<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>ENGINEERING DATA TRANSMITTAL</p> <p>MAY 27 1999</p> </div> <div style="text-align: right;"> <p>Page 1 of 1</p> <p>1. EDT 625119</p> </div> </div>

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Verification and Validation of XSDRNPM Code for Tank Waste Calculations

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Abstract: This validation study demonstrates that the XSDRNPM computer code accurately calculates the infinite neutron multiplication for water-moderated systems of low enriched uranium, plutonium, and iron. Calculations are made on a 200 MHz Bravo MS 5200M personal computer using the SCALE 27-group ENDF/B-IV and 44-group ENDF/B-V cross section libraries. Upper Safety Limits of 0.881 and 0.882 are found for the 27-group and 44-group cross sections, respectively.

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Verification and Validation of XSDRNPM Code for Tank Waste Calculations

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EXECUTIVE SUMMARY

This validation study demonstrates that the XSDRNPM computer code accurately calculates k_{∞} for water-moderated systems of low enriched uranium, plutonium, and iron. XSDRNPM is contained in the Standardized Computer Analysis for Licensing Evaluation (SCALE-4.3) nuclear criticality safety software for use on a personal computer. Calculations are made on a 200 MHz AST Bravo MS 5200M personal computer using the SCALE 27-group ENDF/B-IV and the SCALE 44-group ENDF/B-V cross-section libraries.

An Upper Safety Limit (USL) is determined that defines the upper bounds on k_{eff} for acceptable calculations. The USL incorporates an administrative margin of subcriticality of 0.10, such that an acceptable calculation must not exceed a k_{eff} of 0.90. After taking into account code bias and after subtracting calculational uncertainty at the 95% confidence level, the USL is found to be 0.881 and 0.882 for the SCALE 27-group ENDF/B-IV and 44-group ENDF/B-V cross section libraries, respectively.

The range of applicability for XSDRNPM calculations is defined by: (1) uranium of any ^{235}U enrichment; (2) plutonium containing up to 20 wt% ^{240}Pu ; (3) iron in any proportion; (4) an energy for average lethargy of neutrons causing fissioning (AEF) between 0.029 and 0.344 eV; and (5) geometric configurations for which neutron leakage is negligible. When the hydrogen-to-fissile atom (H/X) ratio falls between 125 and 3694, a system is assured of having an AEF within the range of applicability. Neutron leakage is negligible when the smallest dimension is large enough such that the neutron multiplication constant (k_{eff}) is indistinguishable from the neutron multiplication constant for an unlimited volume (k_{∞}).

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LIST OF TERMS

AEF	energy of the average lethargy causing fission
AEG	average energy group causing fission
cm	centimeter
CSAS	criticality safety control sequence
CSRL	criticality safety reference library
Fe	iron
Fe/HM	mass ratio of iron to heavy metal
g	grams
H/X	hydrogen-to-fissile atom ratio
HM	heavy metal
k_{eff}	effective multiplication factor
k_{∞}	infinite multiplication factor
L	liter
LTB	lower tolerance band
LWR	light water reactor
N/A	not applicable
PCTR	Physical Constants Test Reactor
RSICC	Radiation Shielding Information Computational Center
TWRS	Tank Waste Remediation Systems
USL	upper safety limit
wt%	weight percent

1.0 INTRODUCTION

This report presents the results of a validation study performed to: (1) demonstrate that the XSDRNPM (Greene and Petrie 1995) computer code may be used to accurately calculate k_{∞} for water-moderated systems of enriched uranium, plutonium and iron; (2) establish the subcritical margin in the form of an Upper Safety Limit (USL) for calculations being performed and; (3) clearly define the range of applicability for the validation and subcritical margins.

The XSDRNPM computer code is used to calculate k_{∞} for configurations of tank waste in long-term storage at the Hanford Site tank farms. Tank waste is characterized by low concentrations of plutonium mixed with low enriched uranium and a wide variety of neutron absorbing materials. The neutron absorber of greatest interest is iron because of its ability to coprecipitate and to agglomerate with plutonium and uranium.

The sludge type of primary interest in this validation study is K Basin sludge. This sludge is to be removed from fuel storage basins and is composed of irradiated uranium from N Reactor fuel elements mixed with basin debris. The plutonium produced by irradiation remains in the uranium. Before disposal at tank farms, iron will be added to provide neutron absorption to ensure compatibility with the technical basis for criticality safety at Hanford tank farms. The calculational model for K Basin sludge consists of a homogeneous mixture of low enriched uranium, plutonium, iron, and water.

This validation study demonstrates that the XSDRNPM computer code accurately calculates homogenous systems of low enriched uranium and low concentrations of plutonium for simple geometries. The version of XSDRNPM being validated is contained in Version 4.3 of the Standardized Computer Analysis for Licensing Evaluation (SCALE-4.3) nuclear criticality safety software for use on a personal computer (ORNL 1995a). Calculations are made on a 200 MHz AST Bravo MS 5200M personal computer. Validation is performed for both the SCALE 27-group ENDF/B-IV and the SCALE 44-group ENDF/B-V cross-section libraries.

Guide to Verification and Validation of the SCALE-4 Criticality Safety Software, NUREG/CR-6483, by Emmett and Jordan (1996) is a primary reference for the method of validation used and is the source of many of the experimental benchmarks calculated. Emmett and Jordan (1996) performed validation calculations for both XSDRNPM and KENO V.a (Petrie and Landers 1995) using the SCALE 4.2 code system with the 27-group ENDF/B-IV cross-section library. They performed calculations for ^{233}U , ^{235}U , ^{239}Pu and ^{240}Pu systems over a broad range of geometries and fuel forms. A subset of these benchmark problems is used as the basis for this validation report.

XSDRNPM calculations for 46 benchmark experiments were performed for this validation. These cases are categorized according to the type of fissile material, and subdivided according to the degree of moderation. Systems most similar to K Basin sludge are those thermal systems with uranium of low enrichment and with a high water content.

An USL is defined as the upper bounds on k_{eff} for acceptable calculations. The USL incorporates an administrative margin of subcriticality, any code bias identified in the validation

process, and calculational uncertainties at the 95 percent confidence level. A primary objective of this validation study is the determination of a USL for the systems being modeled.

Based on evaluation of thermal ^{235}U and Pu systems, subgroupings of these systems, and systems mixed with iron, the USL (with a 0.10 administrative margin) is found to be 0.881 for the 27-group cross section set and 0.882 for the 44-group cross section set. These USLs will be valid for XSDRNPM calculations provided the energy of the average lethargy causing fission (AEF) is in the range from 0.029 to 0.344 eV. A configuration whose hydrogen-to-fissile atom ratio (H/X) falls between 125 and 3694 is assured of having an AEF within this range of applicability. These values for AEF and H/X define the range of applicability of this validation effort.

2.0 SCALE CODE PACKAGE DESCRIPTION

SCALE 4.3 is a collection of modules designed to perform criticality, shielding, and thermal calculations. SCALE 4.3 was obtained from the Radiation Shielding Information Center (RSICC). Calculations were made using compiled executables. The criticality modules are being validated in this report. Functional modules may be run individually or called in a prescribed sequence, designated as a criticality safety control sequence (CSAS). A control sequence is also referred to as a control module. Control sequences that call XSDRNPM end in the letter X. When only a XSDRNPM calculation is needed, the CSAS1X sequence is run.

The functional modules, BONAMI (Greene 1995), NITAWL-II (Greene et al. 1995), and XSDRNPM are used in the CSAS1X sequence. Emmett and Jordan provide the following descriptions of these modules:

- BONAMI performs resonance shielding calculations using the Bondarenko shielding factor method. BONAMI reads an AMPX (Greene et al. 1992) master format cross-section library and applies Bondarenko corrections to produce a Bondarenko-corrected master format library. No data processing is performed in BONAMI for the 27-group cross-section library, although it is used with the 44-group library.
- NITAWL-II applies the Nordheim Integral Treatment to perform neutron cross-section processing in the resolved resonance range for ENDF/B resonance parameter data. This technique numerically integrates ENDF/B resonance parameters using a calculated flux distribution across each resonance and subsequent weighting of the cross-section to the desired broad group structure. NITAWL-II completes the processing of the problem-dependent master library from BONAMI. NITAWL-II assembles the group-to-group transfer arrays from the elastic and inelastic scattering components and produces a problem-dependent AMPX working format cross-section library for KENO V.a. The analyst specifies resonance parameters based on two options. The first option is for a homogeneous medium in which the resonance region is treated as if the fissile material were in an infinite homogeneous media. The second option is for the fissile material to be treated as a finite lump.
- XSDRNPM is a general purpose, 1-D discrete-ordinates code used for several purposes in SCALE. In the CSAS1X criticality sequence, XSDRNPM is used to solve the 1-D Boltzmann equation in slab, cylindrical, or spherical geometry. XSDRNPM can also be run as a standalone code.

The CSAS1X control sequence prepares input for the 3 functional modules described above. User-specified data include the cross-section library, specifications for mixtures, information for resonance region cross-section processing of nuclides (size, geometry, and temperature), and model-specific geometry for the XSDRNPM calculation. Physical and neutronics information not supplied explicitly, but required by the functional modules (such as theoretical density, molecular weights, average resonance region background cross sections), are supplied by the Standard Composition Library or calculated by the Materials Information Processor (Emmett and Jordan 1996).

The 27-group and 44-group cross section libraries are broad-group libraries collapsed from the 218-group Criticality Safety Reference Library (CSRL) and from the 238-group Library to Analyze Radioactive Waste (LAW), respectively. The 27- and 218-group libraries are based on ENDF/B-IV data, and the 44- and 238-group libraries are based on ENDF/B-V data (ORNL 1995a).

3.0 CODE VERIFICATION FOR AST BRAVO 5200M PC

Software verification is the assurance that a computer code correctly performs the operations intended. Verification is usually accomplished by comparing calculated results to known results (e.g. hand calculations, analytical solutions or approximations, or baseline calculations certified by the code developers). Verification demonstrates that software has been properly coded, installed on a computer, and performs the intended functions.

Emmett and Jordan (1996) (NUREG/CR-6483) describe more than 600 benchmark experiment calculations used to provide a comprehensive validation of SCALE-4.2 Criticality Safety Software using the 27-group ENDF/B-IV library. Benchmark experiment descriptions were compiled from three reports: ORNL/CSD/TM-238 (Jordan et al. 1986), ORNL/TM-12374 (Primm 1993), and ORNL/TM-12460 (DeHart and Bowman 1994).

The verification described in this report was performed by executing 46 of the Emmett and Jordan (1996) benchmark calculations on the AST Bravo 5200M PC. Results were compared with NUREG/CR-6483 (Emmett and Jordan 1996) values. The intent of the verification process is to verify that the codes were successfully installed. The acceptance criterion for verification was to execute the test problems with less than 0.5 percent discrepancies in the calculated k_{∞} results.

Table 3-1 compares results calculated on the AST Bravo 5200M PC (SCALE 4.3 with the 27-group library) with values from NUREG/CR 6483 (SCALE 4.2 with the 27-group library). The calculated values were found to be in very close agreement with the corresponding NUREG/CR-6483 values. In 13 out of 46 cases, the values agreed to within 0.00001 (0.001percent). In 41 cases agreement is within 0.00050 (0.049 percent). Three cases (2110_07, zpr67, and zpr66a) were found to differ by more than 0.00200 (0.2 percent). The largest difference for any case was found to be 0.00290 (0.283 percent). The exact reason for the differences in results is unknown, but it is thought to result from differences between SCALE-4.2 and SCALE-4.3. The acceptance criterion of 0.5% is satisfied in all cases. Therefore, the conclusion is that the modules are installed correctly.

Figures 3-1 through 3-7 list the banner information printed by SCALE-PC version 4.3 for execution of CSAS, BONAMI, NITAWL, XSDRNP, and the libraries, respectively. Banners contained the statement: "This is not a SCALE-PC configuration controlled code." Normally, this statement is not printed. It was printed for this evaluation because the location of executable files on the hard drive did not match the location indicated in the quality assurance table (i.e., file QATABLE). This discrepancy developed when program files were moved from the D drive to the C drive without updating QATABLE. Cases run with the correct drive specified in QATABLE did not print this statement. This discrepancy does not affect calculations made by the codes.

Table 3-1. Verification Calculations. (2 sheets)

Case	NUREG/CR-6483 ¹ k_{∞}	AST Bravo ² k_{∞}	Absolute Difference	Percent Difference
111_20	1.01417	1.01400	0.00017	0.017
111_25	1.02694	1.02686	0.00008	0.008
1727_01	0.96717	0.96713	0.00004	0.004
1727_02	0.98106	0.98107	0.00001	0.001
1727_03	0.97929	0.97928	0.00001	0.001
1727_04	0.97601	0.97600	0.00001	0.001
1727_05	0.97674	0.97669	0.00005	0.005
1727_06	0.97641	0.97634	0.00007	0.007
1727_07	0.99629	0.99619	0.00010	0.010
1727_08	0.98401	0.98395	0.00006	0.006
1727_09	1.00709	1.00800	0.00091	0.090
1727_10	1.00112	1.00113	0.00001	0.001
1727_14	0.97630	0.97626	0.00004	0.004
1727_15	0.98259	0.98256	0.00003	0.003
2109_25	1.01055	1.01053	0.00002	0.002
2110_01	1.00486	1.00487	0.00001	0.001
2110_02	1.01617	1.01567	0.00050	0.049
2110_03	1.01669	1.01722	0.00053	0.052
2110_04	1.01852	1.01751	0.00101	0.099
2110_07	1.01999	1.01712	0.00287	0.281
2110_30	1.01804	1.01845	0.00041	0.040
2110_32	1.01618	1.01653	0.00035	0.034
BAPL1	1.00883	1.00928	0.00045	0.045
BAPL2	1.01266	1.01302	0.00036	0.036
BAPL3	1.01471	1.01498	0.00027	0.027
BIG10	1.00153	1.00153	0.00000	0.000
FLAT25	1.00885	1.00885	0.00000	0.000
GODIVA	1.00622	1.00622	0.00000	0.000
H2OX1	1.00869	1.00875	0.00006	0.006
HI240R	1.00417	1.00435	0.00018	0.018
JEZB23	0.96475	0.96475	0.00000	0.000
ORNL1	0.99804	0.99832	0.00028	0.028
ORNL10	0.99592	0.99592	0.00000	0.000
ORNL2	0.99788	0.99788	0.00000	0.000
ORNL3	0.99492	0.99492	0.00000	0.000
ORNL4	0.99644	0.99644	0.00000	0.000

Table 3-1. Verification Calculations. (2 sheets)

Case	NUREG/CR-6483 ¹ k_{∞}	AST Bravo ² k_{∞}	Absolute Difference	Percent Difference
PNL3	1.00057	1.00059	0.00002	0.002
PNL6B	1.01678	1.01657	0.00021	0.021
TRX1	1.01237	1.01341	0.00104	0.103
TRX2	1.01804	1.01868	0.00064	0.063
UH3NI	1.06144	1.06137	0.00007	0.007
UH3UR	1.02171	1.02183	0.00012	0.012
ZPR311	1.00693	1.00688	0.00005	0.005
ZPR312	1.01285	1.01261	0.00024	0.024
ZPR66A	1.01792	1.01554	0.00238	0.234
ZPR67	1.02638	1.02348	0.00290	0.283
Average			0.00036	0.035
Maximum			0.00290	0.283

Note: ¹Emmett and Jordan (1996), calculations performed using SCALE 4.2.

²TWRS calculations performed using SCALE 4.3.

Figure 3-1. Banner Printed by SCALE-PC Version 4.3 for CSAS.

```

PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:          SCALE-PC VERSION:    4.3
PROGRAM:              CSAS
CREATION DATE:        3-08-96
VOLUME:               CROOT
LIBRARY:              C:\SCALE43\EXE
THIS IS NOT A SCALE-PC CONFIGURATION CONTROLLED CODE1

```

¹This is printed because the hard drive, where files are stored (i.e., drive C), does not match the drive designated shown in the quality assurance tables (i.e., drive D). This discrepancy does not affect the calculations.

Figure 3-2. Banner Printed by SCALE-PC Version 4.3 for BONAMI

```

PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:          SCALE-PC VERSION:    4.3
PROGRAM:              0000081 or BONAMI
CREATION DATE:        9-15-95
VOLUME:               CROOT
LIBRARY:              C:\SCALE43\EXE
THIS IS NOT A SCALE-PC CONFIGURATION CONTROLLED CODE2

```

¹Numeric identifier used when executed through CSAS, alphabetic identifier used when executed individually.

²See note for Figure 3-1.

Figure 3-3. Banner Printed by SCALE-PC Version 4.3 for NITAWL.

```

PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:          SCALE-PC VERSION:    4.3
PROGRAM:              0000021 or NITAWL
CREATION DATE:        9-28-95
VOLUME:               CROOT
LIBRARY:              C:\SCALE43\EXE
THIS IS NOT A SCALE-PC CONFIGURATION CONTROLLED CODE2

```

¹Numeric identifier used when executed through CSAS, alphabetic identifier used when executed individually.

²See note for Figure 3-1.

Figure 3-4. Banner Printed by SCALE-PC Version 4.3 for XSDRNPM .

```

PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:          SCALE-PC VERSION:      4.3
PROGRAM:              0000011 or XSDRN
CREATION DATE:        9-28-95
VOLUME:               CROOT
LIBRARY:              C:\SCALE43\EXE
THIS IS NOT A SCALE-PC CONFIGURATION CONTROLLED CODE2

```

¹Numeric identifier used when executed through CSAS, alphabetic identifier used when executed individually.

²See note for Figure 3-1.

Figure 3-5. Banner Printed by SCALE-PC Version 4.3 for Standard Composition Library.

STANDARD COMPOSITION LIBRARY DATA

```

UNIT NUMBER:      89
DATASET NAME:     C:\scale43\DATALIB\FT89F001
LIBRARY TITLE:    SCALE-4 STANDARD COMPOSITION LIBRARY
                  637 STANDARD COMPOSITIONS, 490 NUCLIDES
                  90 ELEMENTS WITH VARIABLE ISOTOPIC
                  DISTRIBUTIONS
CREATION DATE:    6/30/95

```

Figure 3-6. Banner Printed by SCALE-PC Version 4.3 for 27-Group Cross Section Library.

