APPENDIX D BENCHMARK CONSIDERATIONS FOR MIXED OXIDE RADIOACTIVE MATERIALS AND SPENT NUCLEAR FUEL

D.1 Experimental Benchmarks

The information and guidance in this appendix applies to both mixed oxide (MOX) radioactive materials and spent nuclear fuel (SNF) packages. This appendix does not address considerations for burnup credit for commercial MOX SNF, whether irradiated in a pressurized-water reactor or a boiling-water reactor; the considerations are for analyses that assume the MOX fuel is unirradiated. Benchmarking for any commercial MOX SNF would need to address additional considerations, such as those indicated in the discussion about MOX burnup credit in Section 6.4.7 of this SRP.

Substantial guidance on how to select an appropriate set of criticality benchmark experiments for low-enriched uranium (LEU) fissile systems is given in NUREG/CR-5661, "Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages," issued April 1997 (Dyer and Parks 1997), and in NUREG/CR-6361, "Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages," issued March 1997 (Lichtenwalter et al. 1997). Considerably fewer benchmark experiments exist for MOX than for LEU. As a consequence, the guidance provided in NUREG/CR-5661 and NUREG/CR-6361 cannot be applied directly to the evaluation of MOX fissile systems. The benchmarks needed for the criticality analyses of MOX packages are in the thermal energy range. This condition results because, for essentially all types of MOX, the most reactive configuration is a flooded containment.

As an alternative, the 2001 edition of the "International Handbook of Evaluated Criticality Safety Benchmark Experiments" (IHECSBE) has 11 evaluated thermal-energy studies involving MOX fuel pins in various lattice experiments and five evaluated thermal-energy studies involving MOX liquids in tank experiments (NEA, 2001). These can be divided into 18 sets of experiments involving different fissile oxide compositions and configurations in lattices and 13 sets of experiments involving different liquid fissile nitrate compositions and configurations in tanks. The total number of essentially different experiments is 131. Since the 2001 edition, an additional four evaluated thermal-energy studies involving MOX fuel pins and an additional four evaluated thermal-energy studies involving MOX liquids have been added to the IHECSBE (NEA, 2014) that include experiments evaluated to be acceptable to use as benchmarks. Other benchmark experiments are available throughout the world but are not as readily available. The vast majority have not been rigorously evaluated in the manner of those found in the IHECSBE and are consequently of limited use for benchmark criticality analyses for MOX packages. More evaluated MOX thermal benchmarks may be included in future editions of the IHECSBE.

The 18 sets of experiments involving fissile oxides in lattices and 13 sets of experiments involving fissile nitrate liquids in tanks from the 2001 edition of the IHECSBE have been organized and shown in Tables D–1 through D–5. The various tables are separated on two features. The first is between lattice and tank experiments, and the second is on weight percent of plutonium to total plutonium plus uranium (Pu/(Pu+U). Table D–1 has lattice experiments with Pu/(Pu+U) to 5 percent. Table D–2 has lattice experiments with Pu/(Pu+U) from 5 percent to 15 percent. Table D–3 has lattice experiments with Pu/(Pu+U) greater than 15 percent. Table D–4 has tank experiments with Pu/(Pu+U) to 31 percent (there are no experiments with Pu/(Pu+U) less than 22 percent). Table D–5 has tank experiments with Pu/(Pu+U) greater than

31 percent. Lists of meaningful, experimental characteristics are recorded for each set of experiments together with characteristics of their corresponding computational evaluations.

Experimental plutonium benchmarks should also be taken into account as part of the initial set of benchmark experiments to be considered for a MOX package application. About four times as many thermal-plutonium-tank-liquid benchmarks exist in the IHECSBE as thermal-MOX-tank-liquid benchmarks. However, fewer thermal-plutonium-lattice benchmarks exist in the IHECSBE than thermal-MOX-lattice benchmarks.

