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Benchmark of SCALE (SAS2H) Isotopic Predictions of Depletion Analyses for San Onofre PWR MOX Fuel

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ABSTRACT

The isotopic composition of mixed-oxide (MOX) fuel, fabricated with both uranium and plutonium, after discharge from reactors is of significant interest to the Fissile Materials Disposition Program. The validation of the SCALE (SAS2H) depletion code for use in the prediction of isotopic compositions of MOX fuel, similar to previous validation studies on uranium-only fueled reactors, has corresponding significance. The EEI-Westinghouse Plutonium Recycle Demonstration Program examined the use of MOX fuel in the San Onofre PWR, Unit 1, during cycles 2 and 3. Isotopic analyses of the MOX spent fuel were conducted on 13 actinides and ^{148}Nd by either mass or alpha spectrometry. Six fuel pellet samples were taken from four different fuel pins of an irradiated MOX assembly. The measured actinide inventories from those samples has been used to benchmark SAS2H for MOX fuel applications.

The average percentage differences in the code results compared with the measurement were −0.9% for ^{235}U and 5.2% for ^{239}Pu. The differences for most of the isotopes were significantly larger than in the cases for uranium-only fueled reactors. In general, comparisons of code results with alpha spectrometer data had extreme differences, although the differences in the calculations compared with mass spectrometer analyses were not extremely larger than that of uranium-only fueled reactors. This benchmark study should be useful in estimating uncertainties of inventory, criticality and dose calculations of MOX spent fuel.

1. INTRODUCTION

A major requirement of the Department of Energy's Fissile Materials Disposition Program[1] (FMDP) is the ability to predict the characteristics of mixed-oxide (MOX) spent fuel. Any fuel-depletion code used for this purpose must be evaluated to determine how the accuracies of the spent fuel content computations compare with those of the more common low-enriched-uranium (LEU)-fueled light-water reactors (LWRs). Validation studies have been conducted for the SCALE code system fuel-depletion analyses (applying SAS2H[2]) of spent fuel for both pressurized-water reactors[3] (PWRs) and boiling-water reactors[4] (BWRs). During the operation of these reactors, the plutonium gradually increases in the fuel that initially contained only uranium oxide. Additional validation of predicted inventories of MOX spent fuel is necessary because there is a much more dominant influence on the flux and depletion characteristics from the plutonium in the MOX fuel: the average plutonium concentration is several times that of spent LEU fuel, and its average absorption and fission probabilities are significantly higher than those of depleted LEU fuel.

The EEI-Westinghouse Plutonium Recycle Demonstration Program, sponsored by Edison Electric Institute, Westinghouse Electric Corporation, and the Atomic Energy Commission, was conducted between 1968 and 1974. A significant part of the program involved the measurement of isotopic compositions of uranium, plutonium, and a few other actinides in depleted MOX fuel withdrawn from the San Onofre PWR Unit 1, a reactor having a Westinghouse design and operated by Southern California Edison and San Diego Gas & Electric companies. Four MOX fuel assemblies were loaded at the start of cycle 2 of the San Onofre Nuclear Generation Station Unit 1 and irradiated during both cycles 2 and 3. Isotopic composition analyses were conducted by Westinghouse Electric Corporation on six sample pellets from four fuel rods of the MOX test assembly D51X. The measured actinide inventories have been used to benchmark the use of SCALE/SAS2H depletion calculations for MOX fuel.

The operating and design data required by the SCALE depletion calculation have been taken from a large number of sources[5–12] and compiled for depletion codes into a single report.[13]

2. MOX FUEL ASSEMBLY DESIGN DATA

The basic parameters of the six MOX spent fuel samples are listed in Table 1. Natural uranium was used, and three different weight percent fissile plutonium ($^{239}Pu + ^{241}Pu$) compositions were applied in the initial MOX fuel. Details of the determination of the case burnups listed in Table 1 are given in Appendix A. A basic description of the SCALE/SAS2H depletion computation is given in Appendix B.

The fuel assembly design and fuel compositions for the four San Onofre MOX assemblies are presented in this section. The MOX fuel assembly design data required by SAS2H input are listed in Table 2. Some of the data were calculated, as noted, from other data in the table. The average measured soluble boron during cycle 2 was approximately 500 wt-ppm.[5] The same value was assumed for cycle 3, because the available boron data were incomplete. The guide tube dimensions were taken from data for the uranium-only assemblies. Although the tube sizes and boron content could have been different, the change would probably not have a significant influence on results.

The initial isotopic compositions of the uranium and the plutonium in the MOX fuel of the San Onofre PWR are given in Table 3. Two deficiencies were noted in the initial plutonium data of the table. First, it is known that the plutonium in the initial MOX fuel is recycled plutonium from spent fuel and that $^{238}Pu/^{239}Pu$ ratios are usually from 0.02 to 0.04 in typical PWR spent fuel.[3] However, no ^{238}Pu is listed in the available data, and its absence needs to be considered in evaluating the uncertainty related to predicted ^{238}Pu results. The other deficiency in the initial Pu data is that the decay of the 14.35-year half-life ^{241}Pu is not considered in the specified initial composition. During the MOX fuel assembly fabrication program, 17 analyses were made on ^{239}Pu and ^{241}Pu in revised analyses (as indicated in Table 3) for accountability. The change in ^{241}Pu composition during a 605-d decay time, thus, can be taken into account.

The fractional compositions of UO_2 and PuO_2 for different values of weight percent fissile plutonium are presented in Table 4. The weight fraction of UO_2 and PuO_2 in the MOX fuel is useful in determining fuel atomic densities or, more directly, in the "arbitrary material input data" description of the fuel as applied by SAS2H. These weight fractions were calculated from the fuel stack density of Table 2, the initial isotopic atom compositions of Table 3 and the atomic weights[14] of the U and the Pu isotopes. The initial Pu isotopic data were used because the revised data are incomplete. However, the decay time for the ^{241}Pu to change (5.2 to 4.8 at. %) was calculated to be 1.66 years, or 605 d. The SAS2H input, here, applies a 605-day step of decay (for a low 10^{-8} megawatt power) that precedes the irradiation cycles to account for the ^{241}Pu decay.

The locations of the four fuel pins analyzed from the MOX fuel assembly D51X, listed in Table 1, are shown in Fig. 1. A complete description of the assembly, showing the fissile plutonium enrichment pattern, is presented in Fig. 2. The locations of the four MOX fuel assemblies in the reactor core, during cycles 2 and 3, are shown in Fig. 3.

Table 1. Basic parameters of measured MOX spent fuel samples

Case No.	ID of test assembly	Pin ID	Cycle No.	Initial enrichment		Location ht[b] (in.)	Burnup[c] (MWd/MTHM)[d]
				(at. % ^{235}U)[a]	(wt % fissile Pu)		
1	D51X	067	2	0.72	3.31	53.0	8,167
2	D51X	141	2	0.72	2.84	95.5	6,808
3	D51X	079	2, 3	0.72	3.10	49.0	20,891
4	D51X	167	2, 3	0.72	2.84	16.5	17,447
5	D51X	167	2, 3	0.72	2.84	95.5	18,713
6	D51X	167	2, 3	0.72	2.84	114.0	11,065

[a]Taken from ref. 14.
[b]Height above bottom of active fuel.
[c]Determination from ^{148}Nd measurements described in Appendix A.
[d]Megawatt days per metric ton heavy metal (U + Pu).
Source: ref. 12, unless otherwise specified.

Table 2. San Onofre MOX fuel assembly design data

Parameter	Data
Assembly general data	
Designer	Westinghouse Electric
Rod lattice	14 × 14
Number of assemblies/core[a]	157
MOX assemblies in cycles 2 and 3	4
Total MOX loading, metric ton heavy metal, MTHM[b]	1.335
MOX fuel/assembly, kg U + Pu[c]	333.75
Number of MOX fuel rods	180
Number of instrument tubes[d]	1
Number of guide tubes[d]	15
Equivalent core diameter, cm (in.)[a]	282 (111)
Assembly pitch, cm (in.)[c]	19.941 (7.851)
H_2O moderator pressure, psia[a]	2100
Average moderator temperature, K (°F)[b]	576.5 (578)
Average moderator density, g/cm^3 [c]	0.7179
Average clad temperature, K (°F)[b]	615 (648)
Soluble boron (approximated), ppm (wt)[e]	500
Fuel rod data	
Type of fuel pellet	UO_2 plus PuO_2 (or MOX)
Stack density, g/cm^3 [c]	10.2235
Rod pitch, cm (in.)	1.41224 (0.556)
Clad OD, cm (in.)	1.07188 (0.422)
Diametrical gap, cm (in.)	0.01905 (0.0075)
Clad thickness, cm (in.)	0.06172 (0.0243)
Clad ID, cm (in.)[c]	0.94844 (0.3734)
Pellet OD, cm (in.)	0.92939 (0.3659)
Active fuel length, cm (in.)	303.28 (119.4)
Clad material	Zircaloy-4
Guide tubes	
Material	Stainless steel-304
Tube ID, cm (in.)[f]	1.29794 (0.511)
Tube OD, cm (in.)[f]	1.35890 (0.535)

[a]Taken from ref. 6.
[b]Taken from ref. 5.
[c]Calculated from other data in table.
[d]Taken from ref. 10 or 11.
[e]Assumed cycle 3 average boron concentration equals that of cycle 2.
[f]Assumed similar to that of U assemblies, taken from ref. 7.
Source: ref. 9, unless otherwise specified.

Table 3. Initial compositions of the uranium and plutonium

Isotope	At. % in U or Pu, ppm ^{241}Am		
Uranium[a]			
^{234}U	0.0055		
^{235}U	0.7200		
^{238}U	99.2745		
Plutonium[b]	Initial	Revised	Decay time, d
^{239}Pu	80.6	80.7	–[d]
^{240}Pu	13.4	–[c]	–[d]
^{241}Pu	5.2	4.8	605[e]
^{242}Pu	0.8	–[c]	–[d]
Other			
^{241}Am[f]	5000		

[a]Taken from ref. 14.
[b]Initial from ref. 5; revised from ref. 9.
[c]No revised measurement reported.
[d]Decay time not calculated.
[e]Calculated decay time required to change ^{241}Pu from the initial to the revised composition.
[f]In ppm (wt) of Pu, from ref. 9.

Table 4. Fractional composition[a] of UO_2 and PuO_2 in the MOX fuel

Case	Pin ID	No. of same type pins	Wt % fissile Pu	Weight fraction in MOX (UO_2 + PuO_2)	
				UO_2	PuO_2
1	067	24	3.31	0.961423	0.038577
2	141	64	2.84	0.966901	0.033099
3	079	92	3.10	0.963870	0.036130
4, 5, 6	167	64	2.84	0.966901	0.033099

[a]Computed from data in Tables 2 and 3 and atomic weights of ref. 14.