CROSS SECTION LIBRARY DATA

```

UNIT NUMBER:      82
DATASET NAME:     C:\scale43\DATALIB\FT82F001
LIBRARY TITLE:    SCALE 4.2 - 27 GROUP NEUTRON GROUP LIBRARY
                  BASED ON ENDF-B VERSION 4 DATA
                  COMPILED FOR NRC:      1/27/89
                  LAST UPDATED:          8/12/94
                  L. M. PETRIE - ORNL

```

Figure 3-7. Banner Printed by SCALE-PC Version 4.3 for 44-Group Cross Section Library.

CROSS SECTION LIBRARY DATA

UNIT NUMBER: 83
DATASET NAME: C:\scale43\DATA\LIB\FT83F001
LIBRARY TITLE: scale 4.3 – 44 neutron group library
based on endf-b version 5 data
collapsed with a light water reactor cell flux spectrum from 238
groups
compiled for nrc: 9/01/94
last updated: 5/14/96
m. d. dehart & l. m. petrie nuclear eng. appl. - cped - ornl

4.0 UPPER SAFETY LIMIT

Software validation is the assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended. This is usually accomplished by comparing code results to either physical data or a validated code designed to perform the same type of analysis. Validation is the process of demonstrating that the software predicts "correct" results for the "systems for which it is intended." The validation process uses critical experiment models covering the applicable range of system parameters.

4.1 REQUIREMENTS TO ESTABLISH SUBCRITICALITY

To establish that a system or process will be subcritical under all normal and credible abnormal conditions, it is necessary to establish acceptable subcritical limits. DOE Standard 3007-93, *Guidelines for Preparing Criticality Safety Evaluations at DOE Non-Reactor Facilities*, (DOE 1993) lists four acceptable methods for establishing subcritical limits:

- By reference to national standards that present subcritical limits.
- By reference to widely accepted handbooks of subcritical limits.
- By reference to experiments with appropriate adjustments to ensure subcriticality when the uncertainties of parameters reported in the experiment documentation are considered.
- By validated calculational techniques.

Hanford Site requirements for validation of analysis methods are found in HNF-PRO-539, *Criticality Safety Evaluations* (FDH 1997b). A code used for criticality safety evaluation is required to be appropriate for the complexity of the problem, be validated, and be identified by code version and date last modified. In addition, each neutron cross section set used for calculations must be properly identified and must be validated in conjunction with validation of the criticality code. The analyst using the code to perform criticality safety calculations must demonstrate sufficient familiarity with the code and the cross section libraries used. The validation report must show comparison with known critical and/or subcritical systems.

4.2 CRITERIA FOR SUBCRITICALITY

American National Standard ANSI/ANS-8.1 (ANS 1983) requires a determination of the calculational bias by "correlating the results of criticality experiments with results obtained for these same systems by the method being validated." The analyst shall use "sufficient correlation to determine if major changes in the bias can occur over the range of variables in the operation being analyzed. Where the extrapolation is large, supplement the method with other calculation methods to provide a better estimate of the bias in the extended area."

American National Standard ANSI/ANS-8.17 (ANS 1994), Section 5.1, provides the following criteria to establish subcriticality:

Where methods of analysis are used to predict neutron multiplication factors, the calculated multiplication factor, k_s , shall be equal to or less than an established allowable neutron multiplication factor:

$$k_s \leq k_c - \Delta k_s - \Delta k_c - \Delta k_m \quad (\text{Eq. 1})$$

where

- k_s = the calculated allowable maximum multiplication factor, k_{eff} , of the system being evaluated for all normal or credible abnormal conditions or events.
- k_c = the mean k_{eff} that results from the calculation of benchmark criticality experiments using a particular calculational method. If the calculated k_{eff} s for the criticality experiments exhibit a trend with a parameter, then k_c shall be determined by extrapolation on the basis of a best fit to the calculated values. The criticality experiments used as benchmarks in computing k_c should have physical compositions, configurations, and nuclear characteristics (including reflectors) similar to those of the system being evaluated.
- Δk_s = uncertainty in the value of k_s
- Δk_c = uncertainty in the value of k_c
- Δk_m = an arbitrary administrative margin to ensure the subcriticality of k_s .

Sources of uncertainty which determine Δk_s include:

- (a) statistical and/or convergence uncertainties
- (b) material and fabrication tolerances
- (c) limitations in the geometric and/or material representations used.

Sources of uncertainty which determine Δk_c include:

- (a) uncertainties in critical experiments
- (b) statistical and/or convergence uncertainties in the computation
- (c) extrapolation outside of the range of experimental data
- (d) limitations in the geometric and/or material representations used.

HNF-PRO-537 (FDH 1997a) establishes the following minimum subcritical limit criteria:

- If reliable experimental data are available for closely similar systems and adequate calculational techniques exist for relatively small extrapolations of the data, the k_{eff} of spheres and cylinders must not exceed 0.98 and the k_{eff} of slabs must not exceed 0.97. The k_{eff} of complicated geometries must not exceed 0.95.

- If limited experimental data exist for a similar system and relatively large but reasonable interpolations or extrapolations are necessary, the calculated k_{eff} of the system must not exceed 0.95.
- If no applicable experimental data are available, such that calculations must be based on very large extrapolations from experimental data, the calculated k_{eff} of the system must not exceed 0.90.

Subcritical limits will be established for evaluation of K Basin sludge in the Hanford Site Tank Farms by validating the calculational techniques.

4.3 THE UPPER SAFETY LIMIT

An assurance of subcriticality requires the determination of an acceptable margin based on known biases and uncertainties. The Upper Safety Limit (USL) is defined as the upper bounds for an acceptable calculation.

Critical benchmark experiments used to determine calculational bias (β) should be similar in composition, configuration, and nuclear characteristics to the system under examination. The range of applicability may be extended beyond the range of conditions represented by the benchmark experiments by extrapolating the trends established for the bias. For critical systems β is related to k_c as follows:

$$\beta = k_c - 1 \quad (\text{Eq. 2})$$

$$\Delta\beta = \Delta k_c. \quad (\text{Eq. 3})$$

Using this definition of bias, the condition for subcriticality is rewritten as:

$$k_s + \Delta k_s \leq 1 - \Delta k_m + \beta - \Delta\beta \quad (\text{Eq. 4})$$

A system is acceptably subcritical if a calculated k_{eff} plus calculational uncertainties lies at or below the USL.

$$k_s + \Delta k_s \leq \text{USL} \quad (\text{Eq. 5})$$

The USL can be written as:

$$\text{USL} = 1 - \Delta k_m + \beta - \Delta\beta. \quad (\text{Eq. 6})$$

Bias is negative if $k_c < 1$ and positive if $k_c > 1$. For conservatism a positive bias is set equal to zero for the purpose of defining the USL. $\Delta\beta$ is determined at the 95 percent confidence level.

The USL takes into account bias, uncertainties, and administrative and/or statistical margins such that the calculated configuration will be subcritical with a high degree of confidence.

β is related to system parameters and may not be constant over the range of a parameter of interest. If k_{eff} s for benchmark experiments vary as a function of a system parameter, such as enrichment or degree of moderation, then β can be determined from a best fit as a function of the parameter upon which it is dependent. Extrapolation outside the range of validation must take into account trends in the bias.

Both $\Delta\beta$ and β can vary with a given parameter, and the USL is typically expressed as a function of the parameter. The most important system parameter which affect bias is the degree of moderation of the neutrons. This parameter can be expressed in several different ways, such as the neutron energy of the average lethargy causing fission (AEF), average energy group (AEG), or hydrogen-to-fissile atom (H/X) ratio.

Generally, the "bias" can be broken down into components caused by system modeling error, code modeling inaccuracies, cross-sectional inaccuracies, and so forth. Biases associated with individual inaccuracies are usually combined into a total bias to represent the combined effect from all sources that prevent code and cross-sections from calculating the experimental value of k_{eff} .

One or two calculations are insufficient to determine calculational bias. In practice, it is necessary to determine the "average bias" for a group of experiments. A statistical analysis of the variation of biases around this average value is used to establish an uncertainty associated with the bias value when it is applied to a future calculation of a similar critical system. The lower limit of this band of uncertainty establishes an upper bound for which a future calculation of k_{eff} for a similar critical system can be considered subcritical with a high degree of confidence.

Lichtenwalter et al. (1997) discusses two methods of determining the USL from the bias and uncertainties associated with calculations. The first method applies a statistical calculation of the bias and its uncertainty plus an administrative margin to a linear fit of critical experimental benchmark data. The second method applies a statistical calculation to determine a combined lower confidence band and subcritical margin. Both methods assume that the distribution of data points is normal. The following discussion of each method follows Lichtenwalter et al. (1997) very closely, and is based on equations and techniques described in Dyer et al. (1991), Easter (1985), Bowden and Graybill (1966), Johnson (1968), and Cain (1995).

4.3.1 Method 1: Confidence Band with Administrative Margin

USL Method 1 applies a statistical calculation of the bias and its uncertainty plus an administrative margin to a linear fit of critical experiment benchmark data. A lower confidence band is statistically determined based on the existing data and a specified level of confidence. The width of the confidence band, W , is strongly influenced by the standard deviation in the data and the confidence level desired. This confidence band, accounts for uncertainties in the experiments, the calculational approach, and in calculational data (e.g., cross sections), and is therefore a statistical basis for $\Delta\beta$, the uncertainty in the value of β . When γ_1 is the specified margin of confidence, W is defined for a confidence level of $(1-\gamma_1)$ using the relationship

$$W = \max\{w(x) | x_{\min}, x_{\max}\}, \quad (\text{Eq. 7})$$

where $w(x)$ is the confidence band on the linear regression for a "single future calculation" expressed as

$$w(x) = t_{1-\gamma, s_p} \left[1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1,n} (x_i - \bar{x})^2} \right]^{\frac{1}{2}}, \quad (\text{Eq. 8})$$

and

n = the number of critical calculations used in establishing $k_c(x)$

$t_{1-\gamma,}$ = the Student - t distribution for $1 - \gamma$ and $n - 2$ degrees of freedom

$\bar{x}$ = the mean value of parameter x in the set of calculations

s_p = the pooled standard deviation for the set of criticality calculations.

For simplicity, it is desirable to obtain a constant width margin. Hence, for conservatism, the confidence band width W is defined as the maximum of $(w(x_{min}), w(x_{max}))$, where x_{min} and x_{max} are the minimum and maximum values of the independent parameter x , respectively. Typically, W is determined at a 95 percent confidence level.

The pooled standard deviation is obtained from the pooled variance $(S_p = \sqrt{S_p^2})$, where s_p is given as:

$$S_p^2 = S_{k(x)}^2 + S_w^2 \quad (\text{Eq. 9})$$

where $S_{k(x)}^2$ is the variance (or mean square error) of the regression fit, and is given by:

$$S_{k(x)}^2 = \frac{1}{(n-2)} \left[\sum_{i=1,n} (k_i - \bar{k})^2 - \frac{\left\{ \sum_{i=1,n} (x_i - \bar{x})(k_i - \bar{k}) \right\}^2}{\sum_{i=1,n} (x_i - \bar{x})^2} \right] \quad (\text{Eq. 10})$$

and S_w^2 is the within-variance of the data:

$$s_w^2 = \frac{1}{n} \sum_{i=1,n} \sigma_i^2 \quad (\text{Eq. 11})$$

where σ_i is the standard deviation associated with the convergence of k_i for a Monte Carlo calculation. It is recommended that the individual standard deviations for Monte Carlo

calculations be roughly uniform in value for the best results. For deterministic codes that do not have a standard deviation associated with a computed value of k , the standard deviation is zero.

In USL Method 1, Δk_m is an arbitrary administrative value. HNF-PRO-537 (FDH 1997a) requires the selection of a minimum of Δk_m to depend on the similarity and adequacy of the benchmark data. Based on this criterion, Δk_m may range from 0.02 to 0.10 compared with the configuration being evaluated.

Having determined the constant W and substituting for $\Delta\beta$ in Equation 6, the expression for the USL based on Method 1 may be written as:

$$USL_1(x) = 1.0 - \Delta k_m - W + \beta(x). \quad (\text{Eq. 12})$$

4.3.2 Method 2: Single-Sided Uniform Width Closed Interval

USL Method 2, sometimes referred to as a lower tolerance band (LTB) method, applies statistical techniques to determine a combined lower confidence band plus subcritical margin. This differs from USL Method 1 in which Δk_m and $\Delta\beta$ are determined independently.

The purpose of this method is to determine a uniform tolerance band over a specified closed interval for a linear least-squares model. The level of confidence in the limit being calculated is α and is typically in the range from 0.90 to 0.999.

The USL based on Method 2 is defined as

$$USL_2(x) = 1.0 - (C_{\alpha/P} \cdot s_p) + \beta(x), \quad (\text{Eq. 13})$$

where s_p is the pooled variance of k_c described earlier. The term $C_{\alpha/P} \cdot s_p$ provides a band for which there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band. For example, a $C_{95/99.5}$ multiplier produces a USL for which there is a 95 percent confidence that 995 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the USL.

The analysis is over the closed interval from $x = a$ to $x = b$. $C_{\alpha/P}$ is calculated according to the following equations:

$$C_{\alpha/P} = C^* + z_p \cdot \sqrt{\frac{n-2}{\chi^2}}, \quad (\text{Eq. 14})$$

where

z_p is the Student t statistic depending on n and P

χ^2 is the chi square distribution, a function of $n-2$ and a .

C^* is determined using the following parameters:

$$g = \sqrt{\frac{1}{n} + \frac{(a - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (\text{Eq. 15})$$

$$h = \sqrt{\frac{1}{n} + \frac{(b - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (\text{Eq. 16})$$

$$\rho = \frac{1}{gh} \cdot \left\{ \frac{1}{n} + \frac{(a - \bar{x})(b - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \right\} \quad (\text{Eq. 17})$$

$$A = \frac{g}{h} \quad (\text{Eq. 18})$$

For values of A between 0.5 and 1.5 ($0.5 \leq A \leq 1.5$) the value of ρ determined from the above formula is used to obtain a value for D from Table 3 in Bowden (1966), and

$$C^* = D \cdot g. \quad (\text{Eq. 19})$$

When A is outside the above range, A is replaced by $1/A$ for the determination of D , and C^* is given by

$$C^* = D \cdot h. \quad (\text{Eq. 20})$$

This approach provides a statistically based subcritical margin, Δk_m , which can be determined as the difference $(C_{\alpha/P} \cdot s_p) - W$. In criticality safety applications, such a statistically determined approach generally serves to illustrate the adequacy of the administrative margin. It is recommended that Method 2 be applied in tandem with Method 1 to verify that the administrative margin is conservative relative to a purely statistical basis. This concurrent application of Method 2 is especially important when a limited number of data points are used in the determination of $k_c(x)$, or when the calculated values have a large standard deviation. In these cases, a larger value of the statistically based subcritical margin may indicate the need for a larger administrative margin.

Lichtenwalter et al. (1997) documents a computer program called USLSTATS that was developed to perform the required statistical analysis and calculate USLs based on Methods 1 and 2 (see Appendix A).

4.4 APPLICATION OF THE UPPER SAFETY LIMIT

The equations USL for Methods 1 and 2 (Equations 12 and 13) represent an upper bound to assure subcriticality for a given configuration when the calculated k_{eff} plus uncertainty for the configuration is less than the USL. An USL may be determined as a function of any one of a number of independent parameters. When more than one USL is determined, the subcritical limit is chosen as the smallest from among the possible USLs.

For a given parameter, the USL is valid over the range of that parameter in the set of calculations used to determine the USL. However, ANSI/ANS-8.1 (ANS 1983) allows the range of applicability to be extended beyond this range by extrapolating the trends established for the bias. No precise guidelines are specified for the limits of extrapolation. Thus, engineering judgement should be applied when extrapolating beyond the range of the parameter bounds.

5.0 VALIDATION

A criticality safety evaluation of long-term storage in large underground tanks of sludge removed from the floor of large water storage basins located in the 100-K Areas on the Hanford Site has been undertaken. For the purpose of calculating k_{∞} , a model of K Basin sludge was developed for input into the XSDRNPM code. This sludge model is composed of irradiated low enriched uranium mixed with iron and water. Plutonium generated during irradiation of uranium is assumed to remain associated with the uranium. The highest ^{235}U enrichment possible in sludge uranium is 1.25 wt%, the enrichment in unirradiated uranium. During irradiation the ^{235}U enrichment decreased, and much of the actual uranium in this sludge is depleted with ^{235}U content as low as 0.60 wt%. However during the irradiation process the plutonium content increased to as much as 0.30 wt% of the uranium. Evaluation of this sludge requires that calculations be made over the range of possible combinations of these waste components.

The plutonium used in the sludge model is composed of ^{239}Pu and ^{240}Pu . Although other isotopes are present, they are of lesser importance to criticality safety and are not taken into account explicitly in calculations. Isotopes not specifically identified in the model are treated as if they were ^{239}Pu or ^{240}Pu . The ^{240}Pu content might be as high as 16 wt% of the plutonium.

Iron is added to sludge to ensure long term chemical compatibility and subcriticality. The iron content is specified in terms of the ratio of its mass to the mass of uranium (i.e., the Fe/U mass ratio), and this ratio is expected to exceed 0.70. This means that the Fe/Pu and the Fe/ ^{235}U mass ratios will exceed 200. No restriction is placed upon the water content. Although calculation of k_{∞} is made over the entire range of possible water concentration, the configuration of interest to criticality safety is that which results in the largest k_{∞} .

Basically, tank wastes modeled in this validation are characterized by low concentration of plutonium mixed with low enriched uranium and with iron as a neutron absorbing material. This section describes previously published benchmarking results and the results from current TWRS (AST Bravo 5200M PC) benchmarking calculations. Experiments are chosen for calculation based upon their possessing isotopes characteristic of tank waste and upon other physical similarities.

5.1 PREVIOUS VALIDATIONS

Several documents providing detailed guidance for the validation of the SCALE code system and the validation of SCALE for general use have been published. This section presents results from two such reports for benchmark experiments applicable to this validation effort.