Also, there is a set of 156 configurations known as the French Haut Taux de Combustion (HTC) experiments. The descriptions of these experiments are provided in the four reports by Fernex listed in Section D3.0 and are considered commercial proprietary. Note that these experiments were set up to simulate the isotopic compositions of irradiated LEU fuel; so, the compositions will not be the same as for MOX fuel and will include other radionuclides that are not present in MOX fuel. Thus, use of the HTC experiments requires appropriate consideration of the differences between the HTC compositions and those of MOX fuel, whether irradiated and unirradiated. An evaluation of the HTC experiment data is described in NUREG/CR-6979, "Evaluation of the French Haut Taux de Combustion (HTC) Critical Experiment Data," issued September 2008, though this evaluation was done for the purpose of using the data to benchmark burnup credit analyses for LEU SNF.

D.2 Summary of Bias and Uncertainty Evaluation

There are two measures of the accuracy of an experiment and its associated calculation. The first measure is the effective bias (Eff-Bias) between calculation and benchmark experiment. The multiplication coefficient for a fissile system is designated as k_{eff}. Designate the calculated k_{eff} for the benchmark experiment as k_{calc} and the benchmark experimental k_{eff} as k_{exp}. If the calculational bias, β, is defined as $\beta = k_{calc} - k_{exp}$, then a quantity Δk can be defined as follows:

$$\Delta k = \begin{pmatrix} \beta \ if \ k_{calc} \leq k_{exp} \\ 0 \ if \ k_{calc} > k_{exp} \end{pmatrix} \qquad \text{(D-1)}$$

or a given experimental benchmark set, Δk_{max} is chosen as the largest absolute value of the Δk given by Equation D-1 for all experiments in the set. The 95 percent confidence limit of k_{calc} is k_{calc} plus twice the calculated standard deviation, which is designated by 2σ. The Eff-Bias value is then given by the following:

$$\text{Eff-Bias} = \Delta k_{max} - 2\sigma \qquad \text{(D-2)}$$

Eff-Bias, as defined here, is always *less* than zero. If k_{calc} is greater than k_{exp} for all experiments in a set, the Eff-Bias value is just the negative of twice the calculated standard deviation.

The second measure is the total experimental uncertainty (Exp-Uncer) that was determined by the evaluator after assessing all sources of uncertainty for the experiments in a set.[1] A worst-case difference between k_{calc} and k_{exp} can be assigned as the difference of the total experimental uncertainty and the effective bias (Exp-Uncer - Eff-Bias) for the experimental set in question. This worst-case difference (WCD), as defined here, is always *greater* than zero. It represents the upper limit of the inherent uncertainties in the ability of the computer code,

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1 The evaluator included sources of experimental bias or error in each k_{exp}. This does not represent an uncertainty and so is not included in the value for total experimental uncertainty.

together with the cross-section set used, to accurately determine the k_{eff} of a critical benchmark experiment. Therefore, a bounding multiplication coefficient, k_{safe}, at the 95 percent confidence limit, can be chosen to be equal to 0.95 minus WCD, where an administrative margin of safety of 0.05 has been included.[2]

Values for the variable WCD for each experimental set vary between 0.0071 to 0.0192 (0.71 percent to 1.92 percent), 0.0043 to 0.0328 (0.43 percent to 3.28 percent), 0.0023 to 0.0138 (0.23 percent to 1.38 percent), 0.0044 to 0.0180 (0.44 percent to 1.80 percent), and 0.0044 to 0.0150 (0.44 percent to 1.50 percent) for the experimental sets in Tables D–1, D–2, D–3, D–4, and D–5, respectively. No particular correlation seems to exist between WCD and the lattice configuration or pitch. Neither does there seem to be a correlation with plutonium composition type. The plutonium composition types are given in Table B–1 of Appendix B to this SRP and are designated as weapons grade (WG), fuel grade (FG), and power grade (PG).