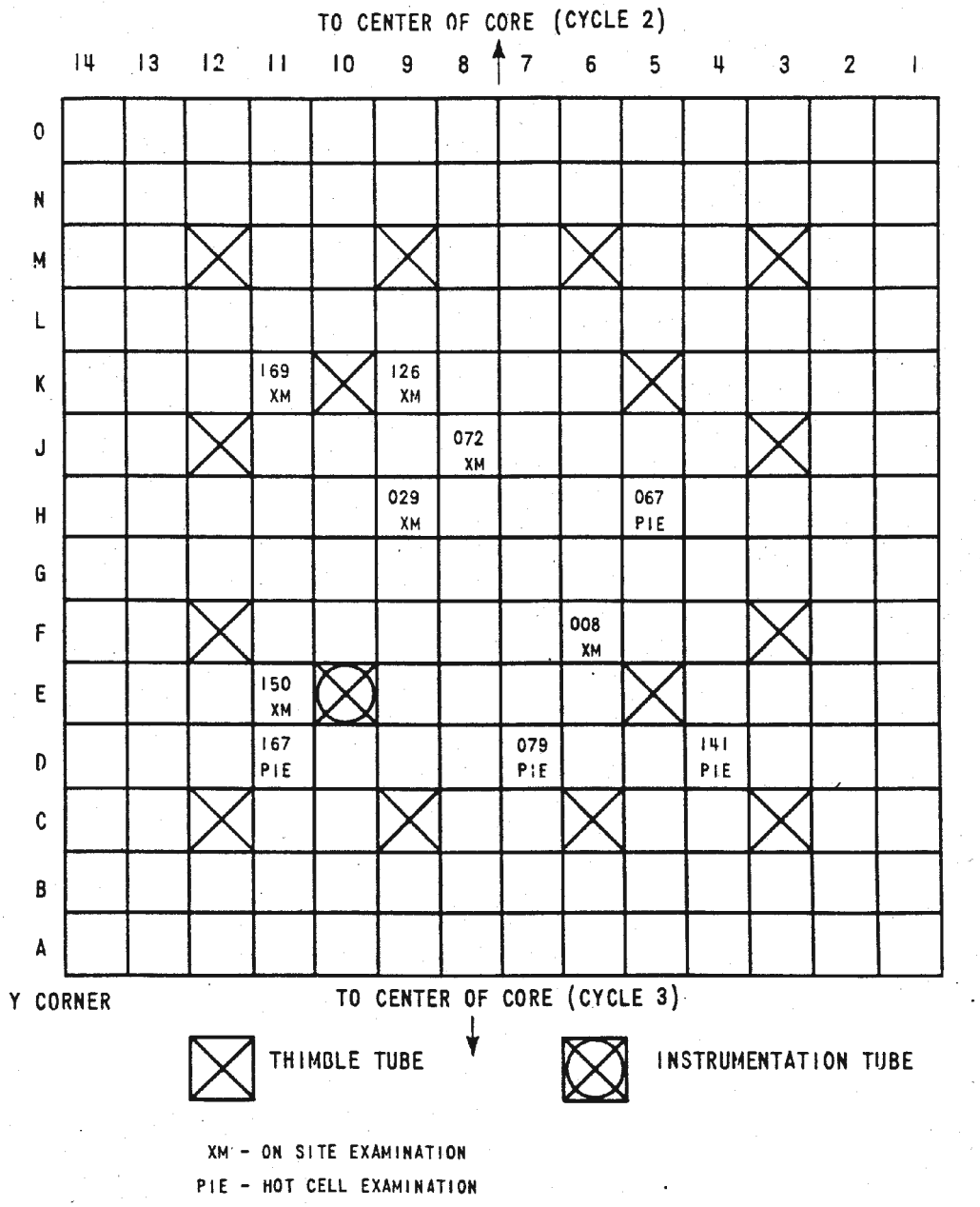

Fig. 1. Location of rods removed from San Onofre Plutonium Demonstration Assembly D51X for post-irradiation examination. *Source:* ref. 11.

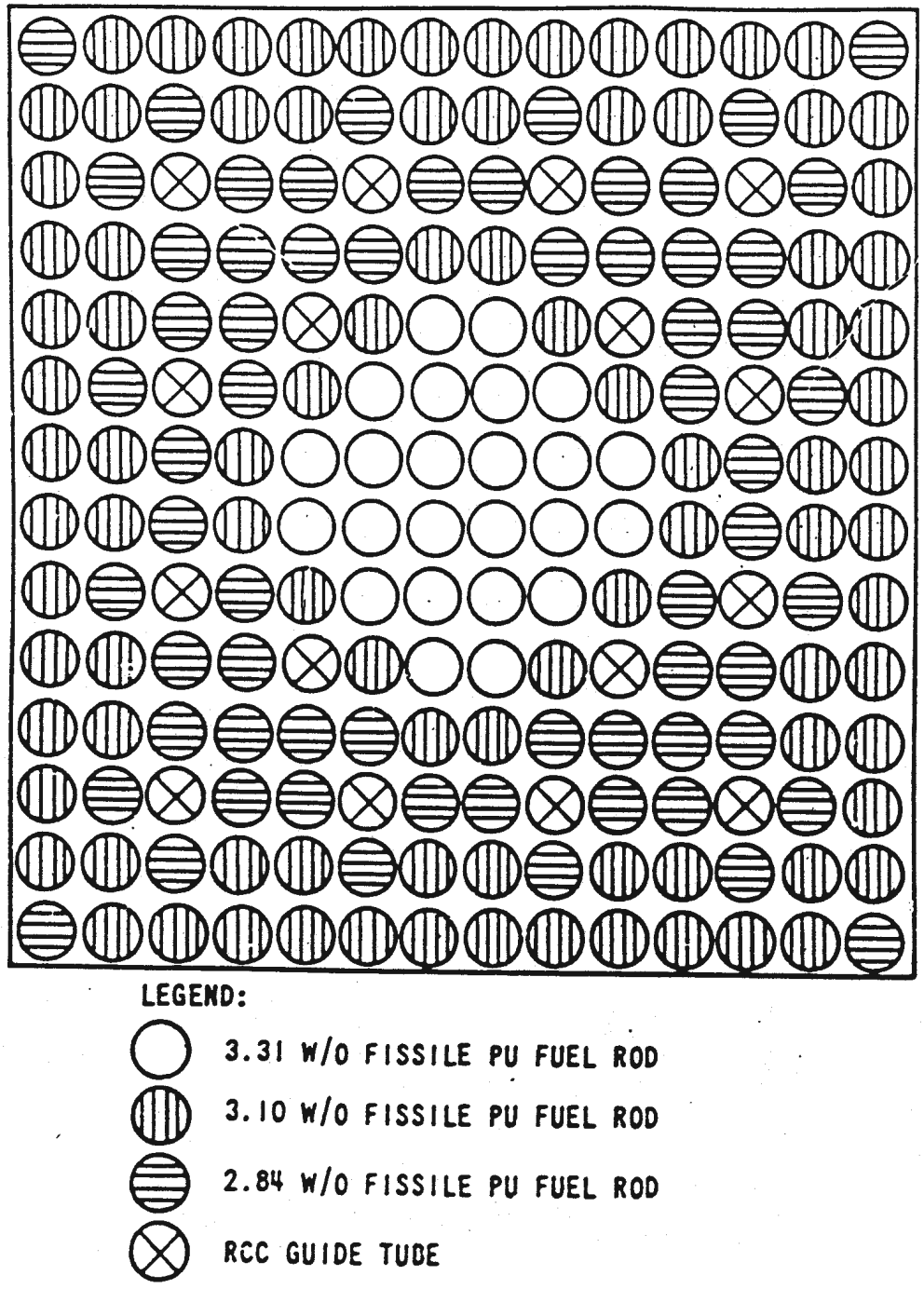

Fig. 2. Enrichment pattern for the four plutonium assemblies.
Source: refs. 6 and 9.

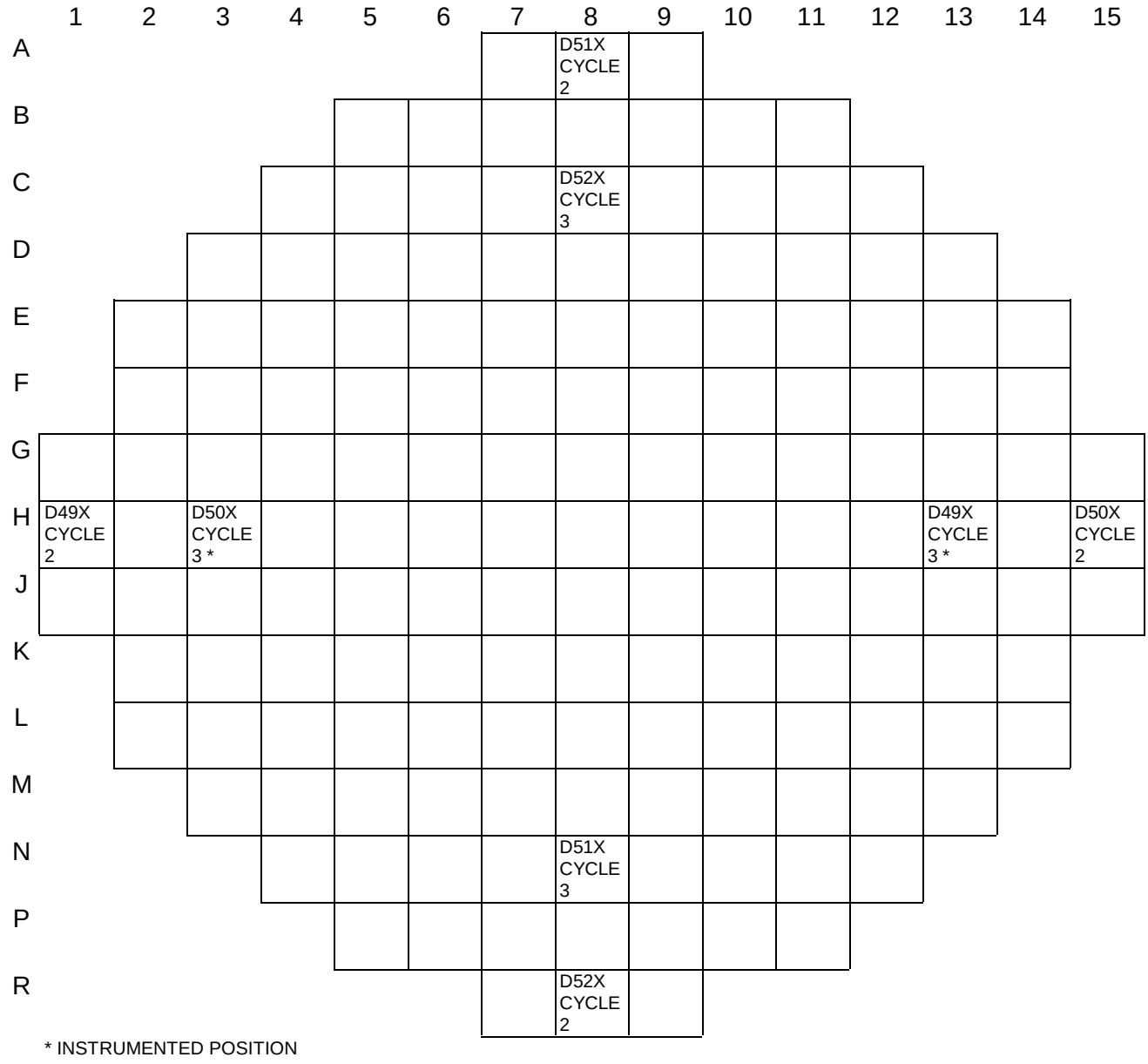

Fig. 3. Location of plutonium demonstration assemblies in San Onofre cycle 2 and cycle 3. *Source:* refs. 10 and 11.

3. THE PWR OPERATIONS DATA AND MODEL OF ASSEMBLIES

The San Onofre PWR Unit 1, operating data, pertaining to the MOX fuel assemblies in cycles 2 and 3, are presented in Table 5. The MOX fuel sample burnups were derived from the ^{148}Nd measurements, as described in the Appendix A. The average cycle power experienced by each of the six pellet samples were calculated from the burnup and cycle time.

Additional operating condition data are listed in Table 2, including the clad and moderator temperatures.[5] The moderator density was obtained by interpolation of data in the temperature-pressure-density table[2] at 578°F and 2100 psia.

