TSUNAMI Analysis of the Applicability of Proposed Experiments to Reactor-Grade and Weapons-Grade Mixed-Oxide Systems

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The applicability of proposed critical experiments for the criticality code validation of a series of prototypic reactor-grade and weapons-grade mixed-oxide systems has been assessed with the TSUNAMI methodology from SCALE 5. The application systems were proposed by the Nuclear Energy Agency (NEA) Organization for Economic Cooperation and Development (OECD) Working Party on Nuclear Criticality Safety MOX Experimental Needs Working Group. Forty-eight application systems were conceived to envelope the range of conditions in processing and fabrication of reactor-grade and weapons-grade MOX fuel. The applicability of 303 existing critical benchmarks to each of the 48 applications was assessed, and validation coverage was found to be lacking for certain applications. Two series of proposed critical experiments were also considered in this analysis. The TSUNAMI analysis has revealed that both series of proposed experiments are applicable to numerous configurations of the reactor-grade and weapons-grade systems. A detailed assessment of which experiments were revealed by TSUNAMI to be most applicable to specific prototypic fuel processing systems has been performed.

KEYWORDS: TSUNAMI, MOX, experiment

1. Introduction

Oak Ridge National Laboratory (ORNL) has applied the **T**ools for **S**ensitivity and **Un**certainty **A**nalysis **M**ethodology **I**mplementation (TSUNAMI)[1,2] from the SCALE code system[3] to assess the applicability of existing experiments and conceptual experiment designs for the validation of criticality safety codes for the analysis of weapons-grade (WG) and reactor-grade (RG) mixed-oxide (MOX) fuel. TSUNAMI includes one-dimensional and three-dimensional sensitivity analysis sequences that compute the sensitivity of k_{eff} to the neutron cross-section data. These sensitivity data can be used to compute relational integral indices that assess the similarity of two systems based on the nuclide-reaction-specific and energy-dependent sensitivity data. TSUNAMI has been demonstrated as an effective method for determining the applicability of benchmark experiments for use in code validation.[4]

The applicability of 303 existing benchmark experiments and 9 proposed critical experiments are evaluated relative to 48 configurations of MOX fuel, representative of those that could be encountered in MOX fuel processing and fabrication.

2. TSUNAMI Analysis Techniques

TSUNAMI techniques from SCALE 5 were used to assess the similarity of the existing and proposed benchmark experiments to prototypic MOX fuel systems. The TSUNAMI-3D sequence utilizes the KENO V.a Monte Carlo code and computes the sensitivity of k_{eff} to cross-section data on a group-wise and nuclide-reaction specific basis.[2] These sensitivity data can be coupled with the uncertainty in the cross-section data to produce an uncertainty in k_{eff} due to uncertainties in the basic nuclear data.[1] As cross-section data are believed to be a likely cause of computational biases, a benchmark experiment with uncertainties in k_{eff} that are highly correlated to the uncertainties in the design system will provide a good indication of the expected computational bias. The SCALE 5 code TSUNAMI-IP processes the

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sensitivity data and cross-section-covariance data and produces a correlation coefficient, denoted c_k, that provides an indication of the similarity of a given benchmark experiment to a design system in terms of the correlations in the uncertainties between the two systems. This correlation coefficient is normalized such that a c_k value of 1.0 indicates that the two systems are identical, and a c_k value of 0.0 indicates that the two systems are completely dissimilar. The c_k correlation coefficient is a global integral index in that it produces a single value from information about all nuclides and all reactions of both systems on an energy-dependent basis. Thus, the computed value of c_k provides an indication of the overall similarity of two systems.

TSUNAMI-IP also provides the ability to use sensitivity data to investigate the coverage provided by a benchmark experiment for a certain nuclide-reaction pair and to quantify the uncertainty in the application due to nuclides and reactions that are not fully covered by the benchmark data. However, due to the brevity of this format, these results from this study are not presented. All of the TSUNAMI techniques are explained in greater detail in the SCALE 5 manual.[3)]

3. Prototypic MOX Applications

The Nuclear Energy Agency (NEA), Organization for Economic Cooperation and Development (OECD) Working Party on Nuclear Criticality Safety MOX Experimental Needs Working Group proposed 48 prototypic application systems to envelope the range of conditions in processing and fabrication of reactor-grade and weapons-grade MOX. The proposed applications have a MOX density of 5 g/cm^3, PuO_2 contents of 10–30 wt %, water contents of 0–5 wt %, and bare and water-reflected conditions. Some properties of the 48 prototypic applications are shown in Table 1. The TSUNAMI-1D analysis sequence from SCALE 5 was used to generate sensitivity data for each MOX application with the SCALE 238-group ENDF/B-V library.