5.1.1 Results Reported in NUREG/CR-6483

Emmett and Jordan (1996) describe more than 600 benchmark experiment calculations used to provide a comprehensive validation of the SCALE-4 criticality safety software. This includes both KENO V.a (Petrie and Landers 1995) and XSDRNPM. The CSAS criticality sequences

and the SCALE 27-group library were used to calculate k_{eff} over broad ranges of ^{233}U , ^{235}U , and ^{239}Pu critical systems. Of these experiments, about 70 were also calculated using XSDRNPM.

These critical experiment validation models were classified as follows:

1. Experiments from Jordan et al. (1986) that cover a broad range of geometry, fissile fuel mixture, moderator, and reflector combinations.
 - a. Low-enriched ^{235}U systems.
 - b. Primarily homogeneous water-moderated single units and arrays of large units. These include arrays of large low-enriched uranium metal billets moderated and reflected by water.
 - c. Models for highly enriched ^{235}U systems.
 - d. ^{233}U systems.
2. Experiments from Primm (1993) that include a harder spectra over a broad range of fissile materials and materials of construction.
 - a. ^{233}U metal systems, water-moderated systems at various concentrations, and arrays of large units.
 - b. Highly enriched ^{235}U systems. Highly thermal systems are excluded in order to validate harder thermal, epithermal, and fast systems.
 - c. ^{239}Pu systems. These include systems with variable ^{240}Pu content as well as systems with a range of fissile material form geometry and moderation level. Several arrays of large units are included.
3. Benchmark experiments from DeHart and Bowman (1994):
 - a. Fast and thermal systems. These include ^{233}U , ^{235}U , and ^{239}Pu unreflected and water- and metal-reflected systems, graphite-moderated systems, and UH_3 systems.
 - b. Thermal systems. These include highly enriched ^{235}U water-moderated systems, low-enriched ^{235}U lattices, and water-moderated ^{239}Pu systems.
 - c. Low-enriched light-water-reactor (LWR) reactor lattices. Both UO_2 and mixed-oxide UO_2 - PuO_2 lattices are included.
 - d. Fast-reactor mixed-oxide lattices and homogeneous ^{235}U systems.

The large number and variety of critical experiments included by Emmett and Jordan (1996) make the results of their validation general. For specific applications their bias and calculational acceptance k_{eff} s may be overly restrictive. When validating these codes for a specific application, an appropriate subset of the validation cases may be used to establish a problem specific bias and acceptance criterion.

A paper in the transactions of the American Nuclear Society (Bowman et al. 1998) describes the verification and the validation process used for the SCALE code package. Bowman et al. provides a summary comparison of calculations of the 600 critical experiment models described in NUREG/CR-6483. Comparison is made of SCALE 4.2 using the 27-group ENDF/B-IV cross-section library with SCALE 4.3 using the 44-group ENDF/B-V library.

5.1.2 Results Reported in NUREG/CR-6361

Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages (NUREG/CR-6361) by Lichtenwaller et al. (1997) reports validation calculations for SCALE 4.3 using the 44-group ENDF/B-V cross-section library. In all, 180 benchmark experiment cases were compiled from 24 reports. Models of these experiments were input into KENO V.a to calculate values of k_{eff} .

Biases are discussed as a function of problem type. Calculations were repeated using the 238-group ENDF/B-V library to determine the adequacy of the 44-group structure. On average, the 238-group cross-sections returned results that were 0.35 percent lower than for the 44-group cross-sections. These benchmark calculations demonstrate that criticality safety calculations can be made using the 44-group ENDF/B-V cross-section library for a wide range of applications.

5.2 RESULTS FROM AST BRAVO 5200M PC CALCULATIONS

Calculational results for 46 benchmark experiments are described in Tables 5-1 through 5-4. The SCALE-4.3 calculations were performed on a 200 MHz AST Bravo MS 5200 personal computer using both the 27- and 44-group cross-sections. The 46 experiments are a subset of the benchmarks listed in NUREG/CR-6483 (Emmett and Jordan 1996) (see Appendix B).

Experiments are grouped according to type. ^{233}U benchmark experiments are listed in Table 5-1; plutonium benchmarks in Table 5-2; uranium benchmarks in Table 5-3, and iron benchmarks in Table 5-4. These groupings are then further broken down into configurations where fissioning results primarily from slow neutrons (i.e., moderated systems) and configurations where fissioning results primarily from fast neutron (i.e., unmoderated systems). The tables list the calculated k_{∞} for each experiment, along with the AEG, AEF, H/X ratio, and isotopic weight percent (wt%) of interest.

5.2.1 Experiments with ^{233}U

Table 5-1 lists XSDRNPM results for calculations of ^{233}U systems. There are two thermal experiments (uranyl nitrate-water solutions) and eleven fast systems (metal spheres). While the uranium in the K Basin sludge does not contain a significant fraction of ^{233}U , the calculations do support the ability of XSDRNPM to calculate critical systems. The results are divided into thermal and fast results. The AEF for the moderated systems fall in the narrow range from 0.0459 to 0.0578 eV, corresponding to an H/X atom ratio from 405 to 658. The AEF for the fast (unmoderated) systems fall in the range from 0.728 to 1.08 MeV, corresponding to an H/X atom ratio of 0. Agreement of the calculated k_{∞} with the benchmark experiments is good for both sets

of cross sections in both energy ranges. However, the 44-group ENDF/B-V cross sections provided consistently better results than the 27-group ENDF/B-IV cross sections.

5.2.2 Experiments with Plutonium

Table 5-2 lists XSDRNPM results for the plutonium benchmark experiments. There are ten thermal experiments (plutonium-water solutions) and four fast systems (metal spheres). Most of the calculations are for plutonium with a ^{240}Pu content close to 5 wt%. One experiment is for high burnup plutonium in which the ^{240}Pu content is 45 wt%. In all cases the calculated k_{eff} values agree well with experimental data. The plutonium in K Basin sludge has a ^{240}Pu content up to 16 wt%. The results are divided into thermal and fast systems. The AEF for the moderated systems fall in the range from 0.0371 to 0.311 eV, corresponding to an H/X atom ratio from 125 to 3,694. For thermal systems the average calculated k_{∞} is 1.0129 ± 0.0068 for 27-group cross sections and 1.0077 ± 0.0065 for 44-group cross sections. The AEF for the fast (metal) systems fall in the range from 0.079 to 1.16 MeV (i.e., an H/X of 0). For fast systems the average calculated k_{∞} is 1.0108 ± 0.0094 for 27-group cross sections and 1.0112 ± 0.0167 for 44-group cross sections.

5.2.3 Experiments with ^{235}U

Table 5-3 lists XSDRNPM results for the ^{235}U benchmark experiments. There are ten thermal systems (uranium rod lattices in water and highly enriched uranium nitride in water) and nine fast systems (metal spheres). The five rod lattice experiments are for 1.3 wt% ^{235}U enriched uranium rod lattices in water. The rod diameters are either 0.9728 cm or 0.9830 cm diameter and lattice pitch is varied between 1.5578 cm and 2.1740 cm. There are five experiments of highly enriched uranium nitride in water over the range of H/X ratio from 972 to 1835. The ^{235}U enrichment ranges from 91.2 to 95.3 wt%. The nine fast calculations are for unmoderated uranium metal spheres with various reflectors. The AEF for moderated systems fall between 0.0292 and 0.344 eV, and the H/X atom ratio fall between 214 and 1835. For thermal (moderated) lattices with an AEF between 0.113 and 0.344 eV the average calculated k_{∞} is 1.0139 ± 0.0034 for 27-group cross sections and 1.0231 ± 0.0037 for 44-group cross sections. For homogeneous solutions with an AEF between 0.0292 and 0.0339 eV the average calculated k_{∞} is 0.9967 ± 0.0014 for 27-group cross sections and 0.9972 ± 0.0013 for 44-group cross sections. The AEF for the fast (metal) systems fall between 2.77 and 878 keV with an H/X atom ratio between 0. and 3.2. For fast systems the average calculated k_{∞} is 1.01595 ± 0.0180 for 27-group cross sections and 1.0109 ± 0.0091 for 44-group cross sections. When all ^{235}U experiments are combined, the average k_{∞} is found to be 1.0103 ± 0.0148 for the 27-group and 1.0105 ± 0.0115 for the 44-group cross sections. These values are almost identical.

5.2.4 Experiments With Iron

A primary component in K Basin sludge when received at tank farms will be iron. The mass ratio of iron to plutonium in the actual waste is expected to exceed 200. Table 5-4 lists XSDRNPM results for systems that contain iron. There are two thermal experiments and four fast experiments listed. However, the mass ratio of iron to heavy metal in the thermal systems is no greater than 0.005, a value far less than in K Basin sludge. Although the iron to heavy metal mass ratio is higher for the fast systems, they are still less than the mass ratio in K Basin sludge. In addition, these systems do not represent the high water content found in K Basin sludge (i.e., the highly moderated state).

Heterogeneous experimental benchmarks are available in which iron is a component of steel in rod cladding, reflector walls, or separator plates. Both NUREG/CR-6483 (Emmett and Jordan 1996) and NUREG/CR-6361 (Lichtenwalter et al. 1997) contain numerous cases in which iron is used in this manner, but these cases are complex and are not adequately modeled by XSDRNPM. Nevertheless, the agreement between KENO V.a results and experiments is found to be good for these experiments. Table 5-5 lists results from a subset of these calculations using KENO V.a with the 27- and 44-group libraries, calculated on the AST Bravo PC.

This supports the conclusion that cross section sets validated for KENO V.a will provide accurate results when run using XSDRNPM. Even in these configurations, however, the iron content is still considerably less than in K Basin sludge.

For one and two dimensional systems, Emmett and Jordan (1996) found XSDRNPM and KENO V.a agree to within 1.0% Δk , and in most cases agreement was closer than 0.3% Δk . Systems modeled in one or two dimensions are calculated as accurately with XSDRNPM as with KENO V.a. Bias for one or two dimension systems are expected to be nearly identical for XSDRNPM as for KENO V.a.

Table 5-1. XSDRNPM Calculations for ^{233}U Benchmark Experiments¹

Moderated Configurations – Solutions							
Case	k_{∞} 27-Group	k_{∞} 44-Group	AEG ²	AEF ² (eV)	H/X Ratio	^{233}U wt%	Description
111_20	1.01400	0.99854	36.8	5.78E-02	405	98.7	Uranyl nitrate-water solution
111_25	1.02686	1.01431	37.4	4.59E-02	658	98.7	Uranyl nitrate-water solution
Average ± Std. Dev.	1.02043 ± .00909	1.00643 ± .01115					
Fast Configurations							
1727_01	0.96713	0.99768	7.9	1.08E+06	0	98.1	Bare metal sphere, no reflector
1727_02	0.98107	0.99746	8.6	7.90E+05	0	98.1	Reflected metal spheres, uranium reflector
1727_03	0.97928	0.99664	8.3	9.01E+05	0	98.2	Reflected metal spheres, uranium reflector
1727_04	0.97600	0.99790	8.2	9.78E+05	0	98.2	Reflected metal spheres, uranium reflector
1727_05	0.97669	1.00894	8.5	8.34E+05	0	98.2	Reflected metal spheres, tungsten alloy reflector
1727_06	0.97634	1.00751	8.3	9.32E+05	0	98.2	Reflected metal spheres, tungsten alloy reflector
1727_07	0.99619	1.00767	8.6	7.28E+05	0	98.2	Reflected metal spheres, natural uranium reflector
1727_08	0.98395	1.00344	8.3	9.03E+05	0	98.2	Reflected metal spheres, tungsten alloy reflector
1727_14	0.97626	1.00118	8.0	1.04E+06	0	98.1	Reflected metal spheres, enriched uranium reflector
1727_15	0.98256	1.00360	8.1	1.03E+06	0	98.1	Reflected metal spheres, enriched uranium reflector
JEZB23	0.96475	0.99525	8.0	1.06E+06	0	98.1	Bare metal sphere, no reflector
Average ± Std. Dev.	0.97820 ± .00838	1.00157 ± .00494					
Combined Average (Moderated and Fast Configurations)							
Overall Average ± Std. Dev.	0.98470 ± .001780	1.00232 ± .00583					

Notes: ¹ All experiments from NUREG/CR-6483 (Emmett and Jordan 1996) ² Uses 44-group cross-sections.

Table 5-2. XSDRNPM Calculations for Plutonium Benchmark Experiments¹

Case	k _∞ 27-Group	k _∞ 44-Group	AEG ²	AEF ² (eV)	H/X Ratio	²⁴⁰ Pu wt%	Description
Moderated Configurations – Solutions							
2110_01	1.00487	1.00139	38.1	3.71E-02	3694	0.0	Pu-water solution
PNL3	1.00059	0.99577	37.1	4.93E-02	1154	4.2	Pu-water solution, bare sphere
2110_30	1.01845	1.01424	37.2	4.91E-02	1067	4.6	Pu-water solution, Pu(NO ₃) ₄
2110_32	1.01653	1.01245	37.1	5.05E-02	1031	4.6	Pu-water solution, Pu(NO ₃) ₄
2110_03	1.01722	1.01199	37.0	5.18E-02	980	0.5	Pu-water solution, Pu(NO ₃) ₄
2110_04	1.01751	1.01280	36.5	6.06E-02	758	4.6	Pu-water solution, Pu(NO ₃) ₄
2110_07	1.01712	1.01282	35.4	8.69E-02	422	4.7	Pu-water solution, Pu(NO ₃) ₄
2110_02	1.01567	1.00745	31.6	3.11E-01	125	4.6	Pu-water solution, Pu(NO ₃) ₄
PNL6B	1.01657	1.00840	31.7	3.00E-01	125	4.6	Pu-water solution, bare sphere
HI240R	1.00435	0.99990	36.9	5.43E-02	623	42.9	Pu nitrate-water, high ²⁴⁰ Pu wt.%, water reflected
Average ± Std. Dev.	1.01289 ± 0.00677	1.00772 ± 0.00649					
Fast Configurations							
1727_09	1.00800	1.00436	12.0	7.90E+04	0	5.2	Pu metal sphere, water reflector
1727_10	1.00113	1.00027	7.8	1.16E+06	0	4.9	Pu metal sphere, enriched uranium reflector
2109_25	1.01053	1.00414	8.4	8.75E+05	0	4.8	Pu metal sphere, natural uranium reflector
ZPR67	1.02348	1.03614	10.9	9.89E+04	0	11.8	Pu in depleted uranium, Pu/U = 0.174, DU reflector
Average ± Std. Dev.	1.01079 ± 0.00935	1.01123 ± 0.01671					
Combined Average (Moderated and Fast Plutonium Configurations)							
Overall Average ± Std. Dev.	1.01229 ± .00727	1.00872 ± .00982					

Notes: ¹All experiments from NUREG/CR-6483 (Emmett and Jordan 1996) ² Uses 44-group cross-sections.

Table 5-3. XSDRNPM Calculations for Uranium Benchmark Experiments¹ (2 sheets)

Case	k_{∞} 27-Group	k_{∞} 44-Group	AEG ²	AEF ² (eV)	H/X Ratio	²³⁵ U wt%	Description
Moderated Configurations – UO₂ Triangular Lattices In Water							
BAPL1	1.00928	1.01836	34.6	2.09E-01	250	1.31	Fuel OD = 0.9728 cm, pitch = 1.5578 cm
BAPL2	1.01302	1.02140	35.3	1.56E-01	319	1.31	Fuel OD = 0.9728 cm, pitch = 1.6523 cm
BAPL3	1.01498	1.02252	36.0	1.13E-01	438	1.31	Fuel OD = 0.9728 cm, pitch = 1.8057 cm
TRX1	1.01341	1.02478	33.6	3.44E-01	214	1.29	Fuel OD = 0.9830 cm, pitch = 1.8060 cm
TRX2	1.01868	1.02830	35.2	1.67E-01	376	1.29	Fuel OD = 0.9830 cm, pitch = 2.1740 cm
Average ± Std. Dev.	1.01387 ± 0.00340	1.02307 ± 0.00373					
Moderated Configurations – Solutions							
ORNL10	0.99592	0.99766	38.8	2.92E-02	1835	91.2	Uranium nitride – water solution
ORNL1	0.99832	0.99832	38.7	3.05E-02	1378	93.2	Uranium nitride – water solution
ORNL2	0.99788	0.99815	38.6	3.19E-02	1177	95.3	Uranium nitride – water solution, 10B
ORNL3	0.99492	0.99519	38.5	3.32E-02	1033	93.8	Uranium nitride – water solution, 10B
ORNL4	0.99644	0.99666	38.4	3.39E-02	972	93.5	Uranium nitride – water solution, 10B
Average ± Std. Dev.	0.99670 ± 0.00140	0.99720 ± 0.00129					
Fast Configurations							
BIG10	1.00153	1.01868	9.2	4.69E+05	0	10.1	U metal sphere, depleted uranium reflector
FLAT25	1.00885	0.99811	8.6	7.75E+05	0	93.2	U metal sphere, natural uranium reflector
GODIVA	1.00622	1.00139	8.4	8.78E+05	0	93.7	U metal sphere, bare
H2OX1	1.00875	1.00432	13.7	2.82E+04	0	93.9	U metal sphere, water reflector
UH3NI	1.06137	1.01040	14.5	2.87E+03	3.2	93.1	U metal sphere, C/ ²³⁵ U = 1.2, nickel reflector
UH3UR	1.02183	1.00676	14.5	2.77E+03	3.2	93.1	U metal sphere, C/ ²³⁵ U = 1.2, natural uranium reflector
ZPR311	1.00688	1.02001	9.3	4.47E+05	0	11.6	U metal sphere, depleted uranium reflector

Notes: ¹All experiments from NUREG/CR-6483 (Emmett and Jordan 1996)² Uses 44-group cross-sections.

Table 5-3. XSDRNPM Calculations for Uranium Benchmark Experiments.¹ (2 sheets)

Case	k_{∞} 27-Group	k_{∞} 44-Group	AEG ²	AEF ² (eV)	H/X Ratio	²³⁵ U wt%	Description
Fast Configurations (Cont'd)							
ZPR312	1.01261	1.01376	9.9	2.69E+05	0	20.8	U metal sphere, depleted uranium reflector
ZPR66A	1.01554	1.02469	11.5	6.02E+04	0	16.4	U metal sphere, depleted uranium reflector
Average ± Std. Dev.	1.01595 ± 0.01801	1.01090 ± 0.00906					
Combined Average (Moderated and Fast Uranium Configurations)							
Overall Average ± Std. Dev.	1.01034 ± .01477	1.01050 ± .01154					

Notes: ¹All Experiments from NUREG/CR-6483 (Emmett and Jordan 1996)²Uses 44-group cross-sections.