The effective fuel temperatures, applied by SCALE in the resonance treatment, were obtained from the fuel-temperature-vs-rod-linear-power curve in Fig. 4, because appropriate data were not available. The curve was developed for the Obrigheim PWR.[15] Similarities are noted in lattice (14 × 14), pellet OD (<1% difference) and moderator temperature (differ by 4.5 K) between the San Onofre and Obrigheim reactors. This method of estimating effective fuel temperature was applied in the validation study of H. B. Robinson PWR analyses.[15] The estimated effective fuel temperatures are given in Table 5.

The unit cell zone geometry data for the assembly model (Path-B, Appendix B) input to SAS2H are listed in Table 6.

A list of the isotopes for which cross sections were updated during each burnup interval of a SAS2H case is shown in Table 7. These include all of the nuclides having the data updated in the latest SAS2H validation study[4] and those isotopes recommended in a burnup-credit sensitivity study[16] as important for depletion calculations. Also, cross sections were updated for ^{236}Pu, ^{237}Pu and ^{238}Pu because they were either a measured isotope or a precursor to a measured isotope.

Applying the data in Tables 2–7, inclusive, the six SAS2H cases were executed using the input listed in Appendix C. The first SAS2H cycle was simulated as an interval at very low power for 605 d to represent the decay of the plutonium fuel from the time of initial inventory analysis to the start of irradiation in the reactor.

Table 5. San Onofre operating data, including sample pellet powers and resonance-type fuel temperatures

Operation data type, Pin ID (height, in.)	Units	Cycle 2	Cycle 3	Total burnup
Cycle times[a]				
Startup date		11/18/70	3/1/72	
Shutdown date		12/26/71	6/2/73	
Uptime	Days	403	459	
Downtime	Days	66	–[b]	
Fuel pellet burnups[c]	MWd/MTHM			
067 (53.0)		8,167	–	8,167
141 (95.5)		6,808	–	6,808
079 (49.0)		7,015	13,877	20,891
167 (16.5)		5,999	11,448	17,447
167 (95.5)		6,434	12,279	18,713
167 (114.0)		3,843	7,222	11,065
Fuel pellet powers[d]	MW/MTHM			
067 (53.0)		20.266	–	
141 (95.5)		16.894	–	
079 (49.0)		17.406	30.232	
167 (16.5)		14.885	24.942	
167 (95.5)		15.965	26.751	
167 (114.0)		9.536	15.735	
Effective fuel temperatures[e]	K			
067 (53.0)		744	–	
141 (95.5)		713	–	
079 (49.0)		718	839	
167 (16.5)		695	787	
167 (95.5)		705	805	
167 (114.0)		650	703	
Shutdown to analysis times[b]	Days			
067 (53.0)		717	–	
141 (95.5)		719	–	
079 (49.0)			194	
167 (16.5)			187	
167 (95.5)			187	
167 (114.0)			192	

[a]Data taken from refs. 10 and 11.
[b]Time from cycle shutdown to sample analysis.
[c]Determined in the appendix from ^{148}Nd measurements.
[d]Calculated directly from the burnup and cycle time.
[e]Effective fuel temperature for resonance treatment.

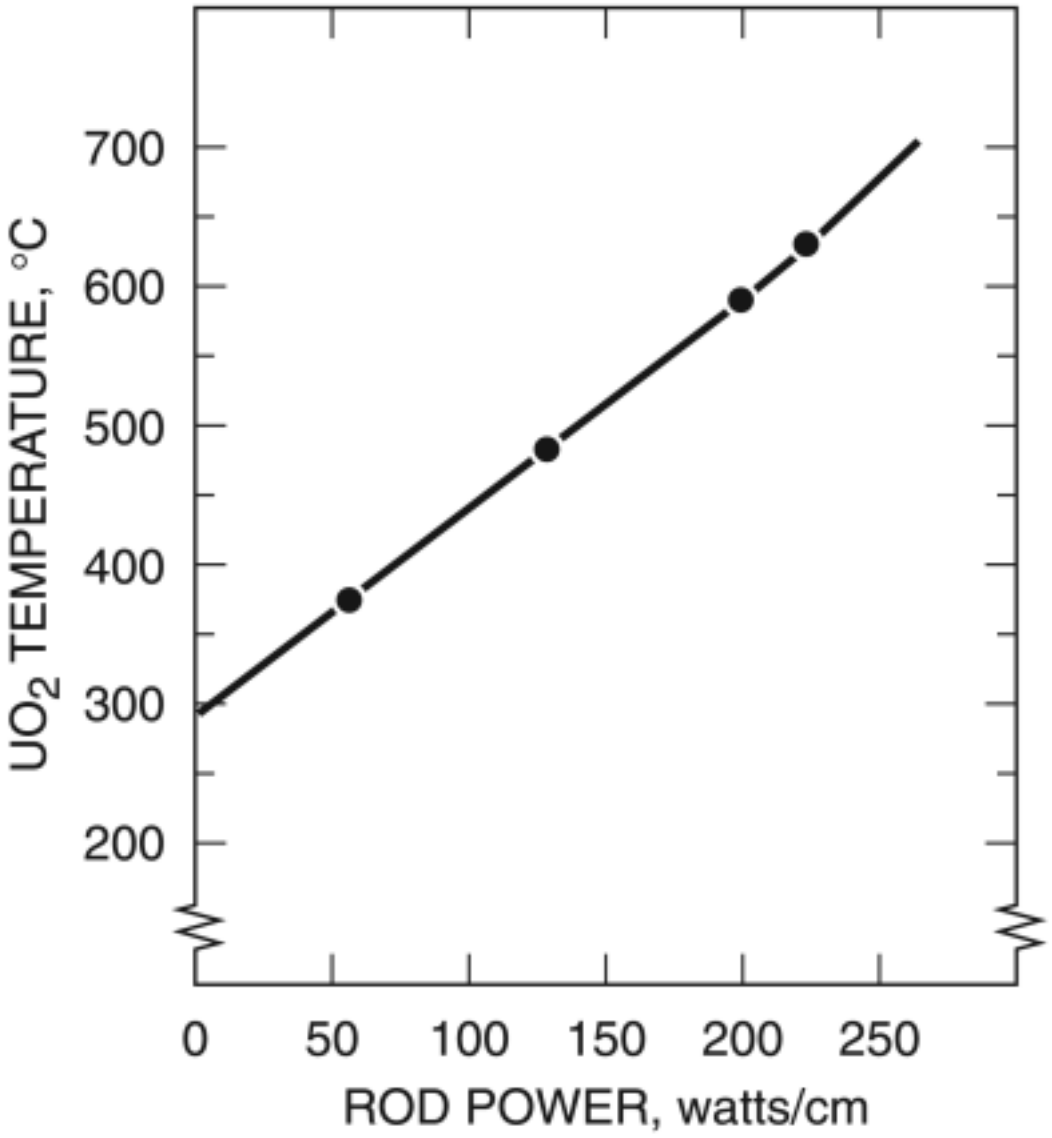

Fig. 4. Fuel-temperature-vs-rod power for Obrigheim PWR. *Source:* ref. 2.

Table 6. Effective SAS2H geometry of the San Onofre MOX assembly model

Cycle	Radial zone	Mixture No.	Composition	Effective radius (cm)
2	1	3	Borated moderator	0.64897
2	2	5	Stainless steel-304	0.67945
2	3	3	Borated moderator[a]	0.79677
2	4	500	Homogenized fuel, clad and borated moderator	2.78870
2	5	3	Borated moderator between assemblies[b]	2.81266
3	1	3	Borated moderator	0.64897
3	2	5	Stainless steel-304	0.67945
3	3	3	Borated moderator[a]	0.84510
3	4	500	Homogenized fuel, clad and borated moderator	2.78870
3	5	3	Borated moderator between assemblies[b]	2.81266

[a]Radius different in cycles 2 and 3 to account for the removal of the two pins indicated in Table 1.
[b]Calculated from assembly pitch and equivalent core diameter in Table 2.

Table 7. Nuclides updated by SAS2H

$^{234}U^{a}$	$^{235}U^{a}$	$^{236}U^{a}$	$^{238}U^{a}$	$^{237}Np^{a}$
^{236}Pu	^{237}Pu	$^{238}Pu^{a}$	$^{239}Pu^{a}$	$^{240}Pu^{a}$
$^{241}Pu^{a}$	$^{242}Pu^{a}$	$^{241}Am^{a}$	$^{242m}Am^{a}$	$^{243}Am^{a}$
$^{242}Cm^{a}$	$^{243}Cm^{a}$	$^{244}Cm^{a}$	^{83}Kr	^{85}Kr
^{90}Sr	^{89}Y	^{93}Zr	^{94}Zr	^{95}Zr
^{94}Nb	^{95}Nb	^{95}Mo	^{99}Tc	^{101}Ru
^{106}Ru	^{103}Rh	^{105}Rh	^{105}Pd	^{108}Pd
^{109}Ag	^{126}Sn	^{124}Sb	^{131}Xe	^{132}Xe
$^{135}Xe^{a}$	^{136}Xe	$^{133}Cs^{a}$	^{134}Cs	^{135}Cs
^{137}Cs	^{136}Ba	^{139}La	^{144}Ce	^{141}Pr
^{143}Pr	^{143}Nd	^{144}Nd	^{145}Nd	^{146}Nd
^{147}Nd	^{148}Nd	^{150}Nd	^{147}Pm	^{148}Pm
^{149}Pm	^{147}Sm	^{148}Sm	^{149}Sm	^{150}Sm
^{151}Sm	^{152}Sm	^{151}Eu	^{153}Eu	^{154}Eu
^{155}Eu	^{155}Gd			

[a] Automatically updated by SAS2H using 44-group library data.

4. PREDICTED AND MEASURED ISOTOPIC COMPOSITIONS

Samples from the San Onofre MOX spent fuel were prepared at the Battelle Memorial Institute hot-cell facility (Columbus, Ohio). The samples were sent to the Westinghouse Waltz Mill Analytical Laboratory for the comprehensive spectrometric analyses of isotopic concentrations. The measured isotopic compositions, usually as atom ratios, of the six MOX sample pellets are given in Table 8. The results pertain to the listed date of analysis. The results for the uranium and plutonium isotopes, except for ^{236}Pu, were adjusted by Westinghouse to the end of irradiation time. The adjusted data are presented in Table 9.

Although no uncertainties of the standard deviations plus systematic biases were reported for the measured data, it was reported[12] that the reanalysis of three samples "showed excellent agreement between initial and repeat results."

The analyses of isotopic ratios of the set of isotopes listed in Table 9 plus the ^{148}Nd/^{238}U atom ratio were determined from mass spectrometer measurements. The ratios involving ^{241}Am, ^{243}Am, ^{236}Pu, ^{238}Pu and ^{237}Np were taken from alpha spectrometer measurements. The averages of results from both analytic methods were applied as the measured values of ^{238}Pu/^{239}Pu.

The reported units of the measured isotopes were atom ratios except for ^{148}Nd, which was given as the mass ratio ^{148}Nd/^{238}U. Several different types of units have been used in the reported measurements applied in previous validation studies.[3,4,15] These units included: weight of the isotope per unit mass of fuel (UO_2 or U), nuclide curies per unit fuel mass, isotopic atom percent of the element, atom ratio between two isotopes, atom ratio of the isotope to the total for the element, and, disintegrations per unit fuel mass. Units were converted to either weight or curies per unit fuel mass, if reported in a different unit. The unit of curies was maintained to avoid causing differences dependent on improvements in half-life data. The application of uniform units for the measurements helped make comparisons between reactors of the nuclide percentage differences both consistent and more meaningful. For example, a comparison of the percentage difference between measured and computed atom percent of the element and the percentage difference in the weight per unit fuel mass for a given isotope may be significantly different if the corresponding values of the element weight per unit fuel mass are considerably different. Thus, in this study, measurements were converted from the reported[12] units specified in Table 8 to milligrams of the isotope per gram of initial heavy metal (uranium plus plutonium). The conversion method applied the nuclide compositions that were computed and written on a concentration file by SAS2H and the atomic mass[14] of required isotopes. The converted data are listed for all six cases in Table 10. The measured and calculated results are also compared in Appendix D.