The maximum value for WCD found in the five tables is 0.0328, or 3.28 percent in k_{eff}. How accurately a criticality computer code can predict the critical value for a criticality experiment depends on the methodology employed by the code and the cross-section set used, together with the detail to which the experimental system is modeled in the input to the computer code. In addition, the basic experimental uncertainty limits the ultimate prediction accuracy possible. Of particular importance is the cross-section set. Values for WCD in the five tables that are significantly less than 0.0100 are due to the fact that k_{calc} is greater than k_{exp}. Therefore, the value for Eff-Bias, in that case, is just the negative of twice the calculated standard deviation, which is approximately 0.0020. The cross-section sets used in the analyses represented in the tables over-predict plutonium reactivity, and this represents some of the reason for the over-prediction for k_{calc} for these experiments. Values for k_{safe} are not expected to be much above 0.93, except when it can be demonstrated that the criticality code and cross section set overestimate the reactivity of the MOX contents.

Analyzing an acceptable number of MOX benchmarks is the preferred way to obtain a bias value for the MOX contents of a package. With the relatively limited number of MOX critical experiments available for use in validation exercises, it is important to determine that the application of interest to the reviewer fits within the area of applicability for the set of critical benchmark experiments selected for validation. Guidance on how to select an appropriate set of benchmark experiments for a fissile system is given in NUREG/CR-5661 and in NUREG/CR-6361. A computational methodology to select an appropriate set of benchmark experiments for a fissile package application has also been developed for SCALE (Broadhead et al. 1999; Broadhead et al. 2004; Rearden and Childs 2000; Rearden and Mueller 2008; Dunn and Rearden 2001).

Beginning with version 5 of SCALE, a set of sensitivity and uncertainty analysis tools have been developed and are included with the code that gives a measure of the similarity of the reactivity of a package application to that of an experimental benchmark. Successive versions of SCALE include an improved and expanded set of tools (Perfetti and Rearden 2016; Rearden et al. 2011; Perfetti et al. 2016; Williams et al. 2013, ORNL 2011). Sensitivity coefficients for both systems are computed and give the sensitivity of each system's k_{eff} to the cross-section

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2 If the benchmarks are applied to a package application where there is a lack of experimental data, the 0.05 administrative margin may not be sufficient, and the reviewer needs to be aware of this issue. In reality, the 0.05 margin should be sufficient, but there needs to be an assessment of the adequacy of the 0.05 to establish the basis. Guidance for deciding on an acceptable choice for the administrative margin is given in NUREG/CR-5661. See also NUREG/CR-6361.

data. These sensitivity coefficients are determined for each energy group in the cross-section library chosen in the analysis, as well as the sum over all energy groups. Two integral parameters for the combined systems are produced from the sensitivity data to determine system-to-system similarities. The first parameter can be used as a gauge of system similarity to sensitivity only. The second parameter can be used as a measure of the similarity of the systems in terms of uncertainty, not just sensitivity. The pair of integral parameter values is determined for every potential benchmark experiment with the package application of interest. When two systems produce an appropriately high value (i.e., a value sufficiently close to 1) for either integral parameter, or both, this indicates the k_{eff} response is similar enough that one system serves well to validate the criticality safety parameters for the other system. Previous analyses using these tools have used the value of 0.8 as a threshold for determining that systems under consideration are similar enough; this is consistent with recommendations the SCALE developer, Oak Ridge National Laboratory, has made. The benchmark experiments chosen for complete validation are those with high integral parameter values (Broadhead et al. 1999; Broadhead et al. 2004; Rearden and Childs 2000; Rearden and Mueller 2008; Dunn and Rearden 2001).

New parameters can also be constructed from the components of the integral parameters and can be used to explore the sensitivity of specific nuclide reactions of benchmark experiments with the package application of interest. For example, if low integral parameter values are found for an application with all benchmark experiments chosen for validation, the new parameters could serve to identify which nuclides would require additional experimental benchmark data for complete validation. Also, in the validation of transportation packages for commercial fuel, numerous benchmark experiments might serve to validate the fission reactions, and thus high integral parameter values would be found. However, the new parameters could be used to find benchmarks to ensure that any poison materials in the package are also well validated by the benchmarks. With the inclusion of these sensitivity and uncertainty analysis tools in the SCALE code, beginning with version 5, the criticality safety analyst now has a powerful set of tools available to perform detailed quantitative analyses to determine the applicability of benchmark experiments to help design package applications under consideration (Broadhead et al. 1999; Broadhead et al. 2004; Rearden and Childs 2000; Rearden and Mueller 2008; Dunn and Rearden 2001).