Table 5-4. XSDRNPM Calculations for Iron Benchmark Experiments¹

Case	k_{∞} 27-Group	k_{∞} 44-Group	AEG ²	AEF ² (eV)	Fe/HM Ratio	Description
Moderated Configurations – Solutions						
PNL3	1.00059	0.99577	37.1	4.93E-02	0.005	Pu-water solution, bare sphere
PNL6B	1.01657	1.00840	31.7	3.00E-01	0.002	Pu-water solution, bare sphere
Average ± Std. Dev.	1.00858 ± .01130	1.00209 ± .00893				
Fast Configurations						
ZPR311	1.00688	1.02001	9.3	4.47E+05	0.034	U metal sphere, depleted uranium reflector
ZPR312	1.01261	1.01376	9.9	2.69E+05	0.062	U metal sphere, depleted uranium reflector
ZPR66A	1.01554	1.02469	11.5	6.02E+04	0.453	U metal sphere, depleted uranium reflector
ZPR67	1.02348	1.03614	10.9	9.89E+04	0.446	Pu in depleted uranium, Pu/U = 0.174, DU reflector
Average ± Std. Dev.	1.01463 ± .00691	1.02365 ± .00945				
Combined Average (Moderated and Fast Iron Configurations)						
Overall Average ± Std. Dev.	1.01646 ± .01391	1.01261 ± .00800				

Notes: ¹ All experiments from NUREG/CR-6483 (Emmett and Jordan 1996).² Uses 44-group cross-sections.

Table 5-5. KENO V.a Calculations for Steel Plate Experiments¹

File	k_{∞} 27-Group	k_{∞} 44-Group	AEF ² (eV)	²³⁵ U wt%	Fe/U Mass Ratio	Plate Thick (cm)	Description
P2438SLG	0.9948 ± 0.0014	0.9981 ± 0.0014	0.073	2.35	0.000	None	Simple square lattice
P2438SS	0.9938 ± 0.0013	0.9961 ± 0.0014	0.074	2.35	0.024	0.485	Stainless steel separator plates
P2615SS	0.9967 ± 0.0016	0.9980 ± 0.0016	0.093	4.31	0.046	0.485	Stainless steel separator plates
P3314SLG	0.9924 ± 0.0016	0.9974 ± 0.0016	0.198	4.31	0.000	None	Simple square lattice
P3314SS1	0.9986 ± 0.0016	1.0025 ± 0.0016	0.211	4.31	0.080	0.302	Steel separator plates
P3314SS2	0.9916 ± 0.0015	1.0043 ± 0.0015	0.204	4.31	0.045	0.302	Steel separator plates
P3314SS3	0.9962 ± 0.0015	0.9988 ± 0.0015	0.213	4.31	0.103	0.485	Steel separator plates
P3314SS4	0.9903 ± 0.0014	1.0010 ± 0.0015	0.132	4.31	0.075	0.485	Steel separator plates
P3314SS5	0.9978 ± 0.0014	0.9974 ± 0.0013	0.233	2.35	0.012	0.302	Steel separator plates
P3314SS6	0.9930 ± 0.0015	1.0015 ± 0.0016	0.194	4.31	0.018	0.302	Steel separator plates
Average	0.9945 ± 0.0015	0.9995 ± 0.0015					

Note: ¹ All experiments from NUREG/CR-6361 (Lichtenwalter et al. 1997).

² Uses 44-group cross-sections.

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6.0 ADDITIONAL COMPARISONS

Additional comparisons are made to demonstrate the ability of XSDRNPM to calculate criticality parameters. Comparisons are made to KENO V.a calculations, and calculations run in the standalone mode are compared to CSASIX sequence calculations. In addition, configurations selected from Paxton and Pruvost (1987) and from the *Criticality Handbook* to represent tank waste are calculated.

6.1 XSDRNPM AND KENO V.a RESULTS

Configurations of primary importance to the evaluation of K Basin sludge are recalculated using KENO V.a, a code using an entirely different method from that used by XSDRNPM. The same cross section sets were used for both calculations. Since these two methods are entirely different and independent, the ability to obtain close agreement for k_{∞} demonstrates that the codes are performing the intended calculations.

XSDRNPM is used to compute k_{∞} for postulated sludge compositions over the entire range of water concentrations. The water content at which the maximum k_{∞} occurs is called the optimum (or optimal) water concentration. Maximum k_{∞} always occurs for a well moderated configuration. Configurations for which the water content provides maximum k_{∞} are shown in Table 6-1.

Maximum k_{∞} for each assumed sludge composition was also calculated using KENO V.a, and the results are shown in Table 6-1 next to the corresponding XSDRNPM value.

Calculations in Table 6-1 are made using the SCALE 4.3 code system using 27-group cross sections. For each calculation the total weight of solids (everything not water) is held constant at 2,000 g/L. Iron is assumed to be present as FeO, plutonium as PuO₂, and uranium as UO₂. Heavy metal (HM) refers to the sum of the plutonium and uranium metal. The AEF falls between 0.09 and 0.19 eV for these configurations.

When the maximum k_{∞} is near 1.0, XSDRNPM usually gives a value that is within 0.004 of the corresponding KENO V.a value. In all cases in Table 6-1, the agreement is to within 0.006. When iron is added, the maximum k_{∞} decreases. When maximum k_{∞} is around 0.70, XSDRNPM gives a maximum k_{∞} which is always larger than the corresponding KENO V.a. The greatest difference is found to be about 0.007 for the configurations examined.

In conclusion, agreement between XSDRNPM and KENO V.a maximum k_{∞} is found to be within 0.007 for the range of sludge types being examined. For well subcritical configurations, as is always the case with tank waste, XSDRNPM tends to give a slightly larger maximum k_{∞} and is therefore slightly more conservative.

Table 6-1. Comparison of XSDRNPM and KENO V.a Calculated k_{∞} (2 sheets)

Identity	$^{235}\text{U/U}$ wt%	Plutonium/Uranium wt%	$^{240}\text{Pu/Pu}$ wt%	Fe/HM Mass Ratio	Water g/cc	XSDRN k_{∞}	KENO V.a k_{∞}	AEF ² eV
F1A-8	1.25	0.0	0.0	0.000	0.35	1.06145	1.0624 ± 0.0008	0.141
F2A-7	0.95	0.0	0.0	0.000	0.30	0.96708	0.9687 ± 0.0011	0.124
F3A-7	0.84	0.0	0.0	0.000	0.30	0.92332	0.9236 ± 0.0011	0.114
F7A-8	0.84	0.20	11.0	0.000	0.35	1.01820	1.0202 ± 0.0012	0.106
F7D-6	0.84	0.20	11.0	0.529	0.25	0.71340	0.7084 ± 0.0008	0.112
F7E-6	0.84	0.20	11.0	0.707	0.25	0.65018	0.6441 ± 0.0007	0.152
F7J-12	0.84	2.00	11.0	0.529	0.60	1.12506	1.1203 ± 0.0012	0.113
F9A-9	0.84	0.30	16.0	0.000	0.40	1.03419	1.0345 ± 0.0012	0.107
F9D-6	0.84	0.30	16.0	0.529	0.25	0.74536	0.7377 ± 0.0008	0.101
F9E-6	0.84	0.30	16.0	0.707	0.25	0.68395	0.6763 ± 0.0007	0.110
F11B-7	0.84	0.60	16.0	0.707	0.30	0.78872	0.7824 ± 0.0009	0.135
F11C-8	0.84	0.90	16.0	0.707	0.35	0.86691	0.8616 ± 0.0009	0.126
F11D-9	0.84	1.20	16.0	0.707	0.40	0.92812	0.9219 ± 0.0011	0.103
F11E-10	0.84	1.50	16.0	0.707	0.45	0.97769	0.9726 ± 0.0009	0.114
F11F-10	0.84	1.80	16.0	0.707	0.45	1.01858	1.0124 ± 0.0011	0.178
F12B-7	0.84	0.60	16.0	0.529	0.30	0.84754	0.8408 ± 0.0010	0.176
F12C-9	0.84	0.90	16.0	0.529	0.40	0.92266	0.9181 ± 0.0010	0.172
F12D-10	0.84	1.20	16.0	0.529	0.45	0.98088	0.9766 ± 0.0010	0.188
F12E-11	0.84	1.50	16.0	0.529	0.50	1.02728	1.0234 ± 0.0011	0.183
F12F-11	0.84	1.80	16.0	0.529	0.50	1.06530	1.0621 ± 0.0012	0.135
F13B-8	0.84	0.60	16.0	0.353	0.35	0.91789	0.9143 ± 0.0010	0.134
F13C-9	0.84	0.90	16.0	0.353	0.40	0.98771	0.9845 ± 0.0011	0.131
F13D-11	0.84	1.20	16.0	0.353	0.50	1.04085	1.0403 ± 0.0012	0.106
F13E-11	0.84	1.50	16.0	0.353	0.50	1.08269	1.0794 ± 0.0012	0.133
F14A-6	0.84	0.30	10.0	0.529	0.25	0.76316	0.7561 ± 0.0009	0.136

Table 6-1. Comparison¹ of XSDRNPM and KENO V.a Calculated k_{∞} (2 sheets)

Identity	²³⁵ U/U wt%	Plutonium/Uranium wt%	²⁴⁰ Pu/Pu wt%	Fe/HM Mass Ratio	Water g/cc	XSDRN k_{∞}	KENO V.a k_{∞}	AEF ² eV
F14B-6	0.84	0.30	5.0	0.529	0.25	0.77865	0.7709 ± 0.0008	0.132
F14C-6	0.84	0.30	0.0	0.529	0.25	0.79493	0.7872 ± 0.0008	0.172
F14D-6	0.75	0.30	16.0	0.529	0.25	0.71951	0.7127 ± 0.0008	0.164
F14E-6	0.80	0.30	16.0	0.529	0.25	0.73412	0.7279 ± 0.0008	0.092
F14F-7	0.90	0.30	16.0	0.529	0.30	0.76207	0.7556 ± 0.0008	0.119
F14G-7	0.95	0.30	16.0	0.529	0.30	0.77577	0.7692 ± 0.0009	0.181
F14H-7	1.00	0.30	16.0	0.529	0.30	0.78890	0.7814 ± 0.0009	0.171

Notes: ¹Assumes 2,000 g solids/L. Uses SCALE 4.3 code system with 27-group cross sections.

²AEF from KENO V.a calculations (using 27-group cross sections).

6.2 COMPARISON BETWEEN CSAS1X AND STANDALONE XSDRNPM

SCALE criticality modules can be executed either individually or using the CSAS sequences. Table 6-2 compares results from XSDRNPM executed individually with results from the CSAS1X sequence. Typical K Basin sludge compositions were selected for this comparison. For the individually executed XSDRNPM cases, cross sections are processed only in NITAWL. However, the CSAS1X sequence processes the cross sections first in BONAMI and then in NITAWL before calculating k_{∞} using XSDRNPM. Table 6-2 shows that the difference between the standalone and CSAS1X results is minimal for calculations with the 27-group cross sections ($<0.0003 \Delta k$). When 44-group cross sections are used, the difference is slightly larger ($<0.0042 \Delta k$). This larger difference for the 44-group cross sections is not unexpected since the 27-group library does not contain any Bondarenko data, and is not processed in BONAMI. However, the 44-group library does contain Bondarenko data for some isotopes and is processed in BONAMI when the CSAS1X sequence is executed.

6.3 COMPARISON TO BENCHMARK EXPERIMENTS AND HANDBOOK DATA

This section compares results from XSDRNPM calculations with published criticality data for infinite homogeneous mixtures of low enriched uranium, plutonium, and water. Calculations in this section were executed in the standalone mode using the 27-group cross-section set.

6.3.1 Minimum Critical Plutonium Concentration in Water

Paxton and Pruvost (1987) state that a limiting critical concentration of $7.6 \text{ g }^{239}\text{Pu/L}$ was deduced at the Hanford Site from experiments with a critical plutonium solution in a 4-ft-diameter sphere. This limiting concentration compares to a value of $8.0 \text{ g }^{239}\text{Pu/L}$ as originally obtained from a Hanford Physical Constants Test Reactor (PCTR) measurement and which was later reduced to $7.2 \text{ g }^{239}\text{Pu/L}$ in a reexamination of the data.

The *Criticality Handbook* (Carter et al. 1969) provides a value of $7.8 \pm 0.3 \text{ g/L}$ for the minimum critical concentration of plutonium in an aqueous solution. This corresponds to an H/Pu atom ratio of 3392 ± 100 .

XSDRNPM calculations of k_{∞} for plutonium oxide as a function of plutonium concentration in water are shown in Figure 6-1. For plutonium containing no ^{240}Pu , criticality occurs when the plutonium concentration is 7.1 g Pu/L . This agrees with the value of $7.2 \text{ g }^{239}\text{Pu/L}$ provided by Paxton and Pruvost (1987).

Figure 6-1 also shows the calculated k_{∞} for plutonium oxide when the ^{240}Pu content is 5, 10, and 15 wt% of the plutonium. No experimental values were found for these three curves. Nevertheless, they do show the degree to which ^{240}Pu influences k_{∞} .

Table 6-2. Comparison of XSDRNPM and CSAS1X Calculated k_{∞}

Description	Cross Section Group	k_{∞} XSDRNPM	k_{∞} CSAS1X	Δk	% Diff
Model of Tank Farm sludge with 0.84 wt% ^{235}U , 0.30 wt% Pu/U, 16.0 wt% ^{240}Pu /Pu, 0.707 Fe/HM mass ratio, and optimal water.	27	0.676459	0.676664	-0.0002	-0.0303%
Model of Tank Farm sludge with 0.84 wt% ^{235}U , 0.30 wt% Pu/U, 16.0 wt% ^{240}Pu /Pu, 0.000 Fe/HM mass ratio, and optimal water.	27	1.035140	1.035420	-0.0003	-0.0270%
	44	1.041160	1.042730	-0.0016	-0.1508%

6.3.2 Comparison to Criticality Handbook Data

This section compares XSDRNPM calculated k_{∞} with values from the *Criticality Handbook* (Carter et al. 1969). Calculations for the *Criticality Handbook* were produced using the GAMTEC-II and HFN codes. The GAMTEC-II code was used to provide 18 neutron energy group cross-section sets which were used in the HFN multigroup one-dimensional diffusion theory code to calculate critical sizes, extrapolation distances and material bucklings. A thorough analysis was made by C. R. Richey (1968) using this method to calculate the effective multiplication factor for critical experiments. Carter et al. (1969) report 11 calculations by Richey (1968). For nine spheres k_{eff} values are well within 1.0 percent of the experimental values. For two short cylinders calculated k_{eff} s are low by 1.5 percent and 2.5 percent. For GAMTEC-II – HFN calculations Carter et al. (1969) conclude that the comparison with experiment shows that this can be slightly non-conservative. Dimensions, which are less than can be obtained with some degree of confidence, can be obtained by reducing the calculated critical values to values equivalent to k_{eff} equal to 0.986 for spheres and 0.980 for infinite slabs and cylinders.

6.3.2.1 PuO₂ in Water

Figure 6-2 shows a comparison between XSDRNPM calculated k_{∞} and values from the *Criticality Handbook*. The comparison is made for an infinite homogeneous volume of PuO₂ in water at concentrations ranging from 10 to 30 g plutonium/liter and for ²⁴⁰Pu contents of 0, 5, 10, and 15 wt% of the plutonium. *Criticality Handbook* data is taken from: (1) Figure III.A.10.100-4 for plutonium metal with no ²⁴⁰Pu; (2) Figure III.A.10.95-4 for plutonium metal with 5 wt% ²⁴⁰Pu; (3) Figure III.A.10(85)-2 for plutonium nitrate with 15 wt% ²⁴⁰Pu; and (4) Figure III.A.10(90)-2 for plutonium nitrate with 10 wt% ²⁴⁰Pu. Although the XSDRNPM calculations were for plutonium oxide in water, the handbook data is for plutonium metal in water and plutonium nitrate systems. In all cases the volume ratio of water to plutonium compound is large, and the difference in plutonium compounds has only a very small effect on k_{∞} .

Over the range of plutonium concentration and ²⁴⁰Pu content examined XSDRNPM calculates k_{∞} about 1.0 percent larger than the handbook value. The slightly poorer agreement at higher plutonium concentration may reflect the small, but increasing, differences in the systems being compared.

6.3.2.2 1.25 wt% UO₂ in Water

Figure 6-3 shows XSDRNPM calculations for 1.25 wt% UO₂ in water. This can be compared with Figure III.B.10(1.25)-2 in the *Criticality Handbook*, which shows a curve of k_{∞} for 1.25 wt% uranium trioxide as a function of concentration in water. A maximum k_{∞} of 1.062 is achieved when the uranium concentration is 3100 g/L. XSDRNPM calculations for 1.25 wt% uranium dioxide in water provides a maximum k_{∞} of 1.0615.

Figure 6-1. k_{∞} or Homogeneous PuO_2 in Water Figure 6-2. Comparison of XSDRNPM with *Criticality Handbook* for PuO_2 in Water

Figure 6-3. XSDRNPM k_{∞} or Homogeneous $U(1.25)O_2$ in Water

7.0 DISCUSSION

Table 7-1 shows the results from a statistical analysis of the results presented in Tables 5-1 through 5-5. The experiments are grouped and analyzed according to fissile isotope, thermal systems, fast systems, all systems, and systems with iron. Within each group, the results are subdivided according to cross section set. The results are correlated against key parameters in each group. Table 7-1 lists the linear regression analysis results, average calculated k_{eff} , standard deviation, and USL_1 and USL_2 values (see Section 4.0 for description) for each statistical analysis. All positive biases are conservatively set to zero.

USL_1 and USL_2 values are shown in Table 7-1 for a variety of experiment groupings. This provides information to validate XSDRNPM for future criticality safety evaluations that might involve configurations different from K Basin sludge. For example, ^{233}U benchmarks were calculated and are included in Table 7-1, but these are not used in the determination of the USL for K Basin sludge.