A summary of the percentage differences between measured and computed isotopic compositions for the six samples of this study are presented in Table 11. Listed in the table are the differences for individual sample results, the averages of all cases and the standard deviations in the individual case differences.

Table 8. Measured atom ratios of San Onofre MOX spent fuel in atom ratios at time of analysis

Pin ID (height, in.)	067 (53.0)	141 (95.5)	079 (49.0)	167 (16.5)	167 (95.5)	167 (114.0)
Date of analysis	12/11/73	12/13/73	12/13/73	12/06/73	12/06/73	12/11/73
Days after shutdown	717	719	194	187	187	192
Burnup, MWd,MTHM	8,167	6,808	20,891	17,447	18,713	11,065
$^{234}U/U \times 10^{-2}$	0.005	0.006	0.005	0.005	0.005	0.005
$^{235}U/U \times 10^{-2}$	0.628	0.641	0.470	0.483	0.479	0.569
$^{236}U/U \times 10^{-2}$	0.023	0.018	0.052	0.050	0.051	0.032
$^{238}U/U \times 10^{-2}$	99.344	99.335	99.473	99.462	99.465	99.394
$^{238}Pu/Pu \times 10^{-2}$	0.557	0.462	0.989	0.860	0.884	0.642
$^{239}Pu/Pu \times 10^{-2}$	71.886	73.218	56.998	57.626	57.130	66.193
$^{240}Pu/Pu \times 10^{-2}$	19.050	18.812	26.422	26.613	26.593	22.401
$^{241}Pu/Pu \times 10^{-2}$	7.210	6.384	12.530	12.047	12.444	9.088
$^{242}Pu/Pu \times 10^{-2}$	1.295	1.124	3.061	2.854	2.949	1.678
$^{239}Pu/^{238}U \times 10^{-2}$	2.619	2.293	1.741	1.594	1.601	1.965
$^{148}Nd/^{238}U \times 10^{-4}$	1.508	1.250	3.875	3.226	3.460	2.046
$^{241}Am/^{239}Pu \times 10^{-2}$	–[a]	–[a]	–[a]	6.51	6.83	1.59
$^{243}Am/^{239}Pu \times 10^{-2}$	–[a]	–[a]	–[a]	1.41	1.55	0.27
$^{236}Pu/^{239}Pu \times 10^{-9}$	4.04	4.60	17.7	12.4	13.4	6.50
$^{238}Pu/^{239}Pu \times 10^{-3}$	7.65	6.16	17.0	14.7	15.2	9.43
$^{237}Np/U \times 10^{-5}$ [b]	–[a]	–[a]	–[a]	9.7	11.1	5.7

[a]No measurement.
[b]In place of atom ratio, units are grams $^{237}Np/g$ U.
Source: ref. 12.

Table 9. Measured atom ratios of San Onofre MOX spent fuel in atom ratios adjusted to shutdown time

Pin ID (height, in.)	067 (53.0)	141 (95.5)	079 (49.0)	167 (16.5)	167 (95.5)	167 (114.0)
Burnup, MWd/MTHM	8,167	6,808	20,891	17,447	18,713	11,065
$^{234}U/U \times 10^{-2}$	0.005	0.006	0.005	0.005	0.005	0.005
$^{235}U/U \times 10^{-2}$	0.628	0.641	0.470	0.483	0.479	0.569
$^{236}U/U \times 10^{-2}$	0.023	0.018	0.052	0.050	0.051	0.032
$^{238}U/U \times 10^{-2}$	99.344	99.335	99.473	99.462	99.465	99.394
$^{238}Pu/Pu \times 10^{-2}$	0.560	0.465	0.986	0.857	0.880	0.639
$^{239}Pu/Pu \times 10^{-2}$	71.345	72.729	56.744	57.379	56.877	65.979
$^{240}Pu/Pu \times 10^{-2}$	18.907	18.686	26.304	26.499	26.495	22.328
$^{241}Pu/Pu \times 10^{-2}$	7.903	7.003	12.919	12.423	12.831	9.382
$^{242}Pu/Pu \times 10^{-2}$	1.285	1.116	3.047	2.842	2.936	1.673
$^{239}Pu/^{238}U \times 10^{-2}$	2.619	2.293	1.741	1.594	1.601	1.965

Source: ref. 12.

Table 10. Measured atom ratios of San Onofre MOX spent fuel converted to milligrams per gram of initial heavy metal

Pin ID (height, in.)	067 (53.0)	141 (95.5)	079 (49.0)	167 (16.5)	167 (95.5)	167 (114.0)
Date of analysis	12/11/73	12/13/73	12/13/73	12/6/73	12/6/73	12/11/73
Days after shutdown	717	719	194	187	187	192
MWd/MTHM	8,167	6,808	20,891	17,447	18,713	11,065
^{234}U	4.698×10^{-2}	5.675×10^{-2}	4.661×10^{-2}	4.688×10^{-2}	4.683×10^{-2}	4.713×10^{-2}
^{235}U	5.926	6.088	4.400	4.548	4.505	5.386
^{236}U	2.180×10^{-1}	1.717×10^{-1}	4.889×10^{-1}	4.728×10^{-1}	4.817×10^{-1}	3.042×10^{-1}
^{238}U	9.495×10^{2}	9.556×10^{2}	9.432×10^{2}	9.485×10^{2}	9.475×10^{2}	9.529×10^{2}
^{236}Pu	9.962×10^{-8}	9.996×10^{-8}	2.882×10^{-7}	1.859×10^{-7}	2.016×10^{-7}	1.207×10^{-7}
^{238}Pu	1.915×10^{-1}	1.366×10^{-1}	2.821×10^{-1}	2.239×10^{-1}	2.327×10^{-1}	1.791×10^{-1}
^{239}Pu	2.497×10^{1}	2.201×10^{1}	1.649×10^{1}	1.518×10^{1}	1.523×10^{1}	1.880×10^{1}
^{240}Pu	6.645	5.678	7.677	7.041	7.121	6.390
^{241}Pu	2.526	1.935	3.656	3.201	3.346	2.603
^{242}Pu	4.555×10^{-1}	3.421×10^{-1}	8.968×10^{-1}	7.614×10^{-1}	7.963×10^{-1}	4.827×10^{-1}
^{237}Np	— [a]	— [a]	— [a]	9.250×10^{-2}	1.057×10^{-1}	5.464×10^{-2}
^{241}Am	— [a]	— [a]	— [a]	9.967×10^{-1}	1.049	3.015×10^{-1}
^{243}Am	— [a]	— [a]	— [a]	2.177×10^{-1}	2.401×10^{-1}	5.162×10^{-2}
^{148}Nd	8.897×10^{-2}	7.423×10^{-2}	2.271×10^{-1}	1.901×10^{-1}	2.037×10^{-1}	1.212×10^{-1}

[a]No measurement.

Table 11. Percentage difference[a] between measured and computed[b] nuclide compositions for the San Onofre PWR MOX fuel samples and averages from Assembly D51X

Fuel Pin ID	067	141	079	167	167	167		
Axial height, in.	53.0	95.5	49.0	16.5	95.5	114.0		
Burnup, MWd/MTHM	8,167	6,808	20,891	17,447	18,713	11,065		
Nuclide							Average	Standard Deviation[c]
^{234}U[d]	1.8	-14.5	-13.1	-10.3	-11.6	-3.1	-8.5	6.4
^{235}U[d]	-0.7	-1.7	-2.0	0.7	-1.6	-0.2	-0.9	1.1
^{236}U[d]	-1.1	14.4	6.6	-0.8	3.2	3.6	4.3	5.7
^{238}U[d]	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{236}Pu[e]	-87.9	-91.6	-59.2	-55.9	-53.0	-73.5	-70.2	16.7
^{238}Pu[d,e]	-61.1	-56.8	-36.3	-34.2	-32.7	-45.3	-44.4	12.2
^{239}Pu[d]	1.6	0.4	5.2	11.1	7.4	5.4	5.2	3.9
^{240}Pu[d]	1.3	1.7	-3.3	-3.8	-4.0	-2.2	-1.7	2.6
^{241}Pu[d]	1.9	11.4	1.5	1.4	0.0	1.9	3.0	4.2
^{242}Pu[d]	7.9	21.4	5.9	3.7	6.1	12.5	9.6	6.5
^{237}Np[e]	—[f]	—[f]	—[f]	-6.3	-11.3	-4.5	-7.4	3.5
^{241}Am[e]	—[f]	—[f]	—[f]	-58.8	-61.5	48.7	-23.9	62.9
^{243}Am[e]	—[f]	—[f]	—[f]	-25.4	-25.2	70.0	6.4	55.0
^{148}Nd[d]	-0.4	-0.5	0.1	-0.2	-0.1	-0.9	-0.3	0.4

[a](Calculated/measured -1) × 100%.
[b]Using SAS2H/ORIGEN-S analysis sequence and the 44-group cross-section library of SCALE-4.4.
[c]One standard deviation in individual data points.
[d]Measurement performed using a mass spectrometer.
[e]Measurement performed using an alpha spectrometer.
[f]No measurement.

The average percentage differences in Table 11 indicate a wide variation in the agreement between calculations and measurements. The largest differences are discussed below, followed by comments concerning the differences for the most significant isotopes.

The average percentage differences in ^{236}Pu, ^{238}Pu and ^{241}Am were excessive, ranging from −23.9 to −70.2%. Another isotope, ^{243}Am, had a very large standard deviation. The isotopes ^{236}Pu, ^{241}Am and ^{243}Am were analyzed by an alpha spectrometer. Information in previous validation studies[3,4,15] and one of their references[17] indicated that uncertainties in alpha-spectrometer measurements may be unusually large. A study[17] on the Obrigheim PWR analyses stated "recent measurements of single KWO pellets — the much more precise method of isotope dilution analysis was used for ^{244}Cm for the first time — show differences from the older alpha-spectrometer measurements which are as much as ±40%," and "with a measurement error of ±25% in ^{241}Am." This may account for the ^{236}Pu, ^{241}Am and ^{243}Am differences, although there may be differences in uncertainties between laboratories and, also, for various isotopes. There is another likely reason the computed values of ^{238}Pu are low (−44.4%). The plutonium composition analysis of the initial MOX fuel did not include a measurement of ^{238}Pu, as shown in Table 3. Thus, none was input to the cases. Estimated ^{238}Pu contents from PWR spent fuel analysis and calculations show that it would be possible for the content to be in the vicinity of twice the computed values, correcting the discrepancy. Note from Table 11 that the average differences of the most significant fissile nuclides, ^{235}U, ^{239}Pu and ^{241}Pu, were −0.9, 5.2 and 3.0%, respectively. Data for the three fissile isotopes, plus ^{238}U, are very significant for criticality k_{eff} calculations. Comparisons for certain fission products not included in this study would be needed to validate better the quality of radioactive dose calculations.

5. SUMMARY

The isotopic composition of spent MOX fuel is important in both criticality and dose determinations of transportation casks and storage of the fuel. Thus, it is necessary to apply computational techniques to estimate the MOX spent fuel compositions, and to apply estimates of the uncertainties of the predictions. Validation studies of the accuracy of the computational methods compared with radiochemical analysis are significant to the Fissile Materials Disposition Program.[1] Previous SCALE/SAS2H validation projects[3,4,15] have pertained to LEU only as the initial reactor fuel.

