I, ',f4.2,' wt % enrichment, ',f5.2,' MW/MTU, ',f5.2,' GWd/MTU ave
B/U, Axial model #',i2.2,/ &
'read parm npg=1000 gen=1005 nsk=5 nub=yes',/ &
!'read parm npg=100 gen=105 nsk=5 nub=yes',/ &
'   lib=4 fdn=yes tme=300 end parm',/ &
'read boun all=mirror end boun',/ &
'read mixt')
1060 format( &
'mix=28',/ &
'  28040000  4.16270E-02',/ &
'  28026000  3.47236E-04',/ &
'  28050116  2.87770E-04',/ &
'  28050120  2.36120E-04',/ &
'mix=29',/ &
'  29001001  6.67692E-02',/ &
'  29008016  3.33846E-02',/ &
'end mixt',/ &
'read geom',/ &
'unit 1')
1065 format(' cylinder   ',i2,' 1  0.47815 ',f7.2,' -182.88')
1070 format( &
' cylinder   0  1  0.49275  182.88  -182.88',/ &
' cylinder   28 1  0.55880  182.88  -182.88',/ &
' cuboid     29 1  2p0.73660  2p0.73660  192.88  -192.88',/ &
'end geom',/ &
'end data',/ &
'end')
end
```

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