As mentioned previously, XSDRNPM will be used to calculate configurations of tank waste. A composition of primary interest is that of K Basin sludge composed of irradiated low enriched uranium and plutonium mixed with iron and water. Plutonium generated during irradiation of uranium is assumed to remain associated with the uranium. The highest ^{235}U enrichment is taken to be 1.25 wt%, the highest enrichment in any uranium in tank waste before irradiation. During the process of irradiation the ^{235}U enrichment decreases, and much of the actual uranium in tank waste is depleted. However, the plutonium content can be as much as 0.30 wt% of the uranium. Scenarios are to be evaluated in which the plutonium is chemically separated from the uranium and is deposited at a higher concentration in a different location. The effect of neutron absorbing solids, especially iron, on the neutron multiplication constant are of interest.

For calculational models the plutonium is assumed composed of the ^{239}Pu and the ^{240}Pu isotopes. Although ^{238}Pu , ^{241}Pu , and ^{242}Pu are present, these isotopes are of lesser importance to criticality safety and are not taken into account specifically in calculations. In practice, calculations may be made with ^{238}Pu and ^{242}Pu replaced by ^{240}Pu or replaced by ^{239}Pu , which is more conservative. The worth of ^{241}Pu can be twice as much as ^{239}Pu . A discussion of the significance of these isotopes should be provided in criticality safety evaluations.

Iron is added to sludge to ensure long-term chemical compatibility and subcriticality. The iron content may be quite high, and the Fe/Pu and the Fe/ ^{235}U mass ratios might exceed 300. No restriction is placed upon the water content, and water is assumed to range from none to a large fraction of the sludge volume. The configuration of interest to criticality safety are those which result in the largest k_{∞} .

7.1 SUMMARY OF USL RESULTS

Table 7-1 summarizes USL calculations for benchmark experiments grouped according to various parameters. Four primary groups contain calculations of experiments with specific components: ^{233}U , ^{235}U , plutonium, and iron. Two primary groups include all component types, but separate configuration according to whether they are thermal or fast, and one primary group includes all calculations for both thermal and fast systems. These calculations were made using XSDRNPM. The final primary group contains KENO V.a calculations of experiments containing iron. Each primary group is subdivided according to 27-group or 44-group cross sections.

7.1.1 USL for all Solution Systems (^{233}U , ^{235}U , and Pu)

For a grouping that includes all solution systems (AEF from 0.029 to 0.344 eV) for ^{233}U , ^{235}U and plutonium, the minimum USL_1 with a 0.05 administrative margin is 0.923 for 27-group cross sections and 0.930 for 44-group cross sections. The minimum USL_2 for this grouping of solution systems is 0.939 for 27-group cross sections and 0.955 for 44-group cross sections. USL_2 is found to be larger than USL_1 for both cross section sets. This indicates that a 0.05 administrative margin applied to USL_1 is adequate for thermal systems as long as the AEF falls within the applicable range (i.e., the correlated parameter is not extrapolated). When the H/X ratio falls between 125 and 3694, the AEF is assured of falling within the applicable range. It should be noted, however, that configurations with an H/X ratio less than 125 can also fall within the applicable AEF range, if additional moderation is provided by other materials.

7.1.2 USL for Thermal Systems (^{235}U and Pu)

For a grouping that includes all ^{235}U and plutonium thermal systems, including moderated ^{235}U lattices, the minimum USL_1 with a 0.05 administrative margin is 0.934 for 27-group cross sections and 0.932 for 44-group cross sections. The minimum USL_2 for this grouping is 0.954 for 27-group cross sections and 0.947 for 44-group cross sections. When ^{235}U lattices are not included, the minimum USL_1 is 0.931 for 27-group cross sections and 0.934 for 44-group cross sections, and the minimum USL_2 is 0.0943 for 27-group cross sections and 0.953 for 44-group cross sections. The AEF for this grouping ranges from 0.029 to 0.344 eV.

7.1.3 USL for K Basin Sludge Analysis

Key configurations of K Basin sludge for which water content is optimized to provide maximum k_∞ are shown in Table 6-1. These configurations are thermal systems with the AEF ranging from 0.092 to 0.188 eV. Configurations with an iron/uranium mass ratio even higher than shown in this table (i.e., greater than 0.707) may be calculated for the evaluation of K Basin sludge. These configurations will nevertheless be thermal systems whose AEF will fall within the range of applicability of this evaluation.

Table 7-1 shows homogeneous systems in which the iron-to-heavy metal (Fe/HM) mass ratio ranges from 0.002 to 0.446. When the administrative margin is 0.05, the minimum USL_1 is 0.933 with 27-group cross sections and 0.926 for 44-group cross sections, and the minimum USL_2 is 0.937 for 27-group cross sections and 0.912 for 44-group cross sections. For the 44-group cross sections USL_2 is smaller than USL_1 . Since the method used to determine USL_2 calculates its own administrative margin, this indicates that the administrative margin applied to USL_1 should be larger than 0.05 for 44-group cross section calculations. The confidence in the 0.05 administrative margin is also brought into question when considering that only two of the XSDRNPM benchmarks are for thermal systems, and the Fe/HM ratio is well below 0.70, the approximate iron content expected K Basin sludge when received at tank farms. Therefore, based on the consideration of iron, it is recommended that an administrative margin of 0.10 be used for the criticality safety evaluation of K Basin sludge in the Hanford Site waste tank.

To increase the confidence in the iron cross sections for thermal systems, KENO V.a calculations for heterogeneous plate experiments were analyzed statistically. For these experiments the AEF ranged from 0.073 to 0.233, and the Fe/HM mass ratio ranged from 0.0 to 0.103. For an administrative margin of 0.05 the minimum USL_1 is 0.936 for 27-group cross sections and 0.941 for 44-group cross sections, and the minimum

USL₂ is 0.968 for 27-group cross sections and 0.974 for 44-group cross sections. This indicates that administrative margin of 0.05 is adequate for systems that fall within this range of benchmark experiments. However, the energy spectrum that the iron encounters in a heterogeneous thermal system is expected to be somewhat different than the spectrum encountered in a homogenous thermal system. In addition, the upper limit of the range of Fe/HM mass ratio covered in these experiments is much less than the values expected for K Basin sludge. In conclusion, although KENO V.a calculations support a 0.05 administrative margin for the range of iron content in available experiments, this range is not broad enough to support a margin of 0.05 for K Basin sludge.

Table 7-1. Summary of Upper Safety Limit Calculations. (3 sheets)

Set ¹	Cross Section Group	Correlated Parameter (x)	No Exps.	K _c (x) Linear Regression	Std. Dev.	Corr. ² Coef. r ²	Average k _c	W	Min USL ₁ (Δk _m = 0.05)	Min USL ₁ (Δk _m = 0.10)	Min USL ₂	Min Δk _m USL ₂
²³³ U Exps	27	AEF (²³³ U - thermal)	2	Insufficient Data								
		AEF (²³³ U - fast)	11	1.0293 + (-5.4695E-08)*x	0.0058	0.582	0.97820	0.0125	0.908	0.858	0.934	0.023
		AEF (²³³ U - all)	13	1.0211 + (-4.5997E-08)*x	0.0060	0.898	0.98470	0.0130	0.908	0.858	0.936	0.022
	44	AEF (²³³ U - thermal)	2	Insufficient Data								
		AEF (²³³ U - fast)	11	1.0202 + (-1.9917E-08)*x	0.0046	0.222	1.00157	0.0100	0.939	0.889	0.970	0.019
		AEF (²³³ U - all)	13	1.0074 + (-6.4425E-09)*x	0.0056	0.164	1.00232	0.0121	0.938	0.888	0.967	0.021
²³⁵ U Exps	27	AEF (²³⁵ U lattices)	5	1.0159 + (-1.0329E-02)*x	0.0038	0.072	1.01387	0.0122	0.938	0.888	0.951	0.036
		AEF (²³⁵ U - solutions)	5	1.0031 + (-2.0248E-01)*x	0.0016	0.084	0.99670	0.0047	0.942	0.892	0.977	0.015
		AEF (²³⁵ U - metal)	9	1.0252 + (-2.8320E-08)*x	0.0163	0.282	1.01595	0.0372	0.913	0.863	0.888	0.075
		AEF (²³⁵ U - all)	19	1.0114 + (-6.6349E-09)*x	0.0151	0.016	1.01034	0.0313	0.919	0.869	0.921	0.048
		Enrichment (²³⁵ U - all)	19	1.0121 + (-3.3535E-03)*x	0.0151	0.010	1.01034	0.0279	0.922	0.872	0.929	0.043
	44	AEF (²³⁵ U lattices)	5	1.0221 + (4.9197E-03)*x	0.0043	0.014	1.02307	0.0138	0.936	0.886	0.945	0.041
		AEF (²³⁵ U - solutions)	5	1.0114 + (-4.4771E-01)*x	0.0011	0.439	0.99720	0.0034	0.943	0.893	0.982	0.011
		AEF (²³⁵ U - metal)	9	1.0142 + (-1.0024E-08)*x	0.0090	0.140	1.01090	0.0205	0.930	0.880	0.938	0.041
		AEF (²³⁵ U - all)	19	1.0114 + (-5.6257E-09)*x	0.0118	0.019	1.01050	0.0244	0.926	0.876	0.939	0.037
		Enrichment (²³⁵ U - all)	19	1.0232 + (-2.4088E-02)*x	0.0044	0.863	1.01050	0.0081	0.942	0.892	0.979	0.013
Pu Exps	27	AEF (Pu - moderated)	10	1.0109 + (1.8944E-02)*x	0.0068	0.089	1.01289	0.0157	0.934	0.884	0.955	0.030
		AEF (Pu - fast)	4	Insufficient Data								
		AEF (Pu - all)	14	1.0135 + (-7.7141E-09)*x	0.0070	0.154	1.01229	0.0159	0.934	0.884	0.958	0.026
		²⁴⁰ Pu wt % (Pu - all)	14	1.0133 + (-1.4462E-02)*x	0.0074	0.045	1.01229	0.0184	0.932	0.882	0.953	0.029
	44	AEF (Pu - moderated)	10	1.0073 + (3.9334E-03)*x	0.0069	0.004	1.00772	0.0157	0.934	0.884	0.955	0.030
		AEF (Pu - fast)	4	Insufficient Data								
		AEF (Pu - all)	14	1.0097 + (-6.4483E-09)*x	0.0099	0.059	1.00872	0.0226	0.927	0.877	0.941	0.037
		²⁴⁰ Pu wt % (Pu - all)	14	1.0093 + (-8.2846E-03)*x	0.0102	0.008	1.00872	0.0253	0.925	0.875	0.935	0.040

Table 7-1. Summary of Upper Safety Limit Calculations. (3 sheets)

Set ¹	Cross Section Group	Correlated Parameter (x)	No Exps.	$k_c(x)$ Linear Regression	Std. Dev.	Corr. ² Coef. r^2	Average k_c	W	Min USL ₁ ($\Delta k_m = 0.05$)	Min USL ₁ ($\Delta k_m = 0.10$)	Min USL ₂	Min Δk_m USL ₂
Thermal Exps	27	H/X Ratio (H/X > 100 - all solutions)	17	$1.0143 + (-5.1756E-06)*x$	0.0096	0.171	1.00901	0.0221	0.923	0.873	0.939	0.034
		AEF (²³⁵ U lattices)	5	$1.0159 + (-1.0329E-02)*x$	0.0038	0.072	1.01387	0.0122	0.938	0.888	0.951	0.036
		AEF (²³⁵ U solutions)	5	$1.0031 + (-2.0248E-01)*x$	0.0016	0.084	0.99670	0.0047	0.942	0.892	0.977	0.015
		AEF (Pu solutions)	10	$1.0109 + (1.8944E-02)*x$	0.0068	0.089	1.01289	0.0157	0.934	0.884	0.955	0.030
		AEF (Pu & ²³⁵ U solutions)	15	$1.0035 + (4.9090E-02)*x$	0.0088	0.357	1.00749	0.0191	0.931	0.881	0.943	0.038
		AEF (Pu & ²³⁵ U systems)	20	$1.0046 + (4.1254E-02)*x$	0.0080	0.283	1.00909	0.0159	0.934	0.884	0.954	0.030
		AEF (all isotopes)	22	$1.0066 + (3.3933E-02)*x$	0.0089	0.133	1.01012	0.0175	0.933	0.883	0.957	0.026
	44	H/X Ratio (H/X > 100 - all isotopes)	17	$1.0073 + (-2.7237E-06)*x$	0.0073	0.089	1.00447	0.0169	0.930	0.880	0.955	0.026
		AEF (²³⁵ U lattices)	5	$1.0221 + (4.9197E-03)*x$	0.0043	0.014	1.02307	0.0138	0.936	0.886	0.945	0.041
		AEF (²³⁵ U solutions)	5	$1.0114 + (-4.4771E-01)*x$	0.0011	0.439	0.99720	0.0034	0.943	0.893	0.982	0.011
		AEF (Pu solutions)	10	$1.0073 + (3.9334E-03)*x$	0.0069	0.004	1.00772	0.0157	0.934	0.884	0.955	0.030
		AEF (Pu & ²³⁵ U solutions)	15	$1.0022 + (2.4748E-02)*x$	0.0072	0.288	1.00421	0.0158	0.934	0.884	0.953	0.031
		AEF (Pu & ²³⁵ U systems)	20	$1.0027 + (5.6254E-02)*x$	0.0091	0.019	1.00893	0.0182	0.932	0.882	0.947	0.034
		AEF (all isotopes)	22	$1.0029 + (5.5356E-02)*x$	0.0091	0.281	1.00870	0.0179	0.932	0.882	0.956	0.026
Fast Exps	27	AEF (²³⁵ U fast)	11	$1.0293 + (-5.4695E-08)*x$	0.0058	0.582	0.97820	0.0125	0.908	0.858	0.934	0.023
		AEF (²³⁵ U - metal)	9	$1.0252 + (-2.8320E-08)*x$	0.0163	0.282	1.01595	0.0372	0.913	0.863	0.888	0.075
		AEF (all isotopes)	24	$1.0252 + (-4.2662E-08)*x$	0.0142	0.523	0.99779	0.0262	0.900	0.850	0.912	0.038
	44	AEF (²³⁵ U fast)	11	$1.0202 + (-1.9917E-08)*x$	0.0046	0.222	1.00157	0.0100	0.939	0.889	0.970	0.019
		AEF (²³⁵ U - metal)	9	$1.0142 + (-1.0024E-08)*x$	0.0090	0.140	1.01090	0.0205	0.930	0.880	0.938	0.041
		AEF (all isotopes)	24	$1.0166 + (-1.5412E-08)*x$	0.0079	0.400	1.00668	0.0145	0.934	0.884	0.963	0.021

Table 7-1. Summary of Upper Safety Limit Calculations. (3 sheets)

Set ¹	Cross Section Group	Correlated Parameter (x)	No Exps.	$k_c(x)$ Linear Regression	Std. Dev.	Corr. ² Coef. r^2	Average k_c	W	Min USL ₁ ($\Delta k_m = 0.05$)	Min USL ₁ ($\Delta k_m = 0.10$)	Min USL ₂	Min Δk_m USL ₂
All Exps	27	AEG (all isotopes, systems) ³	46	$0.9920 + (5.2101E-04)*x$	0.0170	0.153	1.00369	0.0293	0.917	0.867	0.932	0.035
		AEF (all Pu and ²³⁵ U)	33	$1.0123 + (-7.2158E-09)*x$	0.0120	0.009	1.02227	0.0236	0.926	0.876	0.936	0.040
		AEF (all isotopes, systems)	46	$1.0136 + (-2.9667E-08)*x$	0.0130	0.503	1.00369	0.0229	0.906	0.856	0.929	0.028
	44	AEG (all isotopes, systems)	46	$1.0062 + (6.5973E-05)*x$	0.0102	0.008	1.00765	0.0176	0.932	0.882	0.962	0.021
		AEF (all Pu and ²³⁵ U)	33	$1.0107 + (-6.0952E-09)*x$	0.0107	0.006	1.00974	0.0211	0.929	0.879	0.943	0.036
		AEF (all isotopes, systems)	46	$1.0105 + (-8.6221E-09)*x$	0.0095	0.139	1.00765	0.0167	0.933	0.883	0.963	0.020
Fe XSDRN Exps	27	Fe/HM Ratio (thermal)	2	Insufficient Data								
		Fe/HM Ratio (fast)	4	Insufficient Data								
		Fe/HM Ratio (all)	6	$1.0085 + (2.4502E-02)*x$	0.0066	0.454	1.01261	0.0173	0.933	0.883	0.937	0.046
	44	Fe/HM Ratio (thermal)	2	Insufficient Data								
		Fe/HM Ratio (fast)	4	Insufficient Data								
		Fe/HM Ratio (all)	6	$1.0079 + (5.1025E-02)*x$	0.0092	0.650	1.01646	0.0241	0.926	0.876	0.912	0.064
Fe KENO Plate Exps	27	Fe/HM Ratio (ratio = 0)	2	Insufficient Data								
		Fe/HM Ratio (ratio > 0)	8	$0.9944 + (7.1629E-03)*x$	0.0036	0.007	0.99475	0.0085	0.936	0.886	0.968	0.018
		Fe/HM Ratio (all)	10	$0.9940 + (1.2657E-02)*x$	0.0032	0.028	0.99452	0.0073	0.937	0.887	0.973	0.014
	44	Fe/HM Ratio (ratio = 0)	2	Insufficient Data								
		Fe/HM Ratio (ratio > 0)	8	$0.9988 + (2.3311E-02)*x$	0.0033	0.070	0.99995	0.0078	0.941	0.891	0.974	0.017
		Fe/HM Ratio (all)	10	$0.9983 + (3.0451E-02)*x$	0.0030	0.166	0.99951	0.0066	0.942	0.892	0.979	0.013

Notes: ¹Benchmark experiments for ²³³U are described in Table 5-1; experiments for plutonium in Table 5-2; and, experiments for ²³⁵U in Table 5-3.

² r^2 is the coefficient of determination used to compare estimated and actual values. Since the regression curve is linear (i.e., a straight line), a value of 1.0, the largest possible, means that calculated points lie in a straight line. A value less than 1.0 means calculated points do not lie in a straight line, and the smaller the value the less the correlation.

³ All isotopes refers to all ²³³U, ²³⁵U, and plutonium systems combined.