A plutonium recycle demonstration program was conducted by Edison Electric Institute and Westinghouse Electric Corporation during 1968 to 1974. Radiochemical analyses were made on six pellet samples from four MOX fuel pins irradiated for either one or two cycles in the San Onofre PWR Unit 1. Basic parameters of the MOX fuel samples, including the initial fissile contents and the burnups, are shown in Table 1. The MOX fuel assembly design data and initial fuel isotopic compositions are given in Tables 2 and 3. The reactor operating conditions pertaining to the samples are tabulated in Table 5.

The measured isotopic analyses of the MOX spent fuel are listed in Tables 8 and 10. The percentage differences of the SCALE/SAS2H computed results from the measured isotopic compositions, their averages and standard deviations are shown in Table 11. Note that the reason the computed ^{238}Pu is significantly low can likely be attributed to no ^{238}Pu in the initial plutonium isotopic analysis (i.e., none was reported, as shown in Table 3). In general, the differences in the code results and those analyses performed using an alpha spectrometer were large (usually, >25%). Although part of the difference should be from computational error, it has been demonstrated[17] that there were large differences between alpha-spectrometer measurements and those of the more precise method using isotopic dilution analyses, which are comparable to the observed discrepancies. The more important average differences for the fissile isotopes ^{235}U, ^{239}Pu and ^{241}Pu are −0.9, 5.2 and 3.0%, respectively. These values may be compared with the similar differences of ^{235}U, ^{239}Pu and ^{241}Pu from validation studies[3,4] for LEU-only fueled PWRs using 38 samples, which were −0.9, −1.3 and −1.1%, respectively.

It is reasonable to infer that the SCALE-computed compositions of MOX spent fuel for the major actinides, for the limited amount of data observed in this study, are not excessively greater than that obtained for LEU-only fuel. Also, one may note that, due to the small number of samples, the standard deviations of the MOX error estimates could be expected to be larger than that derived from LEU-only initial fuel data. Another limitation to this study is that no fission product results, other than ^{148}Nd, were compared. Validation of several of the dominant-activity fission product gamma-ray emitters would be advisable for validation of transportation and storage radiation source terms.

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APPENDIX A

SAMPLE BURNUP DETERMINATIONS

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This appendix provides an expanded explanation regarding the sample burnup data listed in Table 5. First, the reasons are given why the available burnup data[A.1] are considered inadequate, probably due to the use of methods that have become obsolete. Then, the method applied for converting the ^{148}Nd measurement to burnup is referenced and discussed. Finally, the total burnup results and the separate cycle data are shown.

There is a high degree of confidence in the ANSI/ASTM standards for converting ^{148}Nd measurements to burnup in nuclear research concerning uranium-only fueled LWRs. A total of 68 spent fuel samples from eight different reactors have been used in comparisons of measured and calculated isotopic results in previous validation studies.[A.2–A.4] The referenced burnups were derived from the ^{148}Nd analysis, except for one reactor. In 40 of the sample cases, from five reactors, the ^{148}Nd measured result was given and compared with the SAS2H calculation that applied the ^{148}Nd-derived burnup. The computed/measured ^{148}Nd differences in the 40 cases ranged form −2.4 to 1.7%, with an average of −0.32%. The averages for the five reactors were −1.4, 1.7, 0.4, −2.0 and 0.3%, with an average of 0.20%, or the average of the absolute values of the reactor averages was 1.16%.

The preceding comparisons of analyses and SAS2H results validate that the methods of converting ^{148}Nd measurements to burnups are adequate. However, preliminary computations, using SAS2H, for the MOX fuel cases gave ^{148}Nd differences as large as 4% for 1-cycle cases and 12% for 2-cycle cases. Although the reports giving data that were used in the validation study did not usually give the conversion factors used in determining burnup, the data[A.5] for the Turkey Point PWR did contain the required conversion factors. Thus, the decision was made to apply the conversion factors used with the Turkey Point data in deriving burnups for the MOX fuel for the following reasons. First, applying these factors showed that the referenced burnups[A.1] were too high by approximately the same differences indicated by the ^{148}Nd code-to-measured-results comparisons. Using the same factors from the Turkey Point PWR on data for the Calvert Cliffs PWR, the Cooper BWR and the JPDR BWR gave values for 18 cases within about 1% of the reported burnups. The discussion on the Turkey Point PWR referred to the ANSI/ASTM Standards E321-75 and E267, and that on the Calvert Cliffs PWR and Cooper BWR referred to the ANSI/ASTM Standard E321-79 and E219.

One more question should be considered before using the above ^{148}Nd-burnup conversion method (i.e., factors applied in Turkey Point PWR cases) for MOX spent fuel. Higher concentrations of Pu isotopes and lower concentrations of U isotopes are noted in the average MOX fuel than in the average uranium-only fuel during irradiation. There are two factors that this can change: the average fission yield of ^{148}Nd, and the average recoverable energy per fission. The percent fission yields (based on thermal reactors) for ^{148}Nd (or mass 148) listed in ENDF/B-V[A.6] are 1.670 for ^{235}U, 2.081 for ^{238}U (fast), 1.635 for ^{239}Pu, and 1.990 for ^{241}Pu. An approximate average fission yield for a given case may be calculated by weighting these four fission yields by the average isotopic density times the average microscopic fission cross section of the corresponding isotope (or, rather, the isotopic average macroscopic fission cross section). In two SAS2H trial cases, average macroscopic fission cross sections of the isotopes were estimated from atomic densities and cross sections listed in the case outputs. An estimate of the sum of the weighted fission yields indicated a 1 to 2.5% increase in the average fission yield from MOX fuel compared with that from typical uranium-only fuel. The ORIGEN-S code computes and writes the total recoverable energy per fission for each time step.

The values of the average energy per fission of MOX fueled reactors compared with uranium-only reactors indicate an increase of approximately 1 to 1.5%. The fission yield is in the denominator, and the energy per fission is in the numerator in converting the ^{148}Nd/U atom ratio to burnup. Thus, it is estimated that the burnup could be no greater than 1.5% less for MOX fuel than that produced by the conversion method used for uranium-only fuel cases.

The detailed procedure for converting the measured atom ratio of ^{148}Nd/^{238}U to burnup by using the same conversion factors, C and F_{148}, applied in deriving the Turkey Point data,[A.5] is the following:

$$B = RCAF_u(1 - D_{238}) / F_{148} \ , \tag{A.1}$$

where

B = calculated burnup, MWd/MTHM,

R = atom ratio of (final ^{148}Nd atoms)/(final ^{238}U atoms),

F_{148} = fission fraction for mass 148 = 0.0168,[A.5]

C = 9600 (MWd/MTHM)/at. % of fuel which fissions,[A.5]

A = ^{238}U at. % in natural U, or 99.2745,

F_u = weight fraction of UO_2 in the MOX from Table 4,

D_{238} = ^{238}U fractional depletion, 0.007 per cycle estimated.

F_u should be the atom fraction of U in the U + Pu of the MOX, because each term of the equation is always the ratio of atoms. For the sample compositions, the atom ratio of U to U + Pu is not significantly different than the weight ratio of UO_2 to UO_2 + PuO_2. The estimate of D_{238} is 0.007 ± 0.002, which should cause an error in B no greater than 0.2%. The method in ref. A.5 applied the same factors C and F_{148} in converting R to B, but equivalent measurements were used instead of AF_u (1 – D_{238}).

As an example of using Eq. (A.1), consider the 2-cycle case for pin ID 079, where the value of F_u from Table 4 is 0.963870 and R = 3.875×10^{-4}:

$$\begin{aligned} B &= 3.875 \times 10^{-4} \times 9600 \times 99.2745 \times 0.96387 \times 0.986 / 0.0168 \\ &= 20{,}891.4 \text{ MWd / MTHM.} \end{aligned} \tag{A.2}$$

The reported burnup of 23,500 MWd/MTHM is 12.5% greater than that determined in Eq. (A.2).

Burnups of the six cases computed by Eq. (A.1) are listed in Table A.1. The revised values are given in Table 5. It is seen that the old, or reported, burnups[A.1] are significantly greater than the revised burnups.

The calculation of the burnup for each cycle of the samples irradiated in both cycles 2 and 3 are given in Table A.2. The use of the reported[A.1] linear power for both cycles of the samples permitted the calculation of linear burnups, the fraction of total burnup per cycle, and the final burnup by cycle. These resulting burnups are listed in Table 5, in addition to the computed cycle powers required in depletion code input.

Table A.1 Data applied in determining recommended burnup[a]

Case	R	No. of cycles	$1-D_{238}$	% fissile Pu	F_u	B, MWd/MTHM Revised	B, MWd/MTHM Old	% diff.[b]
1	1.508×10^{-4}	1	0.993	3.31	0.961423	8,167	8,700	6.5
2	1.250×10^{-4}	1	0.993	2.84	0.966901	6,808	7,200	5.8
3	3.875×10^{-4}	2	0.986	3.10	0.963870	20,891	23,500	12.5
4	3.226×10^{-4}	2	0.986	2.84	0.966901	17,447	19,800	13.5
5	3.460×10^{-4}	2	0.986	2.84	0.966901	18,713	21,200	13.3
6	2.046×10^{-4}	2	0.986	2.84	0.966901	11,065	12,500	13.0

[a]Derived B by applying Eq. (A.1), the constants F_{148}, C and A, in addition to data in this table.
[b]$(B_{old}/B_{revised} - 1)$ 100%.

Table A.2 Calculation of burnup for each cycle for 2-cycle cases

	P_{linear}[a] kw/ft		Uptime, d		B_{linear}, kwd/ft		Fraction B_{total}		B_{cycle}, MWd/MTHM	
	Cycle		Cycle		Cycle		Cycle		Cycle	
Case	2	3	2	3	2	3	2	3	2	3
3	3.8	6.6	403	459	1,531.4	3,029.4	0.335774	0.664226	7,015	13,877
4	3.7	6.2	403	459	1,491.1	2,845.8	0.343817	0.656183	5,999	11,448
5	3.7	6.2	403	459	1,491.1	2,845.8	0.343817	0.656183	6,434	12,279
6	2.0	3.3	403	459	806.0	1,514.7	0.347309	0.652691	3,843	7,222

[a]P_{linear} is linear power at the sample height in ref. A.1.

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APPENDIX B

DESCRIPTION OF THE SCALE SAS2H DEPLETION APPROACH

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DESCRIPTION OF THE SCALE SAS2H DEPLETION APPROACH

SCALE is a well-established code system that has been widely used in away-from-reactor (AFR) applications for spent fuel characterization via the SAS2H analysis sequence.[B.1] SAS2H is a multicode sequence that determines the isotopic composition of spent fuel using the ORIGEN-S code[B.2] for depletion and decay calculations and a 1-D neutronics model of an LWR fuel assembly to prepare burnup-dependent cross sections for ORIGEN-S. Isotopic concentrations used in the subsequent spent fuel criticality calculations are based on the results of SAS2H calculations.

The SAS2H control module was originally developed for the SCALE code system to provide a sequence that generated radiation source terms for spent fuel and subsequently utilized these sources with a 1-D shielding analysis of a shipping cask. However, in addition to the calculation of source terms, SAS2H is now often used to obtain decay heat and spent fuel isotopics. Within the scope of validation activities described in this report, SAS2H is used solely for the prediction of spent fuel isotopics.