Table D–1 Important characteristics of lattice experiments with weight percent of Pu/(Pu+U) to 5 percent (from IHECSBE)

Designation for experiments [a]	MCT-009	MCT-002	MCT-002	MCT-006	MCT-007	MCT-008	MCT-004	MCT-005
Facility where experiments conducted	Hanford	Hanford	Hanford	Hanford	Hanford	Hanford	Tokai	Hanford
Computer codes used in evaluations [b]	MCNP/KENO	MCNP	MCNP	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO
Cross section sets used in evaluations [c]	ENDF/B-V/IV	ENDF/B-V	ENDF/B-V	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	JENDL-3.2	ENDF/B-V/IV
Cross section type [d]	cont/27grp	cont	cont	cont/27grp	cont/27grp	cont/27grp	cont/137grp	cont/27grp
Fuel compound [e]	oxide	oxide	oxide	oxide	oxide	oxide	oxide	oxide
Fuel compound form	solid	solid	solid	solid	solid	solid	solid	solid
Density of fuel [f]	86.7%	86.7%	86.7%	86.7%	86.7%	86.7%	55%	86%
Organization of fuel [g]	pins	pins	pins	pins	pins	pins	pins	pins
Cladding used for fuel [h]	Zirc-2	Zirc-2	Zirc-2	Zirc-2	Zirc-2	Zirc-2	Zirc-2	Zirc-2
Pu/(Pu+U) atom percent	1.51%	1.80%	1.80%	1.80%	2.01%	2.01%	3.03%	3.52%
^{235}U atom percent	0.16%	0.71%	0.71%	0.71%	0.72%	0.72%	0.71%	0.71%
^{238}U atom percent	99.84%	99.29%	99.29%	99.29%	99.28%	99.28%	99.29%	99.29%
^{238}Pu atom percent	-	0.01%	0.01%	0.01%	-	-	0.50%	0.28%
^{239}Pu atom percent	91.41%	91.84%	91.84%	91.84%	81.11%	71.76%	68.18%	75.39%
^{240}Pu atom percent	7.83%	7.76%	7.76%	7.76%	16.54%	23.50%	22.02%	18.10%
^{241}Pu atom percent	0.73%	0.37%	0.37%	0.37%	2.15%	4.08%	7.26%	5.08%
^{242}Pu atom percent	0.03%	0.03%	0.03%	0.03%	0.20%	0.66%	2.04%	1.15%
Plutonium type as given in Table B–1	WG	WG	WG	WG	FG	PG	PG	FG-PG
Shape of lattice [i]	cylinder	rectangle	rectangle	cylinder	cylinder	cylinder	rectangle	cylinder
Pitch of lattice	triangle	square	square	triangle	triangle	triangle	square	triangle
Number of experiments in each set	6	3	3	6	5	6	4	7
Fissile moderator used [j]	H_2O	H_2O	B-H_2O	H_2O	H_2O	H_2O	H_2O	H_2O
Reflector used	H_2O	H_2O	B-H_2O	H_2O	H_2O	H_2O	H_2O	H_2O
Maximum effective bias of experiments in set (Eff-Bias)	-0.0112	-0.0052	-0.0026	-0.0089	-0.0040	-0.0068	-0.0097	-0.0037
Maximum uncertainty of experiments in set (Exp-Uncer)	0.0080	0.0059	0.0045	0.0054	0.0061	0.0065	0.0051	0.0042
Exp-Uncer minus Eff-Bias (WCD)	0.0192	0.0111	0.0071	0.0143	0.0101	0.0133	0.0148	0.0079