4. Existing Experiments

To assess the need for new experimental data, ORNL performed a review of existing critical benchmark experiments containing MOX and plutonium. This review of existing experiments included numerous experiments from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE)[5)] as well as benchmarks from other sources.[6,7)] We selected 303 critical configurations for inclusion in this analysis. Summaries of the analyzed experiments are provided in Table 2. Sensitivity data were generated for each of these experiments using the TSUNAMI-3D sensitivity analysis sequence from SCALE 5.

5. IPPE Experiments

The Institute for Physics and Power Engineering (IPPE) has proposed a series of critical experiments to be assembled at the BFS-1 facility in Obninsk, Russia. Each of the critical configurations would consist of stacked pellets of WG plutonium in stainless steel cans and depleted UO_2 in aluminum cans. These fuel stacks will be contained in 5.0-cm-diam aluminum tubes in a hexagonal array with a 5.1-cm pitch. Some configurations will include polyethylene pellets intermixed with the fuel stack and polyethylene dowels inserted between the aluminum tubes. All configurations will have a large depleted UO_2 reflector region. Each of the four proposed experiments is summarized in Table 3. Sensitivity data were generated for each of these experiments using the TSUNAMI-3D sensitivity analysis sequence from SCALE 5.

Table 1 Properties of prototypic MOX application systems

PuO_2 content wt %	^{239}Pu content	Water content wt %	Reflector	Identifier	k_{eff}	EALF (eV)	AECF (eV)	H/(U+Pu)
10	Reactor Grade	0	bare	10r0b	1.01	2.75E+05	1.17E+06	0.00
			reflected	10r0r	1.01	6.72E+03	9.36E+05	0.00
		1	bare	10r1b	1.00	1.86E+04	9.66E+05	0.30
			reflected	10r1r	1.00	1.46E+03	7.99E+05	0.30
		3	bare	10r3b	0.99	1.39E+03	7.51E+05	0.90
			reflected	10r3r	0.99	2.63E+02	6.40E+05	0.90
		5	bare	10r5b	0.99	2.93E+02	6.22E+05	1.50
			reflected	10r5r	0.99	8.53E+01	5.40E+05	1.50
	Weapons Grade	0	bare	10w0b	1.02	2.99E+05	1.18E+06	0.00
			reflected	10w0r	1.01	4.08E+03	9.06E+05	0.00
		1	bare	10w1b	1.00	2.11E+04	9.76E+05	0.30
			reflected	10w1r	1.00	1.11E+03	7.83E+05	0.30
		3	bare	10w3b	1.00	1.29E+03	7.51E+05	0.90
			reflected	10w3r	1.00	1.76E+02	6.17E+05	0.90
		5	bare	10w5b	1.00	2.42E+02	6.14E+05	1.50
			reflected	10w5r	1.00	5.15E+01	5.09E+05	1.50
20	Reactor Grade	0	bare	20r0b	1.01	4.56E+05	1.28E+06	0.00
			reflected	20r0r	1.00	2.61E+03	8.95E+05	0.00
		1	bare	20r1b	1.00	6.43E+04	1.08E+06	0.30
			reflected	20r1r	1.00	1.25E+03	7.91E+05	0.30
		3	bare	20r3b	0.99	5.92E+03	8.37E+05	0.90
			reflected	20r3r	0.99	3.77E+02	6.46E+05	0.90
		5	bare	20r5b	0.99	1.38E+03	6.97E+05	1.50
			reflected	20r5r	0.99	1.63E+02	5.55E+05	1.50
	Weapons Grade	0	bare	20w0b	1.01	4.85E+05	1.28E+06	0.00
			reflected	20w0r	1.00	2.08E+03	8.81E+05	0.00
		1	bare	20w1b	1.00	7.66E+04	1.09E+06	0.30
			reflected	20w1r	1.00	1.04E+03	7.83E+05	0.30
		3	bare	20w3b	1.00	6.37E+03	8.51E+05	0.90
			reflected	20w3r	1.00	3.04E+02	6.39E+05	0.90
		5	bare	20w5b	0.99	1.30E+03	7.02E+05	1.50
			reflected	20w5r	1.00	1.21E+02	5.42E+05	1.50
30	Reactor Grade	0	bare	30r0b	1.01	5.91E+05	1.36E+06	0.00
			reflected	30r0r	1.00	2.77E+03	9.18E+05	0.00
		1	bare	30r1b	1.00	1.33E+05	1.17E+06	0.30
			reflected	30r1r	1.00	1.55E+03	8.21E+05	0.30
		3	bare	30r3b	0.99	1.49E+04	9.21E+05	0.90
			reflected	30r3r	1.00	5.58E+02	6.79E+05	0.90
		5	bare	30r5b	0.99	3.64E+03	7.69E+05	1.50
			reflected	30r5r	0.99	2.65E+02	5.87E+05	1.50
	Weapons Grade	0	bare	30w0b	1.01	6.18E+05	1.37E+06	0.00
			reflected	30w0r	1.00	2.35E+03	9.10E+05	0.00
		1	bare	30w1b	1.00	1.58E+05	1.19E+06	0.30
			reflected	30w1r	1.00	1.34E+03	8.17E+05	0.30
		3	bare	30w3b	1.00	1.72E+04	9.42E+05	0.90
			reflected	30w3r	1.00	4.82E+02	6.78E+05	0.90
		5	bare	30w5b	0.99	3.80E+03	7.84E+05	1.50
			reflected	30w5r	1.00	2.16E+02	5.83E+05	1.50