Six different modules are invoked by the SAS2H sequence for performing a complete fuel depletion analysis. The SCALE-4 system driver provides automated data handling and code execution for each step of the process. This procedure begins with the SCALE Material Information Processor[B.3] which generates number densities and related information, prepares geometry data for resonance self-shielding and flux-weighting cell calculations, and creates data input files for the cross-section processing codes. BONAMI[B.4] applies the Bondarenko method of resonance self-shielding for nuclides which have Bondarenko data included in the cross-section library. NITAWL-II[B.5] performs Nordheim resonance self-shielding corrections for nuclides that have resonance parameters included with their cross-section data. XSDRNPM[B.6] is a 1-D discrete-ordinates code that performs radiation transport calculations based on geometric data passed to it by SAS2H and produces cell-weighted cross sections for fuel depletion calculations. The COUPLE code[B.7] updates cross-section constants included on the ORIGEN-S nuclear data library with data from the cell-weighted cross-section library produced by XSDRNPM. COUPLE also uses the XSDRNPM-computed weighting spectrum to update nuclide cross sections for remaining nuclides. Finally, the ORIGEN-S code is used to perform nuclide generation and depletion calculations for a specified reactor fuel history. The analysis described in this report applied the SCALE 44-group cross-section library.

The process used by SAS2H in calculation of spent fuel isotopics is illustrated schematically in Fig. B.1. The calculation starts with input-specified data describing a fuel assembly as it is initially loaded into a reactor. The initial composition, average temperatures, geometry, and time-dependent specific power of the fuel assembly are required. The SAS2H sequence performs 1-D neutron transport analysis of the reactor fuel assembly using XSDRNPM and a two-part procedure with two separate unit-cell-lattice models. The first model (Path A of Fig. B.1) is a unit fuel-pin cell from which cell-weighted cross sections are obtained. The second model (Path B of Fig. B.1) represents a larger unit cell (e.g., an assembly) within an infinite lattice. The larger unit cell zones can be structured for different assembly designs to account for assembly-specific attributes (i.e., water holes, burnable poison rods, etc.). Problem-dependent resonance self-shielding of cross sections is performed prior to each XSDRNPM calculation using the BONAMI and NITAWL-II codes. The

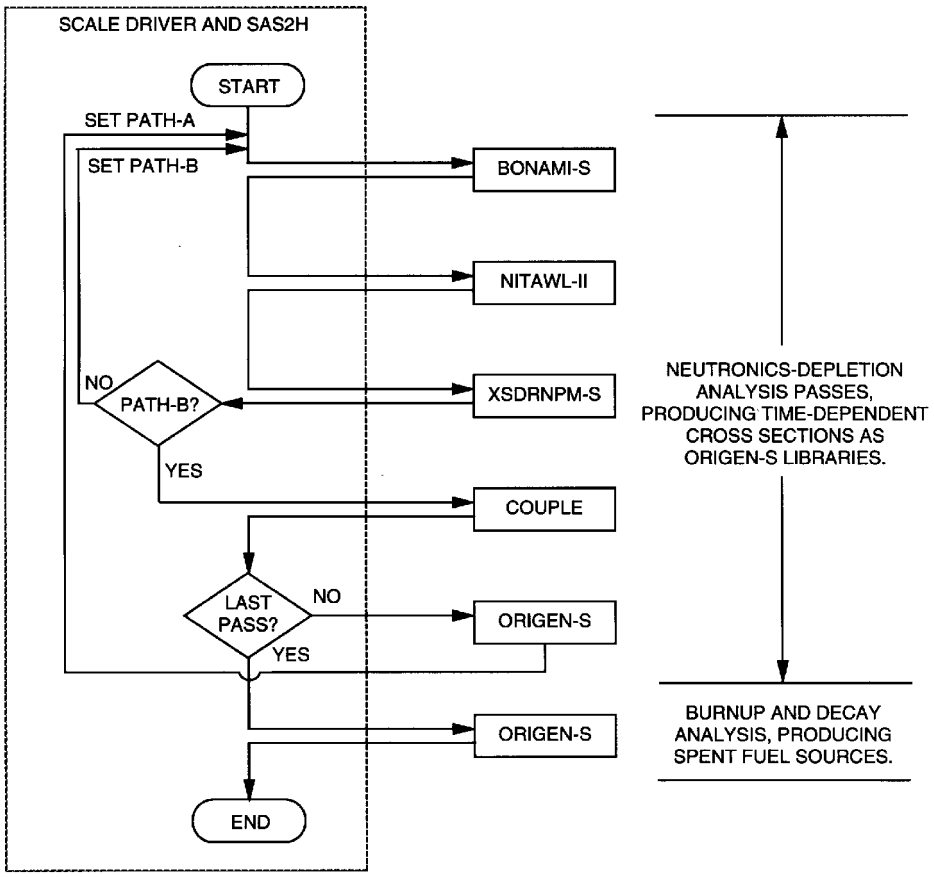

Fig. B.1. Flow path invoked in SAS2H depletion and decay sequences.

neutron flux spectrum obtained from the second (assembly) unit-cell model is used to determine the appropriate nuclide cross sections for the burnup-dependent fuel composition. The cross sections derived from XSDRNPM calculations at each time step are used in an ORIGEN-S point-depletion computation that produces the burnup-dependent fuel compositions to be used in the next spectrum calculation. This sequence is repeated in user-specified burnup steps for a complete assembly operating history. The buildup and decay of nuclides in the fuel assembly is then computed by ORIGEN-S in a final pass based on the assembly's cooling time (i.e., the period of time after final exposure time). Note that ORIGEN-S calculations have no spatial dependence. The neutron flux used to produce the ORIGEN-S cross sections is based on a radial average of an infinitely long uniform assembly with characteristics per input specifications. These specifications (e.g., burnup, specific power, moderator temperature, etc.) can be representative of any axial location along the fuel assembly or an axial average of the fuel assembly.

More than 1000 nuclides are tracked by ORIGEN-S during depletion and decay calculations. (Note that ORIGEN-S tracks all decay chains, but does not account for the loss of volatile isotopes; however, any released nuclides represent an insignificant fraction of the total fission-product inventory, and their inclusion should have an insignificant effect on the isotopic calculations.) Burnup-dependent cross sections are processed by SAS2H only for a select set of user-specified nuclides. These nuclides are those found to be most important for depletion calculations in LWR fuels and are listed in Table B.1. Cross sections for remaining isotopes are obtained from the ORIGEN-S one-group LWR library and are adjusted with burnup using ORIGEN-S spectral parameters (THERM, RES, and FAST)[B.2] calculated using fluxes determined by XSDRNPM. The ORIGEN-S one-group LWR library available in SCALE-4 has been updated to use cross sections from the SCALE-4 44-group burnup library, applied in this study, for approximately 208 nuclides in that library. The update was performed by extracting one-group cross sections from the output of a low-burnup LWR-type fuel.

Table B.1. List of fuel nuclides automatically included by SAS2 for neutronics processing[a]

^{135}Xe	^{238}Pu	^{242m}Am
^{133}Cs	^{239}Pu	^{243}Am
^{234}U	^{240}Pu	^{242}Cm
^{235}U	^{241}Pu	^{243}Cm
^{236}U	^{242}Pu	^{244}Cm
^{238}U	^{241}Am	1/v-absorber[b]
^{237}Np		

[a]Unless overridden by user input, these nuclides are added to the initial fuel mixture with a number density of 10^{-20} atoms/b-cm.

[b]Used to calculate the THERM parameters applied in ORIGEN-S (see Sect. F7 of ref. B.1).

References

B.1 O. W. Hermann and C. V. Parks, "SAS2H: A Coupled One-Dimensional Depletion and Shielding Analysis Code," Sect. S2 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.2 O. W. Hermann and R. M. Westfall, "ORIGEN-S: A SCALE System Module to Calculate Fuel-Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms," Sect. F7 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.3 N. F. Landers et al., "The Material Information Processor for SCALE," Sect. M7 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.4 N. M. Greene, "BONAMI: Resonance Self-Shielding by the Bondarenko Method," Sect. F1 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.5 N. M. Greene, "NITAWL-II: SCALE System Module for Performing Resonance Shielding and Working Library Production," Sect. F2 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.6 N. M. Greene and L. M. Petrie, "XSDRNPM: A One-Dimensional Discrete-Ordinates Code for Transport Analysis," Sect. F3 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

B.7 O. W. Hermann, "COUPLE: SCALE System Module to Process Problem-Dependent Cross Sections and Neutron Spectral Data for ORIGEN-S Analyses," Sect. F6 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (March 1997). Available from Radiation Shielding Information Center as CCC-545.

APPENDIX C

INPUT LISTINGS FOR SAN ONOFRE SAS2H DEPLETION CALCULATION

APPENDIX C

INPUT LISTINGS FOR SAN ONOFRE SAS2H DEPLETION CALCULATION

Pin 067, Height 53.0 in., with a Burnup of 8,167 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre mox-1  pin 067  53" ht, 8,167 mwd/mtm  (3.31 wt% fiss.pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u331  10.2235 4 0 1 0  92234 0.000055  92235 0.0072 92238 0.992745
        8016 2  1  0.961423  744  end
arbm-pu331  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.038577  744  end
pu-236  1 0 1-20 744  end
pu-237  1 0 1-20 744  end
pu-238  1 0 1-20 744  end
kr-83  1 0 1-20 744  end
kr-85  1 0 1-20 744  end
sr-90  1 0 1-20 744  end
 y-89  1 0 1-20 744  end
zr-93  1 0 1-20 744  end
zr-94  1 0 1-20 744  end
zr-95  1 0 1-20 744  end
nb-94  1 0 1-20 744  end
nb-95  1 0 1-20 744  end
mo-95  1 0 1-20 744  end
tc-99  1 0 1-20 744  end
ru-101 1 0 1-20 744  end
ru-106 1 0 1-20 744  end
rh-103 1 0 1-20 744  end
rh-105 1 0 1-20 744  end
pd-105 1 0 1-20 744  end
pd-108 1 0 1-20 744  end
ag-109 1 0 1-20 744  end
sn-126 1 0 1-20 744  end
sb-124 1 0 1-20 744  end
xe-131 1 0 1-20 744  end
xe-132 1 0 1-20 744  end
xe-136 1 0 1-20 744  end
cs-134 1 0 1-20 744  end
cs-135 1 0 1-20 744  end
cs-137 1 0 1-20 744  end
ba-136 1 0 1-20 744  end
la-139 1 0 1-20 744  end
ce-144 1 0 1-20 744  end
pr-141 1 0 1-20 744  end
pr-143 1 0 1-20 744  end
nd-143 1 0 1-20 744  end
nd-144 1 0 1-20 744  end
nd-145 1 0 1-20 744  end
```

```
nd-146 1 0 1-20 744  end
nd-147 1 0 1-20 744  end
nd-148 1 0 1-20 744  end
nd-150 1 0 1-20 744  end
pm-147 1 0 1-20 744  end
pm-148 1 0 1-20 744  end
pm-149 1 0 1-20 744  end
sm-147 1 0 1-20 744  end
sm-148 1 0 1-20 744  end
sm-149 1 0 1-20 744  end
sm-150 1 0 1-20 744  end
sm-151 1 0 1-20 744  end
sm-152 1 0 1-20 744  end
eu-151 1 0 1-20 744  end
eu-153 1 0 1-20 744  end
eu-154 1 0 1-20 744  end
eu-155 1 0 1-20 744  end
gd-155 1 0 1-20 744  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 800.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average, 800 in cyc 2,
'  500 in cyc 3 & 200 in cyc 4
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=4  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5   end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=20.266  burn=134    down=0  end
power=20.266  burn=134    down=0  bfrac=0.625     end
power=20.266  burn=135    down=717  bfrac=0.25    end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