8.0 CONCLUSIONS

The range of applicability for XSDRNPM calculations is defined by: (1) uranium of any ^{235}U enrichment; (2) plutonium containing up to 20 wt% ^{240}Pu ; (3) iron in any proportion; (4) an AEF between 0.029 and 0.344 eV; and (5) geometric configurations for which neutron leakage is negligible. When H/X falls between 125 and 3694, the AEF is assured of falling between 0.029 and 0.344 eV. When moderators are present in addition to water, H/X can be less than 125 while remaining within the applicable AEF range. Neutron leakage is negligible when the smallest dimension is large enough for k_{eff} to be indistinguishable from k_{∞} .

An administrative margin of 0.10 will compensate for the extrapolations from the iron content in the benchmark experiments to the much higher iron content in K Basin sludge. An USL of 0.881 is acceptable for XSDRNPM calculations with 27-group cross sections, and an USL of 0.882 is acceptable with 44-group cross sections.

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APPENDIX A
SAMPLE STATISTICAL CALCULATION

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APPENDIX A

SAMPLE STATISTICAL CALCULATION

uslstats: a utility to calculate upper subcritical

limits for criticality safety applications

Version 1.3.6, December 15, 1998

Oak Ridge National Laboratory

Input to statistical treatment from file:c7z1.i

Title: XSDRN Validation Cases with H/X vs Enrichment (H/X > 100)

Proportion of the population = .995
 Confidence of fit = 950
 Confidence on proportion = 950
 Number of observations = 17
 Minimum value of closed band = 0.00
 Maximum value of closed band = 0.00
 Administrative margin = 0.10

independent dependent
 variable - x variable - y

4.05000E+02	1.01400E+00
6.58000E+02	1.02686E+00
3.69400E+03	1.00487E+00
1.15400E+03	1.00059E+00
1.06700E+03	1.01845E+00
1.03100E+03	1.01653E+00
9.80000E+02	1.01722E+00
7.58000E+02	1.01751E+00
4.22000E+02	1.01712E+00
1.25000E+02	1.01567E+00
1.25000E+02	1.01657E+00
6.23000E+02	1.00435E+00
1.83500E+03	9.95920E-01
1.37800E+03	9.98320E-01
1.17700E+03	9.97880E-01
1.03300E+03	9.94920E-01
9.72000E+02	9.96440E-01

WARNING *** the test for normal may be unreliable because of insufficient data.

chi = 8.5882 (upper bound = 9.49). The data tests normal.

Output from statistical treatment

XSDRN Validation Cases with H/X vs Enrichment (H/X > 100)
 Number of data points (n) 17
 Linear regression, k(x) 1.0143 + (-5.1756E-06)*X
 Confidence on fit (1-gamma) [input] 95.0%
 Confidence on proportion (alpha) [input] 95.0%

Proportion of population falling above	
lower tolerance interval (rho) [input]	99.5%
Minimum value of X	125.0000
Maximum value of X	3694.0000
Average value of	1025.7059
Average value of k	1.00901
Minimum value of k	0.99492
Variance of fit, $s(k,X)^2$	9.2377E-05
Within variance, $s(w)^2$	0.0000E+00
Pooled variance, $s(p)^2$	9.2377E-05
Pooled std. deviation, $s(p)$	9.6113E-03
$C(\alpha, \rho) * s(p)$	5.5789E-02
student-t @ (n-2, 1-gamma)	1.75300E+00
Confidence band width, W	2.2129E-02
Minimum margin of subcriticality, $C*s(p)-W$	3.3659E-02

Upper subcritical limits: (125.00 <= X <= 3694.0)

USL Method 1 (Confidence Band with

Administrative Margin) $USL1 = 0.8922 + (-5.1756E-06)*X$ (X > 2767.1)
 $= 0.8779$ (X <= *****)

USL Method 2 (Single-Sided Uniform

Width Closed Interval Approach) $USL2 = 0.9585 + (-5.1756E-06)*X$ (X > 2767.1)
 $= 0.9442$ (X <= *****)

USLs Evaluated Over Range of Parameter X:

X: 1.25E+2 6.35E+2 1.14E+3 1.65E+3 2.16E+3 2.67E+3 3.18E+3 3.69E+3

 USL-1: 0.8779 0.8779 0.8779 0.8779 0.8779 0.8779 0.8757 0.8731

USL-2: 0.9442 0.9442 0.9442 0.9442 0.9442 0.9442 0.9421 0.9394

Thus spake USLSTATS

Finis.

APPENDIX B

BENCHMARK EXPERIMENTS
DESCRIBED IN NUREG/CR-6483

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APPENDIX B

BENCHMARK EXPERIMENTS
DESCRIBED IN NUREG/CR-6483

This appendix describes validation problems from NUREG/CR-6483 (Emmett and Jordan 1996) used in this report. XSDRNPM cases were run in one of two different modes: (1) using the CSAS1X control module or (2) using the CSASN control module to generate cross sections for the XSDRNPM standalone code. The CSAS1X module calls BONAMI-S, NITAWL-S, and XSDRNPM-S. CSAS1X and CSASN create resonance-corrected, cell-weighted, microscopic libraries in the AMPX working library format. Data is input into CSAS1X in the following format:

```
#CSAS1X
TITLE
CROSS-SECTION LIBRARY NAME
TYPE OF CALCULATION
    INFOHOMMEDIUM
    LATTICECELL
    MULTIREGION
STANDARD COMPOSITION SPECIFICATION DATA
    Terminate data block with END COMP
UNIT CELL GEOMETRY SPECIFICATION
    Optional for INFOHOMMEDIUM
OPTIONAL PARAMETER DATA
    Proceed block with MORE DATA
END
```

B1.0 INPUT LISTINGS

A summary description and a listing of the code input are provided for one representative case from each group of similar experiments. Input listing for all cases can be downloaded from the SCALE website. The home address of the SCALE website is:

<http://www.cad.ornl.gov/cad-nea/text/scale-home.html>

Case 111-xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 29
TM12374 (Primm 1993)/Appendix C

Specific Cases: Case 111_20 Case 111_25

Description for Case 111_20:

²³³U at a concentration of 1.52924E-04 at/b-cm (62.00 g/L) in a 26.4-cm (10.39-in.) diameter sphere of ²³³U nitrate -water solution. Solution is in 0.1-cm thick aluminum shell surrounded by 20-cm (7.87-in.) thick, close-fitting water reflector.

Input Listing for Case 111-20

```
#csas1x
expt. 111-20
```

```

44gr multiregion
h      1 0 6.48995e-02      296.0 end
o      1 0 3.40024e-02      296.0 end
n      1 0 4.26254e-04      296.0 end
u-233  1 0 1.60246e-04      296.0 end
u-234  1 0 8.40645e-07      296.0 end
u-235  1 0 4.02437e-08      296.0 end
u-238  1 0 1.20004e-06      296.0 end
h2o    3 1.0                296.0 end
al      2 0 5.99324e-2       296.0 end
mn      2 0 3.75438e-4       296.0 end
end comp
spherical vacuum reflected 0 end
1 1.32000e+01 oneexterm
2 1.33000e+01 twoexterm
3 3.33000e+01 oneexterm
end zone
end

```

Case 1727-xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 29
 TM12374 (Primm 1993)/Appendix C

Specific Cases:	Case 1727_01	Case 1727_02	Case 1727_03
	Case 1727_04	Case 1727_05	Case 1727_06
	Case 1727_07	Case 1727_08	Case 1727_14
	Case 1727_15		

Description for Case 1727_01:

11.9679 -cm (4.71-in.) diameter, bare, metal, ²³³U sphere.

Input Listing for Case 1727_01

```

#csas1x
la-3067-msr table iv, entry 1, bare, metal, u-233 sphere
44gr
multiregion
u-233  1 0.0 4.67087e-2      300.0 end
u-234  1 0.0 5.92563e-4      300.0 end
u-235  1 0.0 1.27660e-6      300.0 end
u-238  1 0.0 2.84311e-4      300.0 end
end comp
spherical vacuum reflected 0.0 end
1 5.98393 noexterm
end zone
end

```

Case 1727-xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 31
 TM12374 (Primm 1993)/Appendix E

Specific Cases: Case 1727_09 Case 1727_10

Description of Case 1727_09:

8.2434-cm (3.2454-in.) diameter plutonium sphere in 0.0127-cm (0.0050-in.) thick nickel shell with 30.480-cm (12.000-in.) thick close-fitting water reflector. Plutonium contains 5.20 wt% ²⁴⁰Pu.

Input Listing for Case 1727_09

```
#csas1x
la-3067-msr table iii1, entry 13, water ref., metal, pu sphere
44gr
multiregion
pu-239 1 0.0 4.6994e-2 300.0 end
pu-240 1 0.0 2.5757e-3 300.0 end
pu-241 1 0.0 1.4798e-4 300.0 end
pu-242 1 0.0 9.8245e-6 300.0 end
ni      2 1.0 300.0 end
h2o     3 1.0 300.0 end
end comp
spherical vacuum reflected 0.0 end
1 4.1217 oneextermo
2 4.1344 twoextermo
3 34.614 noextermo
end zone
end
```

Case 2109-xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 31
TM12374 (Primm 1993)/Appendix E

Specific Cases: Case 2109_25

Description of Case 2109_25:

9.06454-cm (3.5687-in.) diameter plutonium metal sphere with a 19.52988-cm (7.7200-in.) natural uranium reflector. Plutonium contains 4.81 wt% ²⁴⁰Pu.

Input Listing for Case 2109_25:

```
#csas1x parm=(size=300000)
pu benchmark 25 from 2109, pu metal sphere reflected with nat. u
44gr
multiregion
pu-239 1 0.0 3.713e-2      300.0 end
pu-240 1 0.0 1.870e-3      300.0 end
pu-241 1 0.0 1.164e-4      300.0 end
u-235  2 0.0 3.456e-4      300.0 end
u-238  2 0.0 4.772e-2      300.0 end
end comp
spherical vacuum reflected 0.0 end
1 4.53227 oneextermo
2 24.1411 noextermo
end zone
end
```

Case 2110-xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 31
TM12374 (Primm 1993)/Appendix E

Specific Cases: Case 2110_01 Case 2110_02 Case 2110_03
Case 2110_04 Case 2110_07 Case 2110_30
Case 2110_32

Description of Case 2110_01:

Infinite volume of homogeneous ^{239}Pu -water solution.

Input Listing for Case 2110_01:

```
#csas1x
benchmark#1 infinite homog. critical solution of 239Pu in water
44gr infhommedium
pu-239 1 0 1.8113e-5 end
o      1 0 3.3459e-2 end
h      1 0 6.6918e-2 end
end comp
end
```

Case BAPLx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
TM12460 (Primm 1993)

Specific Cases: Case BAPL1 Case BAPL1-1
Case BAPL2 Case BAPL2-1
Case BAPL3 Case BAPL3-1

Description of Case BAPL1:

Triangular lattice of aluminum clad UO_2 rods in water. Enrichment is 1.31 wt% ^{235}U .

Input Listing for BAPL1:

```
=csasn
bapl-1 lattice cell calc. 44 gr - mdd 5-06-93
44gr latt
u-235 1 0 3.112-4 end
u-238 1 0 2.3127-2 end
o      1 0 4.6946-2 end
al     2 0 6.025-2 end
h      3 0 6.676-2 end
o      3 0 3.338-2 end
end comp
triangpitch 1.5578 0.9728 1 3 1.1506 2 1.0084 0 end
end
=xsdrnprm
bapl-1 lattice, 44gr - mdd - 4-06-93
1$$ 2 3 15 1 3 3 6 8 3 1 10 25 25 0 0
2$$ -2 0 -1 e
3$$ 1 5r0 2 0 4 0 0 0
4$$ -1 44 1 -2 e
5** a6 0.0 55.0310 e t
13$$ 2r3 2 3r1
```



```

14$$$ 3001001 3008016 2013027 1092235 1092238 1008016
15** 6.676-2 3.338-2 4.9028-2 3.112-4 2.3127-2 4.6946-2 t
33** f1.0 t
35** 5i0.0 0.4864 0.5334 6i0.5753 0.8179
36$$$ 6r1 2r2 7r3
39$$$ 1 2 3 40$$$ f3 46$$$ f0
49$$$ 1092235 1092235 1092238 1092238
50$$$ 18 102 18 102
51$$$ 42i1 44 t
end
=xsdrnprm
bapl-1 lattice, 44gr - b-3 calc. - mdd - 4-06-93
0$$$ a3 3 0 4 e
1$$$ 0 1 1 1 3 1 6 8 3 1 10 25 25 0 0
2$$$ -2 0 -1 e
3$$$ 1 5r0 2 0 4 0 0 0
4$$$ -1 2 1 -1 e
5** a6 0.0 55.0310 e t
13$$$ 6r1
14$$$ 3001001 1008016 2013027 1092235 1092238 3008016
15** 3.3730-2 1.6603-2 6.9175-3 1.1006-4 8.1791-3 1.6865-2 t
33** f1.0 t
35** 0.0 0.8179
36$$$ 1
39$$$ 1 40$$$ f3 46$$$ f3
49$$$ 1092235 1092235 1092238 1092238
50$$$ 18 102 18 102
51$$$ 22r1 22r2 t
end

```

Case BIG10

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Description of Case BIG10:

60.96-cm (24.00-in.) diameter uranium metal sphere with 15.24-cm (6.00-in) thick depleted uranium reflector. ²³⁵U enrichment is 10.07 wt%.

Input Listing for Case BIG10:

```

=csasn      parm='size=300000'
big-10 k-calculation -- 44 gr mdd - 5-06-93
44gr multiregion
u-233 1 0.0 1.0-15 end
np-237 1 0.0 1.0-15 end
pu-239 1 0.0 1.0-15 end
u-234 1 0.0 5.00-5 end
u-235 1 0.0 4.84-3 end
u-238 1 0.0 4.268-2 end
u-235 2 0.0 1.00-4 end
u-238 2 0.0 4.797-2 end

```

```

end comp
spherical vacuum reflected 0.0 end
1 30.48 noextermo 2 45.72 noextermo
end zone
end
=xsdrnrm
big-10 s-16, p-3, 44 gr, mdd - 5-06-93
1$$$ 3 3 60 1 0 2 8 16 3 1 10 25 3z
2$$$ -2 0 1 e 3$$$ 8z 6 1 e t
13$$$ 6r1 2r2
14$$$ 1092233 1093237 1094239 1092234 1092235 1092238
      2092235 2092238
15** 3r1-15 5.0-5 4.84-3 4.268-2 1.0-4 4.797-2 t
33** fl.0 t
35** 39i 0 19i 30.48 45.72 36$$$ 1 39r2 20r3
39$$$ 1 1 2 40$$$ f3
49$$$ 1092233 1093237 1094239 1092235 1092238 1092238
50$$$ 5r-18 -102 t
end

```

Case FLAT25

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Description of Case FLAT25:

12.232-cm (4.816-in.) diameter highly enriched (94.2 wt% ²³⁵U) uranium metal sphere
 with 18.014-cm (7.092-in) thick natural uranium (0.698 wt% ²³⁵U) reflector.

Input Listing for FLAT25:

```

=csasn
flattop-25 k-calculation -- 44 gr structure mdd - 5-06-93
44gr multiregion
u-233 1 0.0 1.0-15 end
np-237 1 0.0 1.0-15 end
pu-239 1 0.0 1.0-15 end
u-234 1 0.0 4.90-4 end
u-235 1 0.0 4.449-2 end
u-238 1 0.0 2.70-3 end
u-235 2 0.0 3.40-4 end
u-238 2 0.0 4.774-2 end
end comp
spherical vacuum reflected 0.0 end
1 6.116 noextermo 2 24.13 noextermo
end zone
moredata collapse end
end
1$$$ 3 3 60 1 0 2 8 16 3 1 10 25 3z
2$$$ -2 0 0 e 3$$$ 8z 5 1 e t
13$$$ 6r1 2r2

```

```

14$$$ 1093237 1094239 1092233 1092234 1092235 1092238 2092235
2092238
15** 3r1-15 4.9-4 4.449-2 2.70-3 3.4-4 4.774-2 t
33** f1.0 t
35** 29i 0 29i 6.116 24.13 36$$$ 1 29r2 30r3
39$$$ 1 1 2
40$$$ f3
49$$$ 1093237 1094239 1092233 1092235 1092238
50$$$ 5r-18 t
end

```

Case GODIVA

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Description of GODIVA:

17.482-cm (6.883-in.) diameter, bare, highly enriched (94.7 wt% ²³⁵U) uranium metal sphere.

Input Listing for GODIVA:

```

=csasn      parm='size=300000'
godiva k-calculation -- 44gr mdd - 5-06-93
44gr multiregion
np-237 1 0.0 1.0-15 end
pu-239 1 0.0 1.0-15 end
u-233 1 0.0 1.0-15 end
u-234 1 0.0 4.92-4 end
u-235 1 0.0 4.50-2 end
u-238 1 0.0 2.498-3 end
end comp
spherical vacuum reflected 0.0 end
1 8.741 noextermmod
end zone
moredata collapse end
end
=xsdrrpm
godiva s-16, p-3, 44gr mdd - 5-06-93
1$$$ 3 2 40 1 0 1 6 16 3 1 10 25 3z
2$$$ -1 0 0 e 3$$$ 8z 5 1 e t
13$$$ f1
14$$$ 1093237 1094239 1092233 1092234 1092235 1092238
15** 3r1-15 4.92-4 4.5-2 2.498-3 t
33** f1.0 t
35** 39i 0 8.741 36$$$ 1 39r2
39$$$ 1 1 40$$$ f3
49$$$ 1093237 1094239 1092233 1092235 1092238
50$$$ 5r-18 t
end

```

Case H2OX1

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
TM12460 (DeHart and Bowman 1994)

Description of H2OX1:

13.718-cm (5.400-in.) highly enriched (94.8 wt% ²³⁵U) uranium metal sphere with a
20.14-cm (7.930-in.) thick water reflector.