Table 2 Summary description of existing benchmark experiments analyzed

Experiment identifier	Number of experimental configurations	Range of H/(Pu+U)	Range of Pu/(Pu+U)	Range of EALF (eV)
PU-SOL-THERM-001	6	86.7 to 352.91	1	8.85E-02 to 3.36E-01
PU-SOL-THERM-002	7	299.3 to 508.0	1	7.10E-02 to 9.98E-02
PU-SOL-THERM-003	8	545.3 to 774.1	1	5.82E-02 to 6.87E-02
PU-SOL-THERM-004	13	573.3 to 981.7	1	5.31E-02 to 6.73E-02
PU-SOL-THERM-005	9	557.2 to 866.4	1	5.53E-02 to 6.80E-02
PU-SOL-THERM-006	3	910.9 to 1028.2	1	5.21E-02 to 5.46E-02
PU-SOL-THERM-010	14	259.3 to 825.1	1	5.32E-02 to 1.05E-01
PU-SOL-THERM-011	12	550.7 to 1157.3	1	5.26E-02 to 7.45E-02
PU-SOL-THERM-014	35	210.2	1	1.69E-01 to 1.70E-01
PU-SOL-THERM-015	16	155.3	1	2.41E-01 to 2.43E-01
PU-SOL-THERM-016	11	155.3 to 210.2	1	1.69E-01 to 2.42E-01
PU-SOL-THERM-017	18	210.2	1	1.69E-01
PU-SOL-THERM-020	8	343.0 to 747.2	1	5.89E-02 to 1.06E-01
PU-SOL-THERM-021	2	124.81 to 667.0	1	6.60E-02 to 3.13E-01
PU-COMP-MIXED-001	5	0.04 to 49.6	1	1.54E+00 to 9.57E+05
PU-COMP-MIXED-002	29	0.04 to 49.6	1	6.84E-01 to 4.92E+03
MIX-SOL-THERM-001	11	44.08 to 418.64	0.22 to 0.97	9.25E–02 to 2.84E–01
MIX-SOL-THERM-002	3	481.37 to 1150.66	0.23 to 0.52	4.24E–02 to 4.34E–02
MIX-COMP-THERM-001	4	3.33 to 17.53	0.22	2.11E–04 to 1.61E–03
MIX-COMP-THERM-002	6	1.19 to 3.64	0.020	1.38E–01 to 7.73E–01
MIX-COMP-THERM-003	6	1.68 to 10.75	0.066	1.01E–01 to 9.06E–01
MIX-COMP-THERM-004	11	2.42 to 5.55	0.028 to 0.030	8.02E–02 to 1.46E–01
MIX-COMP-THERM-005	6	2.22 to 11.87	0.040	9.56E-02 to 3.99E-01
PU-8-1 to PU-29-9)	13	2.77 to 7.33	0.08 to 0.29	6.30E-01 to 4.14E+01
BNWL-2129, Table 3)	29	30.6	0.15	1.43E–01 to 2.57E–01
BNWL-2129, Table 4)	18	7.13 to 9.37	0.27 to 0.28	1.51E+00 to 6.13E+00

Table 3 Summary description of proposed IPPE experiments

Identifier	Polyethylene in fuel stack	Polyethylene dowels between tubes	H/(Pu+U) in fuel tube	Pu/(Pu+U)	EALF (eV)
BFS-97-1	No	No	0	0.30	3.56E+05
BFS-97-2	No	Yes	0	0.30	1.16E+05
BFS-97-3	Yes	No	1.38	0.30	5.60E+03
BFS-97-4	Yes	Yes	1.38	0.30	1.88E+03

6. Valduc Experiments

The Valduc Criticality Laboratory has proposed a series of critical experiments to be assembled on Apparatus B. Each critical configuration would be constructed of water-flooded fuel rod arrays of RG MOX. The RG MOX fuel rods have a PuO_2 content of 27.5 wt %, an outer diameter of 0.735 cm, and an active fuel height of 100 cm. The proposed critical configurations place the fuel rods on triangular pitches ranging from 0.96 to 1.04 cm. Each of the five proposed configurations are summarized in Table 4. Sensitivity data were generated for each of these experiments using the TSUNAMI-3D sensitivity analysis sequence from SCALE 5.