Pin 141, Height 95.5 in., with a Burnup of 6,808 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre mox-2 pin 141, 95.5 in. ht. 6,808 mwd/mtm  (2.84 wt% fiss.pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u284   10.2235  4 0 1 0  92234 0.000055  92235 0.0072 92238
  0.992745   8016 2  1  0.966901  713  end
arbm-pu284  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.033099  713  end
pu-236  1 0 1-20 713  end
pu-237  1 0 1-20 713  end
pu-238  1 0 1-20 713  end
kr-83  1 0 1-20 713  end
kr-85  1 0 1-20 713  end
sr-90  1 0 1-20 713  end
 y-89  1 0 1-20 713  end
zr-93  1 0 1-20 713  end
zr-94  1 0 1-20 713  end
zr-95  1 0 1-20 713  end
nb-94  1 0 1-20 713  end
nb-95  1 0 1-20 713  end
mo-95  1 0 1-20 713  end
tc-99  1 0 1-20 713  end
ru-101 1 0 1-20 713  end
ru-106 1 0 1-20 713  end
rh-103 1 0 1-20 713  end
rh-105 1 0 1-20 713  end
pd-105 1 0 1-20 713  end
pd-108 1 0 1-20 713  end
ag-109 1 0 1-20 713  end
sn-126 1 0 1-20 713  end
sb-124 1 0 1-20 713  end
xe-131 1 0 1-20 713  end
xe-132 1 0 1-20 713  end
xe-136 1 0 1-20 713  end
cs-134 1 0 1-20 713  end
cs-135 1 0 1-20 713  end
cs-137 1 0 1-20 713  end
ba-136 1 0 1-20 713  end
la-139 1 0 1-20 713  end
ce-144 1 0 1-20 713  end
pr-141 1 0 1-20 713  end
pr-143 1 0 1-20 713  end
nd-143 1 0 1-20 713  end
nd-144 1 0 1-20 713  end
nd-145 1 0 1-20 713  end
nd-146 1 0 1-20 713  end
nd-147 1 0 1-20 713  end
nd-148 1 0 1-20 713  end
nd-150 1 0 1-20 713  end
pm-147 1 0 1-20 713  end
pm-148 1 0 1-20 713  end
pm-149 1 0 1-20 713  end
sm-147 1 0 1-20 713  end
sm-148 1 0 1-20 713  end
sm-149 1 0 1-20 713  end
sm-150 1 0 1-20 713  end
```

```
sm-151 1 0 1-20 713  end
sm-152 1 0 1-20 713  end
eu-151 1 0 1-20 713  end
eu-153 1 0 1-20 713  end
eu-154 1 0 1-20 713  end
eu-155 1 0 1-20 713  end
gd-155 1 0 1-20 713  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 800.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average, 800 in cyc 2,
'  500 in cyc3 & 200 in cyc4
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=4  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5   end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=16.894  burn=134    down=0   end
power=16.894  burn=134    down=0   bfrac=0.625     end
power=16.894  burn=135    down=719  bfrac=0.25     end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

Pin 079, Height 49.0 in., with a Burnup of 20,891 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre mox-3 pin 079  49" ht, modcy3, 20891 mwd/mtm (3.10 wt% fiss.pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u310   10.2235  4 0 1 0  92234 0.000055  92235 0.0072 92238
  0.992745   8016 2  1  0.963870  718  end
arbm-pu310  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.036130  718  end
pu-236  1 0 1-20 718  end
pu-237  1 0 1-20 718  end
pu-238  1 0 1-20 718  end
kr-83  1 0 1-20 718  end
kr-85  1 0 1-20 718  end
sr-90  1 0 1-20 718  end
 y-89  1 0 1-20 718  end
zr-93  1 0 1-20 718  end
zr-94  1 0 1-20 718  end
zr-95  1 0 1-20 718  end
nb-94  1 0 1-20 718  end
nb-95  1 0 1-20 718  end
mo-95  1 0 1-20 718  end
tc-99  1 0 1-20 718  end
ru-101 1 0 1-20 718  end
ru-106 1 0 1-20 718  end
rh-103 1 0 1-20 718  end
rh-105 1 0 1-20 718  end
pd-105 1 0 1-20 718  end
pd-108 1 0 1-20 718  end
ag-109 1 0 1-20 718  end
sn-126 1 0 1-20 718  end
sb-124 1 0 1-20 718  end
xe-131 1 0 1-20 718  end
xe-132 1 0 1-20 718  end
xe-136 1 0 1-20 718  end
cs-134 1 0 1-20 718  end
cs-135 1 0 1-20 718  end
cs-137 1 0 1-20 718  end
ba-136 1 0 1-20 718  end
la-139 1 0 1-20 718  end
ce-144 1 0 1-20 718  end
pr-141 1 0 1-20 718  end
pr-143 1 0 1-20 718  end
nd-143 1 0 1-20 718  end
nd-144 1 0 1-20 718  end
nd-145 1 0 1-20 718  end
nd-146 1 0 1-20 718  end
nd-147 1 0 1-20 718  end
nd-148 1 0 1-20 718  end
nd-150 1 0 1-20 718  end
pm-147 1 0 1-20 718  end
pm-148 1 0 1-20 718  end
pm-149 1 0 1-20 718  end
sm-147 1 0 1-20 718  end
sm-148 1 0 1-20 718  end
sm-149 1 0 1-20 718  end
sm-150 1 0 1-20 718  end
```

```
sm-151 1 0 1-20 718  end
sm-152 1 0 1-20 718  end
eu-151 1 0 1-20 718  end
eu-153 1 0 1-20 718  end
eu-154 1 0 1-20 718  end
eu-155 1 0 1-20 718  end
gd-155 1 0 1-20 718  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 725.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average,
'  725 in cyc 2 & 4 and 275 in cyc 3 & 5
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=5  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5  mxrepeats=0  end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=17.406  burn=201.5  down=0    end
power=17.406  burn=201.5  down=66   bfrac=0.37931   end
power=30.232  burn=229.5  down=0    tmpfuel=839  end
power=30.232  burn=229.5  down=194  bfrac=0.37931  tmpfuel=839  end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

Pin 167, Height 16.5 in., with a Burnup of 17,447 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre mox-4 pin 167, 16.5" ht. mod-cy3, 17447 mwd/mthm (2.84 wt% fis. pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u284   10.2235  4 0 1 0  92234 0.000055  92235 0.0072 92238
  0.992745   8016 2  1  0.966901  695  end
arbm-pu284  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.033099  695  end
pu-236  1 0 1-20 695  end
pu-237  1 0 1-20 695  end
pu-238  1 0 1-20 695  end
kr-83  1 0 1-20 695  end
kr-85  1 0 1-20 695  end
sr-90  1 0 1-20 695  end
 y-89  1 0 1-20 695  end
zr-93  1 0 1-20 695  end
zr-94  1 0 1-20 695  end
zr-95  1 0 1-20 695  end
nb-94  1 0 1-20 695  end
nb-95  1 0 1-20 695  end
mo-95  1 0 1-20 695  end
tc-99  1 0 1-20 695  end
ru-101 1 0 1-20 695  end
ru-106 1 0 1-20 695  end
rh-103 1 0 1-20 695  end
rh-105 1 0 1-20 695  end
pd-105 1 0 1-20 695  end
pd-108 1 0 1-20 695  end
ag-109 1 0 1-20 695  end
sn-126 1 0 1-20 695  end
sb-124 1 0 1-20 695  end
xe-131 1 0 1-20 695  end
xe-132 1 0 1-20 695  end
xe-136 1 0 1-20 695  end
cs-134 1 0 1-20 695  end
cs-135 1 0 1-20 695  end
cs-137 1 0 1-20 695  end
ba-136 1 0 1-20 695  end
la-139 1 0 1-20 695  end
ce-144 1 0 1-20 695  end
pr-141 1 0 1-20 695  end
pr-143 1 0 1-20 695  end
nd-143 1 0 1-20 695  end
nd-144 1 0 1-20 695  end
nd-145 1 0 1-20 695  end
nd-146 1 0 1-20 695  end
nd-147 1 0 1-20 695  end
nd-148 1 0 1-20 695  end
nd-150 1 0 1-20 695  end
pm-147 1 0 1-20 695  end
pm-148 1 0 1-20 695  end
pm-149 1 0 1-20 695  end
sm-147 1 0 1-20 695  end
sm-148 1 0 1-20 695  end
sm-149 1 0 1-20 695  end
sm-150 1 0 1-20 695  end
```

```
sm-151 1 0 1-20 695  end
sm-152 1 0 1-20 695  end
eu-151 1 0 1-20 695  end
eu-153 1 0 1-20 695  end
eu-154 1 0 1-20 695  end
eu-155 1 0 1-20 695  end
gd-155 1 0 1-20 695  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 725.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average,
'  725 in cyc 2 & 4 and 275 in cyc 3 & 5
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=5  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5  mxrepeats=0  end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=14.885  burn=201.5  down=0    end
power=14.885  burn=201.5  down=66   bfrac=0.37931   end
power=24.942  burn=229.5  down=0    tmpfuel=787     end
power=24.942  burn=229.5  down=187  bfrac=0.37931   tmpfuel=787   end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

Pin 167, Height 95.5 in., with a Burnup of 18,713 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre  mox-5  pin 167, 95.5" ht,mod-cy3, 18713 mwd/mtm(2.84 wt% fiss.pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u284   10.2235  4 0 1 0  92234 0.000055  92235 0.0072 92238
  0.992745   8016 2  1  0.966901  705  end
arbm-pu284  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.033099  705  end
pu-236  1 0 1-20 705  end
pu-237  1 0 1-20 705  end
pu-238  1 0 1-20 705  end
kr-83  1 0 1-20 705  end
kr-85  1 0 1-20 705  end
sr-90  1 0 1-20 705  end
 y-89  1 0 1-20 705  end
zr-93  1 0 1-20 705  end
zr-94  1 0 1-20 705  end
zr-95  1 0 1-20 705  end
nb-94  1 0 1-20 705  end
nb-95  1 0 1-20 705  end
mo-95  1 0 1-20 705  end
tc-99  1 0 1-20 705  end
ru-101 1 0 1-20 705  end
ru-106 1 0 1-20 705  end
rh-103 1 0 1-20 705  end
rh-105 1 0 1-20 705  end
pd-105 1 0 1-20 705  end
pd-108 1 0 1-20 705  end
ag-109 1 0 1-20 705  end
sn-126 1 0 1-20 705  end
sb-124 1 0 1-20 705  end
xe-131 1 0 1-20 705  end
xe-132 1 0 1-20 705  end
xe-136 1 0 1-20 705  end
cs-134 1 0 1-20 705  end
cs-135 1 0 1-20 705  end
cs-137 1 0 1-20 705  end
ba-136 1 0 1-20 705  end
la-139 1 0 1-20 705  end
ce-144 1 0 1-20 705  end
pr-141 1 0 1-20 705  end
pr-143 1 0 1-20 705  end
nd-143 1 0 1-20 705  end
nd-144 1 0 1-20 705  end
nd-145 1 0 1-20 705  end
nd-146 1 0 1-20 705  end
nd-147 1 0 1-20 705  end
nd-148 1 0 1-20 705  end
nd-150 1 0 1-20 705  end
pm-147 1 0 1-20 705  end
pm-148 1 0 1-20 705  end
pm-149 1 0 1-20 705  end
sm-147 1 0 1-20 705  end
sm-148 1 0 1-20 705  end
sm-149 1 0 1-20 705  end
```