Input Listing for Case H2OX1:

```
=csasn
h2ox-1 h2o-refl u-sphere: k-calc - 44 gr , mdd - 5-06-93
44gr multiregion
u-233 1 0.0 1.0-20 end
u-234 1 0.0 4.761-4 end
u-235 1 0.0 4.4515-2 end
u-238 1 0.0 2.3872-3 end
h 2 0 0 6.692-2 end
o 2 0 0 3.346-2 end
end comp
spherical vacuum reflected 0.0 end
1 6.859 oneextermad 2 27.0 noextermad
end zone
end
=xsdrrpm
k-calc&react rates for h2ox-1 h2o-refl 44gr up - mdd - 5-06-93
1$$$ 3 2 70 1 0 2 06 16 3 1 10 40 3z
2$$$ -2 5z -1 3z 3$$$ 7z 1 12 1 e t
13$$$ 4r1 2 2
14$$$ 1092233 1092234 1092235 1092238 2001001 2008016
15** 1-20 4.761-4 4.4515-2 2.3872-3 6.692-2 3.346-2
t
33## fl.0t
35**
3i 0 23i 1.054 1i 5.854 3i 6.109 3i 6.609 4i 6.859 3i 7.2
3i 7.7 8.7 17i 9.0 27.0
36$$$ 38r1 32r2 39$$$ 1 2 40$$$ f3
49$$$ 3r1092233 3r1092234 3r1092235 3r1092238
50$$$ -101 -102 -18 3q3
38** 4z fl.0
t
end
```

Case HI240R

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
TM12460 (DeHart and Bowman 1994)

Description of HI240R:

66.80-cm (26.30-in.) diameter sphere of plutonium nitrate in a 0.08-cm (0.03-in.) thick
steel container with a 20.00-cm (7.87-in.) thick, close-fitting, water reflector. ²⁴⁰Pu
content of 45 wt%.

Input Listing for Case HI240R:

```

#csasn
hi-240 k=calculation -- 44 gr M. D. DeHart 5/17/93
44gr multiregion
H      1 0.0 0.063526 end
O      1 0.0 0.035184 end
N      1 0.0 1.287-3  end
pu-238 1 0.0 2.0537-7 end
pu-239 1 0.0 4.2342-5 end
pu-240 1 0.0 4.3694-5 end
pu-241 1 0.0 1.0955-5 end
pu-242 1 0.0 4.7478-6 end
FE      2 0.0 6.3310-2 end
CR      2 0.0 1.6540-2 end
Ni      2 0.0 6.5100-3 end
H      3 0.0 6.6680-2 end
O      3 0.0 3.3340-2 end
end comp
spherical vacuum reflected 0.0 end
1 33.400
2 33.480
3 53.480
end zone
end
#xsdrnmpm
hi-240 s-08/p-3, 44-grp, rqw 6-19-92
-1$$$ 300000 e
1$$$ 3 3 72 1 0 3 13 8 3 1 10 45 3z
2$$$ -1 5z -1 e 3$$$ 8z 5 1 e t
13$$$ 8r1 3r2 2r3
14$$$ 1001001 1008016 1007014 1094238 1094239 1094240 1094241
      1094242 2026000 2024000 2028000 3001001 3008016
15** 6.3526-2 3.5184-2 1.2870-3 2.0537-7 4.2342-5 4.3694-5
      1.0955-5 4.7478-6 6.3310-2 1.6540-2 6.5100-3 6.6680-2 3.3340-2 t
33** fl.0 t
35** 49i 0 33.400 33.440 19i 33.480 53.480
36$$$ 50r1 2r2 20r3
39$$$ 1 2 3 40$$$ f3
49$$$ 1094239 1094240 1094239 1094240 1001001
50$$$ 2r-18 3r-102 t
end

```

Case JEZBxx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Specific Cases: Case JEZB23 Case JEZBEL Case JEZBPU

Description of JEZBEL:

12.770-cm (5.028-in.) diameter, bare plutonium sphere.

Input Listing for Case JEZBEL:

```
=csasn      parm='size=300000'
jezebel k-calculation -- 44 gr
44gr multiregion
u-233  1 0.0 1.0-15  end
u-235  1 0.0 1.0-15  end
u-238  1 0.0 1.0-15  end
np-237 1 0.0 1.0-15  end
ga      1 0.0 1.375-3 end
pu-239 1 0.0 3.705-2 end
pu-240 1 0.0 1.751-3 end
pu-241 1 0.0 1.17-4  end
end comp
spherical vacuum reflected 0.0 end
1 6.385
end zone
moredata collapse end
end
=xsdrrnpm
jezebel s-16, p-3, 44 gr
1$$$ 3 2 40 1 0 1 8 16 3 1 10 25 3z
2$$$ -1 0 0 e
3$$$ 8z 5 1 e t
13$$$ fl
14$$$ 1092233 1092235 1092238 1093237 1094239 1094240 1094241 1031000
15** 4r1-15 3.705-2 1.751-3 1.17-4 1.375-3 t
33** fl.0 t
35** 39i 0 6.385
36$$$ 1 39r2
39$$$ 1 1
40$$$ f3
49$$$ 1093237 1094239 1092233 1092235 1092238
50$$$ 5r-18 t
end
```

Case ORNLx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32

TM12460 (DeHart and Bowman 1994)

Specific Cases: Case ORNL1 Case ORNL2 Case ORNL3
 Case ORNL4 Case ORNL10

Description of ORNL1:

94.4 wt% ²³⁵U enriched, 69.19-cm (27.24-in.) diameter, bare, sphere of ²³⁵U nitride in water. ²³⁵U concentration is 18.7 g/L.

Input Listing for Case ORNL1:

```
#csasn
```

```

ornl-1 k=calculation -- 44gr mdd - 5-06-93
44gr multiregion
h      1 0.0 0.066228 end
o      1 0.0 0.033736 end
n      1 0.0 1.869-4 end
u-234  1 0.0 5.38-7 end
u-235  1 0.0 4.8066-5 end
u-236  1 0.0 1.38-7 end
u-238  1 0.0 2.807-6 end
end comp
spherical vacuum reflected 0.0 end
1 34.595 noextermod
end zone
end
#xsdrnmpm
ornl-1 s-8, p-3, 44gr , mdd - 5-06-93
-1$$ 300000 e
1$$ 3 2 40 1 0 1 7 8 3 1 10 35 3z
2$$ -1 5z -1 e 3$$ 8z 5 1 e t
1$$ fl
14$$ 1001001 1008016 1007014 1092234 1092235 1092236 1092238
15** 0.066228 0.033736 1.869-4 5.38-7 4.8066-5 1.38-7 2.807-6 t
33** fl.0 t
35** 39i 0 34.595 36$$ 1 39r2
39$$ 1 1 40$$ f3
49$$ 1092235 1092238 1092235 1092238 1001001
50$$ 2r-18 3r-102 t
end

```

Case PNL3

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Specific Cases: Case PNL3 Case PNL6B

Description of PNL3:

45.40-cm-(17.87-in.) diameter, bare, sphere of plutonium, nitrogen, iron, and water.

Input Listing for Case PNL3:

```

#csasn
pnl3fg k=calculation -- 44gr mdd - 5-06-93
44gr multiregion
h      1 0.0 0.064950 end
o      1 0.0 0.034410 end
n      1 0.0 7.393-4 end
fe     1 0.0 1.294-6 end
pu-239 1 0.0 5.3950-5 end
pu-240 1 0.0 2.355-6 end
end comp
spherical vacuum reflected 0.0 end

```

```

1 22.700 noextermo
end zone
end
#xsdrnmp
pnl3fg s-08/p-3, 44gr, mdd - 5-06-93
-1$$$ 300000 e
1$$$ 3 2 50 1 0 1 6 8 3 1 10 45 3z
2$$$ -1 5z -1 e 3$$$ 8z 5 1 e t
13$$$ f1
14$$$ 1001001 1008016 1007014 1026000 1094239 1094240
15** 0.06495 0.03441 7.393-4 1.294-6 5.395-5 2.355-6 t
33** f1.0 t
35** 49i 0 22.700 36$$$ 1 49r2
39$$$ 1 1. 40$$$ f3
49$$$ 1094239 1094240 1094239 1094240 1001001
50$$$ 2r-18 3r-102 t
end

```

Case TRXx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Specific Cases: Case TRX1 Case TRX1-1
 Case TRX2 Case TRX2-1

Description of TRX1:

Triangular lattice of 1.29 wt% ²³⁵U enriched uranium fuel pins in water. Pins clad in aluminum. Cylindrical geometry.

Input Listing for CaseTRX1:

```

=csasn
trx-1 lattice cell calculation -- 44 gr
44gr latt
u-235 1 0 6.253-4 end
u-238 1 0 4.7205-2 end
al 2 0 6.025-2 end
h 3 0 6.676-2 end
o 3 0 3.338-2 end
end comp
triangpitch 1.8060 0.9830 1 3 1.1506 2 1.0084 0 end
end
=xsdrnmp
trx-1 lattice,- 44 gr
1$$$ 2 3 15 1 3 3 5 8 3 1 10 25 25 0 0
2$$$ -2 0 -1 e
3$$$ 1 5r0 2 0 4 0 0 0
4$$$ -1 44 1 -2 e
5** a6 0.0 41.6114 e t
13$$$ 2r3 2 2r1
14$$$ 3001001 3008016 2013027 1092235 1092238

```



```

15** 6.676-2 3.338-2 5.173-2 6.253-4 4.7205-2 t
33** f1.0 t
35** 5i0.0 0.4915 0.5334 6i0.5753 0.9482
36$$ 6r1 2r2 7r3
39$$ 1 2 3 40$$ f3 46$$ f0
49$$ 1092235 1092235 1092238 1092238
50$$ 18 102 18 102
51$$ 42i1 44 t
end
=xsdrnpm
trx-1 lattice, - 44 gr - b-3 calc.
0$$ a3 3 0 4 e
1$$ 0 1 1 1 3 1 5 8 3 1 10 25 25 0 0
2$$ -2 0 -1 e
3$$ 1 5r0 2 0 4 0 0 0
4$$ -1 2 1 -1 e
5** a6 0.0 41.6114 e t
13$$ 5r1
14$$ 3001001 3008016 2013027 1092235 1092238
15** 4.2184-2 2.1092-2 5.1436-3 1.6801-4 1.2683-2 t
33** f1.0 t
35** 0.0 0.9482
36$$ 1
39$$ 1 40$$ f3 46$$ f3
49$$ 1092235 1092235 1092238 1092238
50$$ 18 102 18 102
51$$ 22r1 22r2 t
end

```

Case UH3xx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Specific Cases: Case UH3NI Case UH3NR

Description of UH3NI:

15.595-cm (6.140-in.) diameter sphere of highly enriched UH₃ and carbon with a 20.32-cm (8.000-in.) nickel reflector.

Input Listing for Case UH3NI:

```

#csasn
UH3NI k-calculation -- 44 gr mdd - 5-06-93
44gr multiregion
h 1 0.0 0.0518100 end
o 1 0.0 0.0043600 end
c 1 0.0 1.9360-2 end
u-235 1 0.0 1.62700-2 end
u-234 1 0.0 1.70000-4 end
u-238 1 0.0 1.02000-3 end
ni 2 0.0 9.03100-2 end

```

```

end comp
spherical vacuum reflected 0.0 end
1 7.7978
2 28.1178
end zone
end
#xsdrnpm
UH3-NI s-16/p-3, 44gr, mdd - 5-06-93
-1$$ 300000 e
1$$ 3 3 84 1 0 2 7 16 3 1 10 45 3z
2$$ -1 5z -1 e 3$$ 8z 5 1 e t
13$$ 6r1 2
14$$ 1001001 1006012 1008016 1092234 1092235 1092238 2028000
15** 5.18100-2 1.93600-2 4.3600-3 1.70000-4 1.62700-2 1.020-3 9.03100-2 t
33** f1.0 t
35** 49i0 33i7.7978 28.1178
36$$ 1 49r2 34r3
39$$ 1 1 2 40$$ f3
49$$ 1092235 1092238 1092235 1092238 1001001
50$$ 2r-18 3r-102 t
end

```

Case ZPRxx

References: NUREG/CR-6483 (Emmett and Jordan 1996)/Table 32
 TM12460 (DeHart and Bowman 1994)

Specific Cases: Case ZPR66A Case ZPR67 Case ZPR311
 Case ZPR312

Description of ZPR66A:

191.3-cm (75.3-in.) diameter sphere of enriched uranium oxide mixed with sodium and steel. Surrounded by a 33.8-cm (13.3-in.) thick reflector of depleted uranium and steel.

Input Listing for Case ZPR66A:

```

=csasn parm='size=300000'
zpr-6/6a k-calculation -- 44 gr mdd - 5-06-93
44gr multiregion
u-233 1 0.0 1.0-15 end
np-237 1 0.0 1.0-15 end
pu-239 1 0.0 1.0-15 end
u-235 1 0.0 1.153-3 end
u-238 1 0.0 5.8176-3 end
na 1 0.0 9.2904-3 end
o 1 0.0 1.390-2 end
fe 1 0.0 1.3431-2 end
cr 1 0.0 2.842-3 end
ni 1 0.0 1.291-3 end
mn 1 0.0 2.210-4 end
u-235 2 0.0 8.56-5 end
u-238 2 0.0 3.95508-2 end

```

```

o      2 0.0 2.30-5      end
fe     2 0.0 4.4669-3    end
cr     2 0.0 1.247-3     end
ni     2 0.0 5.407-4     end
mn     2 0.0 9.60-5      end
end comp
spherical vacuum reflected 0.0 end
1 95.67 noextermmod 2 129.48 noextermmod
end zone
moredata collapse end
end
=xsdrmpm
zpr-6/6a k-calculation -- 44gr , mdd - 5-06-93
-1$$$ 300000 e
1$$$ 3 3 60 1 0 2 18 4 3 1 10 25 3z
2$$$ -2 0 1 e 3$$$ 8z 6 1 e t
13$$$ 11r1 7r2
14$$$ 1092233 1093237 1094239 1092235 1092238 1011023 1008016
      1026000 1024000 1028000 1025055
      2092235 2092238 2008016 2026000 2024000 2028000 2025055
15** 3r1-15 1.153-3 5.8176-3 9.2904-3 1.390-2 1.3431-2 2.842-3
      1.291-3 2.21-4 8.56-5 3.95508-2 2.30-5 4.4669-3 1.247-3
      5.407-4 9.529-5 t
33** f1.0 t
35** 39i 0 19i 95.67 129.48 36$$$ 1 39r2 20r3
39$$$ 1 1 2 40$$$ f3
49$$$ 1092233 1093237 1094239 1092235 1092238 1092238
50$$$ 5r-18 -102 t
end

```

B2.0 REFERENCES

- DeHart, M.D., and S. M. Bowman, 1994, *Validation of the SCALE Broad Structure 44-Group ENDF-BV Cross Section Library for Use in Criticality Safety Analyses*, ORNL/TM-12460 (NUREG/CR-6102), Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, September, 1994.
- Emmett, M. B., and W. C. Jordan, 1996, *Guide to Verification and Validation of the SCALE-4 Criticality Safety Software*, NUREG/CR-6483 (ORNL/TM-12834), Lockheed Martin Energy Research Corp., Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Primm, R. T., III, 1993, *Criticality Safety Studies of Building 3019 Cell 4 and In-Line Storage Wells*, ORNL/TM-12374, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, November 1993.

APPENDIX C
INPUT LISTINGS

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APPENDIX C

INPUT LISTINGS

Input listings are provided for cases run for comparison to *Criticality Handbook* (Carter et al. 1969) data. When water concentration is varied, the case shown is for that concentration which provides the largest value of k_{∞} .

C1.0 INPUT LISTINGS FOR CRITICALITY HANDBOOK COMPARISONS

The title cards for each input listing indicates the units for H₂O (water) as g/L, but the appropriate units are g/cc.

C1.1 MINIMUM CRITICAL PLUTONIUM CONCENTRATION IN WATER

k_{∞} is calculated for an infinite volume of ²³⁹Pu oxide at a uniform concentration in water. At a concentration of 7.0 g ²³⁹Pu /L, k_{∞} is 0.991547 (Case F10B-6). At a ²³⁹Pu concentration of 7.5 g ²³⁹Pu /L, k_{∞} is 1.02676. Interpolation provides a k_{∞} of 1.000 at a ²³⁹Pu concentration of 7.1 g/L. The water density is 1 g/cc (1000 g/L).

XSDRNPM Input Listing For Case F10B-6:

```
=nitawl
0$$$ 82 e
1$$$ a2. 7 a8 4 e 1t
2$$$ 1001 8016 26000 92235 92238 94240 94239
3**
92235 293. 0 0. 0. 0. 1.000E-10 1 1.008 1.365E+10
1 16.00 1.406E+09 1 1.
92238 293. 0 0. 0. 0. 1.000E-10 1 1.008 1.365E+10
1 16.00 1.406E+09 1 1.
94240 293. 0 0. 0. 0. 1.757E-10 1 1.008 7.769E+09
1 16.00 8.006E+08 1 1.
94239 293. 0 0. 0. 0. 1.764E-05 1 1.008 7.737E+04
1 16.00 7.973E+03 1 1.

2t
end
=xsdrrn
Case F10B-6, 100% Pu(0.0) Metal, 7.0 G Pu/L, H2O=1.0 g/L
1$$$ 3 1 32 1 1 1 7 16 1 1 20 10 0 0 0
2$$$ a7 -1 e
3$$$ 1 a9 3 1 e
4$$$ 0 4 20 -1 7 ehjjjj
5** 2r1.-5 e 1t
13$$$ 1 1 1 1 1 1 1
14$$$ 1001 8016 26000 92235 92238 94240 94239
```

```

15** 6.690E-02 3.349E-02 1.000E-10 1.000E-10 1.000E-10
      1.757E-10 1.764E-05
16$$ 11001 18016 126000 192235 192238 194240 194239
18## 6HH-1 6HO-16 6HFE-26 6HU-235 6HU-238 6HPU-240 6HPU-239
2t
33## fl 4t
35** 31i0.0 16.0
36$$ fl
49$$ 92235 92235 92238
50$$ 18 27 27
51$$ 5r1 5r2 5r3 12r4 5t
end

```

C1.2 k_{∞} FOR HOMOGENEOUS PuO_2 IN WATER

k_{∞} is calculated for an infinite volume of plutonium oxide in a homogeneous water solution. An example is Case F10C-14 for a concentration of 20 g Pu/L with plutonium composed 95 wt% of ^{239}Pu and 5 wt% of ^{240}Pu . k_{∞} is found to be 1.42858. The water density is 1 g/cc (1000 g/L).