[a]MCT = MIX-COMP-THERM.
[b]Codes MCNP (LANL, 1997) and KENO (ORNL, 1995).
[c]ENDF/B-V/IV means cross section set ENDF/B-V for MCNP and cross section set ENDF/B-IV for KENO. JENDL-3.2 is the cross section set for both MCNP and KENO.
[d]Cross section type is either continuous cross sections (cont.) or group cross sections (27grp, 137grp).
[e]Heavy metal is as an oxide.
MOX density given as percent of theoretical density taken as 11.00 g/cm^3.
[g]Pins means organization of MOX is as pellets in fuel pins.
[h]Zirc-2 means Zircaloy-2 cladding.
[i]Cylinder means shape of lattice is a cylinder. Rectangle means shape of lattice is a rectangle.
[j]B-H_2O means borated water as moderator or reflector.
[f]

Table D–2 Important characteristics of lattice experiments with weight percent of Pu/(Pu+U) from 5 percent to 15 percent (from IHECSBE)

Designation for experiments [a]	MCT-003	MCT-003	MCT-012	MCT-012	MCT-012	MCT-012
Facility where experiments conducted	WREC	WREC	Hanford	Hanford	Hanford	Hanford
Computer codes used in evaluations [b]	MCNP	MCNP	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO
Cross section sets used in evaluations [c]	ENDF/B-V	ENDF/B-V	ENDF/B-V	ENDF/B-V	ENDF/B-V	ENDF/B-V
Cross section type [d]	cont	cont	cont/238grp	cont/238grp	cont/238grp	cont/238grp
Fuel compound [e]	oxide	oxide	oxide-poly	oxide-poly	oxide-poly	oxide-poly
Fuel compound form	solid	solid	solid	solid	solid	solid
Density of fuel [f]	94%	94%	N/A	N/A	N/A	N/A
Organization of fuel [g]	pins	pins	cubes, slabs	cubes, slabs	cubes, slabs	cubes, slabs
Cladding used for fuel [h]	Zirc-4	Zirc-4	plastic 471	plastic 471	plastic 471	plastic 471
Pu/(Pu+U) atom percent	6.63%	6.63%	7.60%	7.89%	14.62%	14.62%
^{235}U atom percent	0.71%	0.71%	0.15%	0.15%	0.15%	0.15%
^{238}U atom percent	99.29%	99.29%	99.85%	99.85%	99.85%	99.85%
^{238}Pu atom percent	-	-	0.59%	-	-	-
^{239}Pu atom percent	90.65%	90.65%	67.97%	91.25%	91.42%	91.42%
^{240}Pu atom percent	8.55%	8.55%	22.95%	8.12%	7.97%	7.97%
^{241}Pu atom percent	0.76%	0.76%	5.57%	0.58%	0.57%	0.57%
^{242}Pu atom percent	0.04%	0.04%	2.92%	0.05%	0.04%	0.04%
Plutonium type as given in Table B–1	WG-FG	WG-FG	PG	WG	WG	WG
Shape of lattice [i]	rectangle	rectangle	3D cube	3D cube	3D cube	3D cube
Pitch of lattice	square	square	square	square	square	square
Number of experiments in each set	5	1	6	7	6	3
Fissile moderator used [j]	H_2O	B-H_2O	polystyrene	polystyrene	polystyrene	polystyrene
Reflector used	H_2O	B-H_2O	Plexiglas	Plexiglas	Plexiglas	none
Maximum effective bias of experiments in set (Eff-Bias)	-0.0063	-0.0030	-0.0270	-0.0016	-0.0016	-0.0020
Maximum uncertainty of experiments in set (Exp-Uncer)	0.0071	0.0052	0.0058	0.0036	0.0027	0.0037
Exp-Uncer minus Eff-Bias (WCD)	0.0134	0.0082	0.0328	0.0052	0.0043	0.0057