```
sm-150 1 0 1-20 705  end
sm-151 1 0 1-20 705  end
sm-152 1 0 1-20 705  end
eu-151 1 0 1-20 705  end
eu-153 1 0 1-20 705  end
eu-154 1 0 1-20 705  end
eu-155 1 0 1-20 705  end
gd-155 1 0 1-20 705  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 725.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average,
'  725 in cyc 2 & 4 and 275 in cyc 3 & 5
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=5  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5  mxrepeats=0  end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=15.965  burn=201.5  down=0    end
power=15.965  burn=201.5  down=66   bfrac=0.37931   end
power=26.751  burn=229.5  down=0    tmpfuel=805  end
power=26.751  burn=229.5  down=187  bfrac=0.37931  tmpfuel=805   end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

Pin 167, Height 114.0 in., with a Burnup of 11,065 GWd/MTHM

```
=sas2h    parm='skipshipdata'
san onofre mox-6 pin 167, 114" ht. mod-cy3 11,065 mwd/mthm (2.84 wt% fis. pu)
44group        latticecell
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
arbm-u284   10.2235  4 0 1 0  92234 0.000055  92235 0.0072 92238
  0.992745   8016 2  1  0.966901  650  end
arbm-pu284  10.2235  6 0 1 0  94239 0.806 94240 0.134 94241 0.052
    94242 0.008 95241 0.005 8016 2  1  0.033099  650  end
pu-236  1 0 1-20 650  end
pu-237  1 0 1-20 650  end
pu-238  1 0 1-20 650  end
kr-83  1 0 1-20 650  end
kr-85  1 0 1-20 650  end
sr-90  1 0 1-20 650  end
 y-89  1 0 1-20 650  end
zr-93  1 0 1-20 650  end
zr-94  1 0 1-20 650  end
zr-95  1 0 1-20 650  end
nb-94  1 0 1-20 650  end
nb-95  1 0 1-20 650  end
mo-95  1 0 1-20 650  end
tc-99  1 0 1-20 650  end
ru-101 1 0 1-20 650  end
ru-106 1 0 1-20 650  end
rh-103 1 0 1-20 650  end
rh-105 1 0 1-20 650  end
pd-105 1 0 1-20 650  end
pd-108 1 0 1-20 650  end
ag-109 1 0 1-20 650  end
sn-126 1 0 1-20 650  end
sb-124 1 0 1-20 650  end
xe-131 1 0 1-20 650  end
xe-132 1 0 1-20 650  end
xe-136 1 0 1-20 650  end
cs-134 1 0 1-20 650  end
cs-135 1 0 1-20 650  end
cs-137 1 0 1-20 650  end
ba-136 1 0 1-20 650  end
la-139 1 0 1-20 650  end
ce-144 1 0 1-20 650  end
pr-141 1 0 1-20 650  end
pr-143 1 0 1-20 650  end
nd-143 1 0 1-20 650  end
nd-144 1 0 1-20 650  end
nd-145 1 0 1-20 650  end
nd-146 1 0 1-20 650  end
nd-147 1 0 1-20 650  end
nd-148 1 0 1-20 650  end
nd-150 1 0 1-20 650  end
pm-147 1 0 1-20 650  end
pm-148 1 0 1-20 650  end
pm-149 1 0 1-20 650  end
sm-147 1 0 1-20 650  end
sm-148 1 0 1-20 650  end
sm-149 1 0 1-20 650  end
sm-150 1 0 1-20 650  end
```

```
sm-151 1 0 1-20 650  end
sm-152 1 0 1-20 650  end
eu-151 1 0 1-20 650  end
eu-153 1 0 1-20 650  end
eu-154 1 0 1-20 650  end
eu-155 1 0 1-20 650  end
gd-155 1 0 1-20 650  end
'   need the following to use endf/b5 library:
zirc2   2  1  615  end
h2o   3  den=0.7179  1  576.5  end
arbm-boron  0.7179  1 1 0 0 5000 100 3 725.0e-6 576.5  end
ss304   5  1  576.5  end
'---------------------------------
'
'  500 ppm boron (wt) in moderator on average,
'  725 in cyc 2 & 4 and 275 in cyc 3 & 5
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch  1.41224  0.92939 1  3  1.07188 2  0.94844  0  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly and cycle parameters:
'
npin/assm=180  fuelngth=908.69  ncycles=5  nlib/cyc=1
printlevel=5 lightel=9  inplevel=2  numzones=5  mxrepeats=0  end
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.79677   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
 3     0.64897    5   0.67945   3  0.84510   500  2.78870
 3   2.81266
power=1-8  burn=10   down=595   end
power=9.536   burn=201.5  down=0    end
power=9.536   burn=201.5  down=66   bfrac=0.37931   end
power=15.735  burn=229.5  down=0    tmpfuel=703  end
power=15.735  burn=229.5  down=192  bfrac=0.37931  tmpfuel=703  end
  o 135  cr  5.9  mn  0.33
  fe 13  co 0.075 ni  9.9
  zr 221 nb  0.71 sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

APPENDIX D

MEASURED AND COMPUTED CONCENTRATIONS FOR SAN ONOFRE MOX FUEL SAMPLES

APPENDIX D

MEASURED AND COMPUTED CONCENTRATIONS FOR SAN ONOFRE MOX FUEL SAMPLES

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 067, 53 in. height, 8.167 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:		milligrams/gram u + pu		
92	u234	4.698E-02	4.781E-02	(1.8%)
92	u235	5.926E+00	5.885E+00	(-0.7%)
92	u236	2.180E-01	2.155E-01	(-1.1%)
92	u238	9.495E+02	9.495E+02	(0.0%)
94	pu236	9.962E-08	1.208E-08	(-87.9%)
94	pu238	1.915E-01	7.440E-02	(-61.1%)
94	pu239	2.497E+01	2.536E+01	(1.6%)
94	pu240	6.645E+00	6.732E+00	(1.3%)
94	pu241	2.526E+00	2.574E+00	(1.9%)
94	pu242	4.555E-01	4.917E-01	(7.9%)
60	nd148	8.897E-02	8.862E-02	(-0.4%)

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 141, 95.9 in. height, 6.808 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:		milligrams/gram u + pu		
92	u234	5.675E-02	4.852E-02	(-14.5%)
92	u235	6.088E+00	5.987E+00	(-1.7%)
92	u236	1.717E-01	1.964E-01	(14.4%)
92	u238	9.556E+02	9.557E+02	(0.0%)
94	pu236	9.996E-08	8.421E-09	(-91.6%)
94	pu238	1.366E-01	5.897E-02	(-56.8%)
94	pu239	2.201E+01	2.209E+01	(0.4%)
94	pu240	5.678E+00	5.773E+00	(1.7%)
94	pu241	1.935E+00	2.155E+00	(11.4%)
94	pu242	3.421E-01	4.151E-01	(21.4%)
60	nd148	7.423E-02	7.389E-02	(-0.5%)

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 079, 49.0 in. height, 20.891 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:	milligrams/gram u + pu			
92	u234	4.661E-02	4.050E-02	(-13.1%)
92	u235	4.400E+00	4.313E+00	(-2.0%)
92	u236	4.889E-01	5.213E-01	(6.6%)
92	u238	9.432E+02	9.433E+02	(0.0%)
94	pu236	2.882E-07	1.175E-07	(-59.2%)
94	pu238	2.821E-01	1.797E-01	(-36.3%)
94	pu239	1.649E+01	1.735E+01	(5.2%)
94	pu240	7.677E+00	7.421E+00	(-3.3%)
94	pu241	3.656E+00	3.711E+00	(1.5%)
94	pu242	8.968E-01	9.498E-01	(5.9%)
60	nd148	2.271E-01	2.273E-01	(0.1%)

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 167, 16.5 in. height, 17.447 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:	milligrams/gram u + pu			
92	u234	4.688E-02	4.207E-02	(-10.3%)
92	u235	4.548E+00	4.581E+00	(0.7%)
92	u236	4.728E-01	4.690E-01	(-0.8%)
92	u238	9.485E+02	9.485E+02	(0.0%)
94	pu236	1.859E-07	8.194E-08	(-55.9%)
94	pu238	2.239E-01	1.473E-01	(-34.2%)
94	pu239	1.518E+01	1.687E+01	(11.1%)
94	pu240	7.041E+00	6.772E+00	(-3.8%)
94	pu241	3.201E+00	3.247E+00	(1.4%)
94	pu242	7.614E-01	7.894E-01	(3.7%)
93	np237	9.250E-02	8.663E-02	(-6.3%)
95	am241	9.967E-01	4.107E-01	(-58.8%)
95	am243	2.177E-01	1.623E-01	(-25.4%)
60	nd148	1.901E-01	1.897E-01	(-0.2%)

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 167, 95.5 in. height, 18.713 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:	milligrams/gram u + pu			
92	u234	4.683E-02	4.137E-02	(-11.6%)
92	u235	4.505E+00	4.431E+00	(-1.6%)
92	u236	4.817E-01	4.970E-01	(3.2%)
92	u238	9.475E+02	9.476E+02	(0.0%)
94	pu236	2.016E-07	9.474E-08	(-53.0%)
94	pu238	2.327E-01	1.566E-01	(-32.7%)
94	pu239	1.523E+01	1.636E+01	(7.4%)
94	pu240	7.121E+00	6.837E+00	(-4.0%)
94	pu241	3.346E+00	3.346E+00	(0.0%)
94	pu242	7.963E-01	8.448E-01	(6.1%)
93	np237	1.057E-01	9.379E-02	(-11.3%)
95	am241	1.049E+00	4.038E-01	(-61.5%)
95	am243	2.401E-01	1.795E-01	(-25.2%)
60	nd148	2.037E-01	2.036E-01	(-0.1%)

san onofre unit 1 pwr mox fuel program
measured and computed irradiated fuel composition, mg/g fuel (u+pu)
fuel assembly d51x, pin id 167, 114 in. height, 11.065 gwd/mthm

run november 1999

..compares cases using 44GROUPNDF5 library..

nuclide, z & name		measured	44groupndf5	%diff
units:	milligrams/gram u + pu			
92	u234	4.713E-02	4.568E-02	(-3.1%)
92	u235	5.386E+00	5.378E+00	(-0.2%)
92	u236	3.042E-01	3.153E-01	(3.6%)
92	u238	9.529E+02	9.529E+02	(0.0%)
94	pu236	1.207E-07	3.200E-08	(-73.5%)
94	pu238	1.791E-01	9.796E-02	(-45.3%)
94	pu239	1.880E+01	1.981E+01	(5.4%)
94	pu240	6.390E+00	6.248E+00	(-2.2%)
94	pu241	2.603E+00	2.652E+00	(1.9%)
94	pu242	4.827E-01	5.432E-01	(12.5%)
93	np237	5.464E-02	5.217E-02	(-4.5%)
95	am241	3.015E-01	4.483E-01	(48.7%)
95	am243	5.162E-02	8.775E-02	(70.0%)
60	nd148	1.212E-01	1.200E-01	(-0.9%)

Statistics for SAS2H vs Measurements

For six irradiation cases

San Onofre PWR using Four Mox Fuel Assemblies

Cross-section source: SCALE 44-group, 44GROUPNDF5

	Nuclide	Cases	Percentage Difference		
			Average	1-Sigma of average	1-Sigma of individual
1	nd148	6	-0.3	0.1	0.4
2	u234	6	-8.5	2.6	6.4
3	u235	6	-0.9	0.4	1.1
4	u236	6	4.3	2.3	5.7
5	u238	6	0.0	0.0	0.0
6	np237	3	-7.4	2.0	3.5
7	pu236	6	-70.2	6.8	16.7
8	pu238	6	-44.4	5.0	12.2
9	pu239	6	5.2	1.6	3.9
10	pu240	6	-1.7	1.0	2.6
11	pu241	6	3.0	1.7	4.2
12	pu242	6	9.6	2.6	6.5
13	am241	3	-23.9	36.3	62.9
14	am243	3	6.4	31.8	55.0

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