XSDRNPM Input Listing for Case F10C-14:

```

=nitawl
0$$ 82 e
1$$ a2 7 a8 4 e 1t
2$$ 1001 8016 26000 92235 92238 94240 94239
3**
92235 293. 0 0. 0. 0. 1.000E-10 1 1.008 1.364E+10
      1 16.00 1.408E+09 11.
92238 293. 0 0. 0. 0. 1.000E-10 1 1.008 1.364E+10
      1 16.00 1.408E+09 11.
94240 293. 0 0. 0. 0. 2.510E-06 1 1.008 5.435E+05
      1 16.00 5.611E+04 11.
94239 293. 0 0. 0. 0. 4.788E-05 1 1.008 2.848E+04
      1 16.00 2.941E+03 11.
2t
end
=xsdnm
Case F10C-14, 100% Pu(5.0) Oxide, 20.0 G Pu/L, H2O=1.0 g/L
1$$ 3 1 32 1 1 1 7 16 1 1 20 10 0 0 0
2$$ a7 -1 e
3$$ 1 a9 3 1 e
4$$ 0 4 20 -1 7 e
5** 2r1.-5 e 1t
13$$ 1 1 1 1 1 1 1
14$$ 1001 8016 26000 92235 92238 94240 94239
15** 6.686E-02 3.353E-02 1.000E-10 1.000E-10 1.000E-10
      2.510E-06 4.788E-05

```



```

16$$ 11001 18016 126000 192235 192238 194240 194239
8## 6HH-1 6HO-16 6HFE-26 6HU-235 6HU-238 6HPU-240 6HPU-239
2t
33## f1 4t
35** 31i0.0 16.0
36$$ f1
49$$ 92235 92235 92238
50$$ 18 27 27
51$$ 5r1 5r2 5r3 12r4 5t
end

```

C1.3 k_{∞} FOR HOMOGENEOUS 1.25 WT% UO_2 IN WATER

k_{∞} is calculated for 1.25 wt% enriched UO_2 over the entire range of water concentration. The maximum k_{∞} of 1.06145 occurs at a water density of 0.35 g/cc (350 g/L) (Case F1A-8). The concentration of UO_2 is held constant at 2000 g/L

XSDRNPM Input Listing for Case F1A-8:

```

=nitawl
0$$ 82 e
1$$ a2 7 a8 4 e 1t
2$$ 1001 8016 26000 92235 92238 94240 94239
3**
92235 293. 0 0.0 0.0 0.0 5.651e-05 1 1.008 8.455e+03 1
1 16.068 1.534e+03 11.
92238 293. 0 0.0 0.0 0.0 4.408e-03 1 1.008 1.082e+02 1
1 16.068 1.967e+01 11.
94240 293. 0 0.0 0.0 0.0 1.000e-08 1 1.008 1.000e+08 1
1 16.068 1.000e+08 11.
94239 293. 0 0.0 0.0 0.0 1.000e-08 1 1.008 1.000e+08 1
1 16.068 1.000e+08 11.
2t
end
=xsdnm
Case F1A-8, U(1.25) Oxide, 2000 g/L, FeO/ $UO_2$ =0.0, H2O=0.35 g/L
1$$ 3 1 32 1 1 1 7 16 1 1 20 10 0 0 0
2$$ a7 -1 e
3$$ 1 a9 3 1 e
4$$ 0 4 20 -1 7 e
5** 2r1.-5 e 1t
13$$ 1 1 1 1 1 1 1
14$$ 1001 8016 26000 92235 92238 94240 94239
15** 2.342-2 2.062-2 1.000-8 5.651-5 4.408-3 1.000-8 1.000-8
16$$ 11001 18016 126000 192235 192238 194240 194239
18## 6HH-1 6HO-16 6HFe-26 6HU-235 6HU-238 6HPu-240 6HPu-239 2T

```

```

33## f1 4t
35** 31i0.0 16.0
36$$ f1
49$$ 92235 92235 92238
50$$ 18 27 27
51$$ 5r1 5r2 5r3 12r4 5t
end

```

KENO V.a Input Listing for Case F1A-8:

```

=csas25
kfla-8
27group infhommedium
u-235 1 0 5.6510e-5 end
u-238 1 0 4.4080e-3 end
pu-239 1 0 1.0000e-8 end
pu-240 1 0 1.0000e-8 end
h 1 0 2.3420e-2 end
o 1 0 2.0620e-2 end
fe 1 0 1.0000e-8 end
end comp
Case F1A-8, U(1.25) Oxide, 2000 g/L, FeO/UO2=0.0, H2O=0.35 g/L
read param gen= 405 npg=600 nsk=5 wrs=34
res=205 nub=yes fdn=yes run=yes plt=no end param
read geom
cuboid 1 1 100.0 -100.0 100.0 -100.0 100.0 -100.0
end geom
read bnds
all=mirror
end bnds
end data
end

```

C2.0 SLUDGE CONFIGURATIONS

Case F9D-6 is representative of tank waste configurations. k_{∞} is calculated for uranium containing 0.84 wt% ^{235}U and 0.30 wt% plutonium. The plutonium contains 16 wt% ^{240}Pu . The FeO/HMO mass ratio is 0.60 (equivalent to a Fe/HM mass ratio of 0.529). The water content is 0.25 g/cc (250 g/L). The XSDRNPM calculated k_{∞} is 0.74536, and the KENO V.a k_{∞} is 0.7377 $\pm$ 0.0008.

XSDRNPM Input Listing for Case F9D-6:

```

=nitawl
0$$ 82 e
1$$ a2 7 a8 4 e 1t
2$$ 1001 8016 26000 92235 92238 94240 94239

```

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```

3**
92235 293. 0 0. 0. 0.      2.366E-05    1      1.008 1.442E+04
                                           1      16.00 3.591E+03   11.
92238 293. 0 0. 0. 0.      2.758E-03    1      1.008 1.237E+02
                                           1      16.00 3.081E+01   11.
94240 293. 0 0. 0. 0.      1.328E-06    1      1.008 2.570E+05
                                           1      16.00 6.399E+04   11.
94239 293. 0 0. 0. 0.      7.002E-06    1      1.008 4.875E+04
                                           1      16.00 1.214E+04   11.

2t
end
=xsdrn
Case F9D-6,[U(0.84), 0.30% Pu(16.0)] Oxide, 2000 G/L,Fe/HM=0.6,H2O=0.25
1$$ 3 1 32 1 1 1 7 16 1 1 20 10 0 0 0
2$$ a7 -1 e
3$$ 1 a9 3 1 e
4$$ 0 4 20 -1 7 e
5** 2r1.-5 e 1t
13$$ 1 1 1 1 1 1 1
14$$ 1001 8016 26000 92235 92238 94240 94239
15** 1.673E-02 2.023E-02 6.287E-03 2.366E-05 2.758E-03
      1.328E-06 7.002E-06
16$$ 11001 18016 126000 192235 192238 194240 194239
18## 6HH-1 6HO-16 6HFE-26 6HU-235 6HU-238 6HPU-240
6HPU-239 2t
33## fl 4t
35** 31i0.0 16.0
36$$ fl
49$$ 92235 92235 92238
50$$ 18 27 27
51$$ 5r1 5r2 5r3 12r4 5t
end

```

KENO V.a Input Listing for Case F9D-6:

```

=csas25
kf9d-6
27group infhommedium
h 1 0 1.6730E-2 end
o 1 0 2.0230E-2 end
fe 1 0 6.2870E-3 end
u-235 1 0 2.3660E-5 end
u-238 1 0 2.7580E-3 end
pu-240 1 0 1.3280E-6 end
pu-239 1 0 7.0020E-6 end
end comp
Case F9D-6,[U(0.84), 0.30% Pu(16.0)] Oxide, 2000 G/L,Fe/HM=0.6,H2O=0.25
read param gen= 205 npg=600 nsk=5 wrs=34

```

```
nub=yes fdn=yes run=yes plt=no end param
read geom
cuboid 1 1 100.0 -100.0 100.0 -100.0 100.0 -100.0
end geom
read bnds
all=mirror
end bnds
end data
end
```

C3.0 REFERENCES

- Carter, R. D., G. R. Kiel, and K. R. Ridgway, 1969, *Criticality Handbook*, ARH-600, Vol. II, Atlantic Richfield Hanford Company, Richland, Washington.
- Greene, N. M., and L. M. Petrie, 1995m "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), Vol. I, II, III, April 1995.
- Petrie, L. M., and N. F. Landers, 1995, "KENO V.a: An Improved Monte Carlo Criticality Program with Supergrouping," *Sect. F11 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, III, April 1995. Available from Radiation Shielding Information Center at Oak Ridge National Laboratory as CCC-545.

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APPENDIX D
INDEPENDENT REVIEW

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APPENDIX D

INDEPENDENT REVIEW

Mr. Warren D. Wittekind of Fluor Daniel Northwest, Criticality & Shielding organization performed an independent peer review. The following is his description of this review.

D1.0 REVIEW

D1.1 LOGIC OF THE CODE VALIDATION

This validation for the XSDRNPM code drew heavily on the software resources available from the SCALE internet web site. The SCALE input files were downloaded from:

http://www.ornl.gov/pub/rsic/scale4.3/critv_v.exe.

This is a self-extracting ZIP file and the SCALE input files are available. Selected cases can then be executed from these input files.

When all the selected cases are executed, then the statistical calculations are also available (the USLSTATS code) from this web site to calculate the upper safety limit based on the SCALE input file results. These upper safety limits were then reported as the main results of this code validation document. The entire process is standardized and automated with reduced chance for error.

D1.2 SCOPE OF THIS INDEPENDENT PEER REVIEW

The SCALE input files were independently recovered from the SCALE internet web site. The independently recovered SCALE input files were checked with listings in this document, and where there was a question about identical values, the SCALE output file was compared directly to these independently downloaded files.

Selected standard SCALE input files were verified: the input was correct and the stated output was correctly translated into the document. The tabulated SCALE case results were used as input files into the USLSTATS code, and this was assumed to have been performed carefully.

Results of the USLSTATS code were then incorporated into tables in this report. The lowest values from the USLSTATS code were then used as the upper safety limits. These values comprise the final result of this validation report, and this was assumed to have been performed carefully.

Conclusions drawn from the results of the USLSTATS code were considered. Any high correlation coefficients were considered, as well as any possible biases introduced from any category of the benchmark cases. The recommendations are consequences of this consideration of the USLSTATS results.

D1.3 COMMENTS ON THE VALIDATION REPORT

The logic of the validation calculation is indisputable. The accuracy of the SCALE input files was verified. The correctness of copying the SCALE output results was verified on selected samples. The entire process is standardized and automated with reduced change for logic error.

The selection of which SCALE input cases are chosen and how the results are grouped for input into USLSTATS is a value judgement, and may differ between criticality safety specialists. The XSDRNPM code is expected to be applied to low enrichment uranium, 0.60 wt% ^{235}U minimum up to 1.25 wt% ^{235}U maximum, smaller proportions of plutonium, up to a maximum of 0.0030 weight fraction of the uranium present, and plutonium compositions with a maximum of 16.6 wt% ^{240}Pu . The iron to uranium composition for the basin sludge is expected to exceed the ratio $\text{Fe}/\text{U}=0.70$.

- There were 19 uranium benchmark cases that were ^{235}U enriched, 5 were enriched to approximately 1.30 wt% ^{235}U , 4 were enriched to 10 to 20 wt% ^{235}U , while the other 10 were very highly enriched at 90 wt% ^{235}U . The correlation coefficient, r^2 , of k_{eff} to ^{235}U enrichment was a high 0.863 for the 44-group calculation and there was an apparent bias due to the uranium ^{235}U enrichment. This bias was in the conservative direction, the low enrichments calculated the highest k_{eff} s.
- There were 14 plutonium benchmark cases and all but 1 involved the ^{240}Pu wt% less than 11.8 wt% ^{240}Pu , that is the expected range. There was no bias apparent due to the plutonium ^{240}Pu composition.
- There were 6 iron critical benchmark cases and the iron composition was a maximum of $\text{Fe}/\text{HM}=0.453$ ratio. Two iron benchmarks were in the thermal neutron energy range (highest $\text{Fe}/\text{HM}=0.005$), while 4, including the highest Fe/HM ratio, were in the fast range. The iron concentration expected in the modeled system $\text{Fe}/\text{HM}=0.7$ contained enough iron to be substantially subcritical. There was no bias apparent due to the Fe/HM mass ratio over the narrow range of the iron benchmarks.
- There were 13 ^{233}U critical benchmark cases that used an isotope that is not of concern in the modeled system. The results are different from all other calculations, as can be seen from the low USL_1 s reported in the final table with USLSTATS results tabulated that an undesirable bias maybe introduced for the 27-group calculations. This bias toward lower USL_1 s are in the fast neutron energy category.
- The 10 iron plate KENO V.a benchmark cases did add confirmation that the iron composition was being correctly calculated by the XSDRNPM code.

The sum of $10+14+6+13+13$ is 52, but 6 were counted in two different categories, so there was only a total of 46 different benchmark cases. There was an obvious consistency between the criticality calculations for all the different situations confirming valid application of the XSDRNPM code to this modeled system. This selection of benchmark cases appears to be adequate for validation.

Another possible value judgement involved how to specify the limits for the XSDRNPM output results into the USLSTATS code. The average energy group (AEG) and the average energy causing fission (AEF) are both output from XSDRNPM and are not subject to value judgements. The hydrogen to heavy metal ration, H/HM for a fast system is very low and may be assumed to be zero.

D1.4 REVIEW COMMENT RECORD

A Review Comment Record (RCR) is provided with comments that required a response by the author. The disposition of these comments is shown on the RCR.

REVIEW COMMENT RECORD (RCR)	1. Date 03/30/99	2. Review No.
	3. Project No.	4. Page 1 of 4

5. Document Number(s)/Title(s) HNF-3950, Rev. 0, Verification and Validation of XSDRNPM Code for Tank Waste Calculations.	6. Program/Project/ Building Number:	7. Reviewer Warren D. Wittekind	8. Organization/Group Fluor Daniel Northwest/ Criticality and Shielding	9. Location/Phone B4-44/ 376-8175
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17. Comment Submittal Approval:

Organization Manager (Optional)

10. Agreement with indicated comment disposition(s)

11. CLOSED

5/13/99
Date
Warren D. Wittekind
Reviewer/Point of Contact
Charles Rogers
Author/Originator

5/13/99
Date
Warren D. Wittekind
Reviewer/Point of Contact
Charles Rogers
Author/Originator

12. Item	13. Comment(s)/Discrepancy(s) (Provide technical justification for the comment and detailed recommendation of the action required to correct/resolve the discrepancy/problem indicated.)	14. Hold Point	15. Disposition (Provide justification if NOT accepted.)	16. Status
1.	A value judgement is the selection of the administrative margin as 0.10 ($k_{\text{limit}} = 0.90$) instead of 0.02 ($k_{\text{limit}} = 0.98$), or 0.05 ($k_{\text{limit}} = 0.95$). This has to do with the simplicity and similarity of the modeled system with the benchmark cases. The dominant constituent is low enrichment uranium, next is the iron, and finally the plutonium. The benchmark cases available considered high ^{235}U enrichment, high ^{235}U enrichment, plutonium systems and some cases with some iron involved. The choice of the 0.10 administrative margin is reasonable, defensible and conservative.		Author concurs with comment. No further action required.	

REVIEW COMMENT RECORD (RCR)			1. Date 03/30/99	2. Review No.
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12. Item	13. Comment(s)/Discrepancy(s) (Provide technical justification for the comment and detailed recommendation of the action required to correct/resolve the discrepancy/problem indicated.)	14. Hold Point	15. Disposition (Provide justification if NOT accepted.)	16. Status
2.	It is recommended to exclude the ²³³ U benchmarks from the final upper safety limit calculation. The ²³³ U benchmarks are fast systems and do seem to introduce some downward bias on the upper safety limit for the 27 group XSDRNPM calculations, from the final upper safety limit calculation. This is relevant because at the end of the conclusions section, the 27 group upper safety limit is recommended for both the 27 group and 44 group calculations.		The Uranium-233 fast data was not included. However, the Uranium-233 thermal data was included. These data will be removed, and the Upper Safety Limit will be recalculated. Table 7-1 will be revised.	

REVIEW COMMENT RECORD (RCR)		1. Date 03/30/99		2. Review No.	
		3. Project No.		4. Page 3 of 4	
12. Item	13. Comment(s)/Discrepancy(s) (Provide technical justification for the comment and detailed recommendation of the action required to correct/resolve the discrepancy/problem indicated.)	14. Hold Point	15. Disposition (Provide justification if NOT accepted.)		16. Status
3.	<p>It is also recommended that the final calculation for the upper safety limit should include both fast and thermal systems together. Since the uranium and plutonium tend to collect in the sludge layer where the H/HM is lower, it makes sense to include both the thermal and fast systems together for the final upper safety limit calculation so that the H/HM range of applicability will not be limited at some arbitrary H/HM ratio. Additionally, four of the six Fe/U benchmarks are for fast systems, and considering only the thermal systems, as was done, includes only two Fe/U and the highest Fe/U=0.005, much lower than the range of application which is expected to be >Fe/U=0.70. Furthermore, consider the description of water content from WHC-SD-SQA-CSA-507, Rev. 0, <i>Criticality Parameters for Tank Waste Evaluation</i>, which states: "Water content in waste varies from very high in supernatant liquid to relatively low in dry waste. ... At the very low plutonium concentration in waste, optimal water content is generally a state of extreme dryness. (section 3.3.2)" This published description infers that the thermal and fast benchmark measurements should both be used in the XSDRNPM validation because there is no artificial H/HM ratio, such as H/HM=100, that divides off an irrelevant area for waste tank criticality code validation.</p>	X	<p>The report includes evaluation of an Upper Safety Limit with all 46 experiments. However, this is not applicable to K Basin Sludge or existing tank wastes because the sludge and/or wastes cannot be dried to the point of producing a fast system.</p> <p>In CSA-507, "optimal water content" means optimal moderation. At that point the system is not a fast system. The H/X range stated in the report applies to the range of benchmark data and is not artificially chosen. The H/X limit has been modified to a description of AEF to more clearly represent moderation in the system.</p>		

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