[a] MCT = MIX-COMP-THERM.
[b] Codes MCNP (LANL, 1997) and KENO (ORNL, 1995).
[c] ENDF/B-V is the cross section set for MCNP and KENO.
[d] Cross section type is either continuous cross sections (cont) or group cross sections (238grp).
[e] Heavy metal is as an oxide. Oxide-poly means mixture of MOX particles and polystyrene pressed into cubes and slabs.
[f] MOX density given as percent of theoretical density taken as 11.00 g/cm^3.
[g] Pins means organization of MOX is as pellets in fuel pins. Cubes, slabs means organization of MOX-polystyrene is as cubes and slabs.
[h] Zirc-4 means Zircaloy-4 cladding. Plastic 471 means cladding is six mil plastic tape MM&M (3M) #471.
[i] Rectangle means shape of lattice is a rectangle. 3D cube means cubes and slabs stacked into the shape of a 3D rectangular cube.
[j] B-H_2O means borated water as moderator or reflector.

Table D–3 Important characteristics of lattice experiments with weight percent of Pu/(Pu+U) greater than 15 percent (from IHECSBE)

Designation for experiments [a]	MCT-001	MCT-011	MCT-012	MCT-012
Facility where experiments conducted	Hanford	Valduc	Hanford	Hanford
Computer codes used in evaluations [b]	MONK	MORET	MCNP/KENO	MCNP/KENO
Cross section sets used in evaluations [c]	UKNDL	JEF2.2	ENDF/B-V	ENDF/B-V
Cross section type [d]	cont	172gp	cont/238grp	cont/238grp
Fuel compound [e]	oxide	oxide	oxide-poly	oxide-poly
Fuel compound form	solid	solid	solid	solid
Density of fuel [f]	89.4%	94.2%	N/A	N/A
Organization of fuel [g]	pins	pins	cubes, slabs	cubes, slabs
Cladding used for fuel [h]	316SS	Z3CND18.12 SS	plastic 471	plastic 471
Pu/(Pu+U) atom percent	19.70%	25.80%	30.00%	30.00%
^{235}U atom percent	0.71%	60.15%	0.15%	0.15%
^{238}U atom percent	99.29%	39.85%	99.85%	99.85%
^{238}Pu atom percent	0.15%	-	-	-
^{239}Pu atom percent	85.54%	89.00%	91.22%	91.22%
^{240}Pu atom percent	11.46%	9.72%	8.13%	8.13%
^{241}Pu atom percent	2.50%	1.21%	0.61%	0.61%
^{242}Pu atom percent	0.35%	0.07%	0.04%	0.04%
Plutonium type as given in Table B–1	FG	WG-FG	WG	WG
Shape of lattice [i]	rectangle	cylinder	3D cube	3D cube
Pitch of lattice	square	triangle	square	square
Number of experiments in each set	4	6	8	3
Fissile moderator used	H_2O	H_2O	polystyrene	polystyrene
Reflector used	H_2O	H_2O	Plexiglas	none
Maximum effective bias of experiments in set (Eff-Bias)	-0.0103	-0.0006	-0.0018	-0.0086
Maximum uncertainty of experiments in set (Exp-Uncer)	0.0025	0.0017	0.0049	0.0052
Exp-Uncer minus Eff-Bias (WCD)	0.0128	0.0023	0.0067	0.0138

a MCT = MIX-COMP-THERM.
b Codes MCNP (LANL, 1997), KENO (ORNL, 1995), MONK, and MORET. MONK is a three-dimensional Monte Carlo radiation transport code that uses point-wise cross sections, developed by A.E.A. Technology of the United Kingdom. MORET is a three-dimensional Monte Carlo criticality code that uses multigroup cross sections, developed by C.E.A. of France.
c ENDF/B-V is the cross section set for MCNP and KENO. UKNDL is the cross section set for MONK. JEF2.2 is the cross section set for MORET.
d Cross section type is either continuous cross sections (cont) or group cross sections (172grp, 238grp).
e Heavy metal is as an oxide. Oxide-poly means mixture of MOX particles and polystyrene pressed into cubes and slabs.
f MOX density given as percent of theoretical density taken as 11.00 g/cm^3.
g Pins means organization of MOX is as pellets in fuel pins. Cubes, slabs means organization of MOX-polystyrene is as cubes and slabs.
h SS means stainless steel cladding. Plastic 471 means cladding is six mil plastic tape MM&M (3M) #471.
i Cylinder means shape of lattice is a cylinder. Rectangle means shape of lattice is a rectangle. 3D cube means cubes and slabs stacked into the shape of a 3D rectangular cube.

Table D–4 Important characteristics of tank experiments with weight percent of Pu/(Pu+U) to 31 percent (from IHECSBE)

Designation for experiments [a]	**MST-001**	**MST-001**	**MST-001**	**MST-001**	**MST-002**	**MST-003**
Facility where experiments conducted	Hanford	Hanford	Hanford	Hanford	Hanford	AWRE
Computer codes used in evaluations [b]	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MONK
Cross section sets used in evaluations [c]	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	UKNDL
Cross section type [d]	cont/27grp	cont/27grp	cont/27grp	cont/27grp	cont/27grp	cont
Fuel compound [e]	nitrate	nitrate	nitrate	nitrate	nitrate	nitrate
Fuel compound form	liquid	liquid	liquid	liquid	liquid	liquid
Density of fuel [f]	1.31–1.68	1.31–1.68	1.31–1.48	1.70	1.09	1.11–1.52
Pu/(Pu+U) atom percent	22%	22%	22%	22%	23%	30.7%
^{235}U atom percent	0.70%	0.70%	0.70%	0.70%	0.70%	0.72%
^{238}U atom percent	99.30%	99.30%	99.30%	99.30%	99.30%	99.28%
^{238}Pu atom percent	0.03%	0.03%	0.03%	0.03%	0.03%	-
^{239}Pu atom percent	91.12%	91.12%	91.12%	91.12%	91.12%	93.95%
^{240}Pu atom percent	8.34%	8.34%	8.34%	8.34%	8.31%	5.63%
^{241}Pu atom percent	0.42%	0.42%	0.42%	0.42%	0.45%	0.42%
^{242}Pu atom percent	0.09%	0.09%	0.09%	0.09%	0.09%	-
Plutonium type as given in Table B–1	WG	WG	WG	WG	WG	WG
Tank fissile liquid is in [g]	N/A	cylinder	cylinder	cylinder	cylinder	slab
Auxiliary tank additional fissile liquid is in [h]	annular	annular	annular	N/A	N/A	N/A
Number of experiments in each set	2	5	2	1	1	10
Fissile moderator used [i]	soln H_2O	soln H_2O	soln H_2O	soln H_2O	soln H_2O	soln H_2O
Reflector used [j]	B_4C-concrete	B_4C-concrete	poly-Cd cover	none	H_2O	H_2O & poly
Maximum effective bias of experiments in set (Eff-Bias)	-0.0101	-0.0164	-0.0028	-0.0068	-0.0020	-0.0038
Maximum uncertainty of experiments in set (Exp-Uncer)	0.0016	0.0016	0.0016	0.0016	0.0024	0.0025
Exp-Uncer minus Eff-Bias (WCD)	0.0117	0.0180	0.0044	0.0084	0.0044	0.0063

[a] MST = MIX-SOL-THERM.
[b] Codes MCNP (LANL, 1997), KENO (ORNL, 1995), and MONK (A.E.A. Technology). MONK is a three-dimensional Monte Carlo radiation transport code that uses point-wise cross sections, developed by A.E.A. Technology of the United Kingdom.
[c] ENDF/B-V/IV means cross section set ENDF/B-V for MCNP and ENDF/B-IV for KENO. UKNDL is cross section set for MONK.
[d] Cross section type is either continuous cross sections (cont) or group cross sections (27grp).
[e] Heavy metal is as a nitrate dissolved in dilute nitric acid solution.
[f] Solution density is in g/ml.
[g] Containers for fissile solution are cylinders or slabs.
[h] Annular tank surrounding central cylindrical tank or just an annular tank.
[i] Soln H_2O means the moderator is the fissile nitrate solution.
[j] B_4C-concrete means borated concrete. Poly-Cd cover means polyethylene reflector coated with Cd.

Table D–5 Important characteristics of tank experiments with weight percent of Pu/(Pu+U) greater than 31 percent (from IHECSBE)

Designation for experiments [a]	MST-004	MST-004	MST-004	MST-005	MST-005	MST-002	MST-001
Facility where experiments conducted	Hanford	Hanford	Hanford	Hanford	Hanford	Hanford	Hanford
Computer codes used in evaluations [b]	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO	MCNP/KENO
Cross section sets used in evaluations [c]	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV	ENDF/B-V/IV
Cross section type [d]	cont/27grp	cont/27grp	cont/27grp	cont/27grp	cont/27grp	cont/27grp	cont/27grp
Fuel compound [e]	nitrate	nitrate	nitrate	nitrate	nitrate	nitrate	nitrate
Fuel compound form	liquid	liquid	liquid	liquid	liquid	liquid	liquid
Density of fuel [f]	1.17–1.67	1.17–1.67	1.17–1.67	1.17–1.67	1.17–1.67	1.05	1.15–1.44
Pu/(Pu+U) atom percent	40%	40%	40%	40%	40%	52%	97%
^{235}U atom percent	0.56%	0.56%	0.56%	0.56%	0.56%	0.70%	2.29%
^{238}U atom percent	99.44%	99.44%	99.44%	99.44%	99.44%	99.30%	97.71%
^{238}Pu atom percent	0.03%	0.03%	0.03%	0.03%	0.03%	0.03%	0.03%
^{239}Pu atom percent	91.12%	91.12%	91.12%	91.12%	91.12%	91.12%	91.57%
^{240}Pu atom percent	8.34%	8.34%	8.34%	8.34%	8.34%	8.34%	7.94%
^{241}Pu atom percent	0.42%	0.42%	0.42%	0.42%	0.42%	0.42%	0.39%
^{242}Pu atom percent	0.09%	0.09%	0.09%	0.09%	0.09%	0.09%	0.07%
Plutonium type as given in Table B–1	WG	WG	WG	WG	WG	WG	WG
Tank fissile liquid is in [g]	cylinder	cylinder	cylinder	slab	slab	cylinder	cylinder
Auxiliary tank additional fissile liquid is in [h]	N/A	N/A	N/A	N/A	N/A	N/A	annular
Number of experiments in each set	3	3	3	3	4	2	3
Fissile moderator used [i]	soln H_2O	soln H_2O	soln H_2O	soln H_2O	soln H_2O	soln H_2O	soln H_2O
Reflector used [j]	none	H_2O	concrete	none	H_2O	H_2O	B_4C-concrete
Maximum effective bias of experiments in set (Eff-Bias)	-0.0060	-0.0048	-0.0024	-0.0114	-0.0026	-0.0020	-0.0032
Maximum uncertainty of experiments in set (Exp-Uncer)	0.0033	0.0033	0.0078	0.0036	0.0037	0.0024	0.0016
Exp-Uncer minus Eff-Bias (WCD)	0.0093	0.0081	0.0102	0.0150	0.0063	0.0044	0.0048

[a] MST = MIX-SOL-THERM.
[b] Codes MCNP (LANL, 1997) and KENO (ORNL, 1995).
[c] ENDF/B-V/IV means ENDF/B-V for MCNP and ENDF/B-IV for KENO.
[d] Cross section type is either continuous cross sections (cont) or group cross sections (27grp).
[e] Heavy metal is as a nitrate dissolved in dilute nitric acid solution.
[f] Solution density is in g/ml.
[g] Containers for fissile solution are cylinders or slabs.
[h] Annular tank surrounding central cylindrical tank.
[i] Soln H_2O means the moderator is the fissile nitrate solution.
[j] B_4C-concrete means borated concrete.

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