Table 4 Summary description of proposed Valduc experiments

Identifier	Triangular pitch (cm)	H/(Pu+U)	Pu/(Pu+U)	EALF (eV)
MOX-96	0.96	0.71	0.27	1.24E+03
MOX-98	0.98	0.94	0.27	7.77E+02
MOX-100	1.00	1.18	0.27	5.47E+02
MOX-102	1.02	1.42	0.27	3.80E+02
MOX-104	1.04	1.66	0.27	2.55E+02

7. Applicability of Existing Experiments

The global integral index c_k was computed for each prototypic MOX application system in relation to each existing experiment. Current guidance[)] states that an experiment is adequately similar to a design application to serve in its code and data validation if the c_k value relating the experiment to the application is 0.9 or higher. The experiment may be applicable to the code validation if its c_k value is 0.8 or higher. Furthermore, to ensure that the correct computational bias is determined for a given application, approximately 15–20 experiments with c_k values of at least 0.9 or 25–40 experiments with c_k values between 0.8 and 0.9 are recommended. It is expected that fewer experiments with c_k values near 1.0 should also provide for an adequate assessment of the computational bias.

The similarity of the 303 existing experiments to the MOX applications was assessed using the integral index c_k generated from the TSUNAMI-IP code. The number of existing experiments with $c_k \geq 0.9$ for each weapons- and reactor-grade application are shown in Figures 1 and 2, respectively. For the weapons-grade applications, several configurations have 15 or more experiments with c_k values ≥ 0.9, but many others do not. For the reactor-grade applications, no application has 15 experiments with $c_k \geq 0.9$. Thus, the need for additional benchmark data is confirmed.

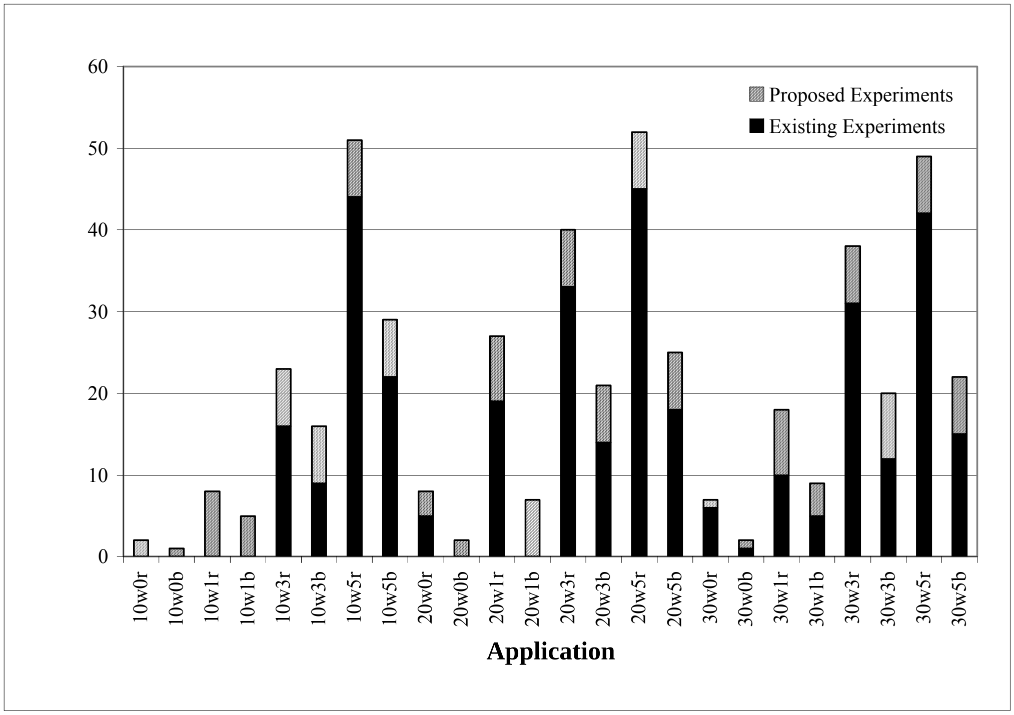

Fig. 1 Number of existing and proposed experiments with $c_k \geq 0.9$ relative to weapons-grade MOX applications.

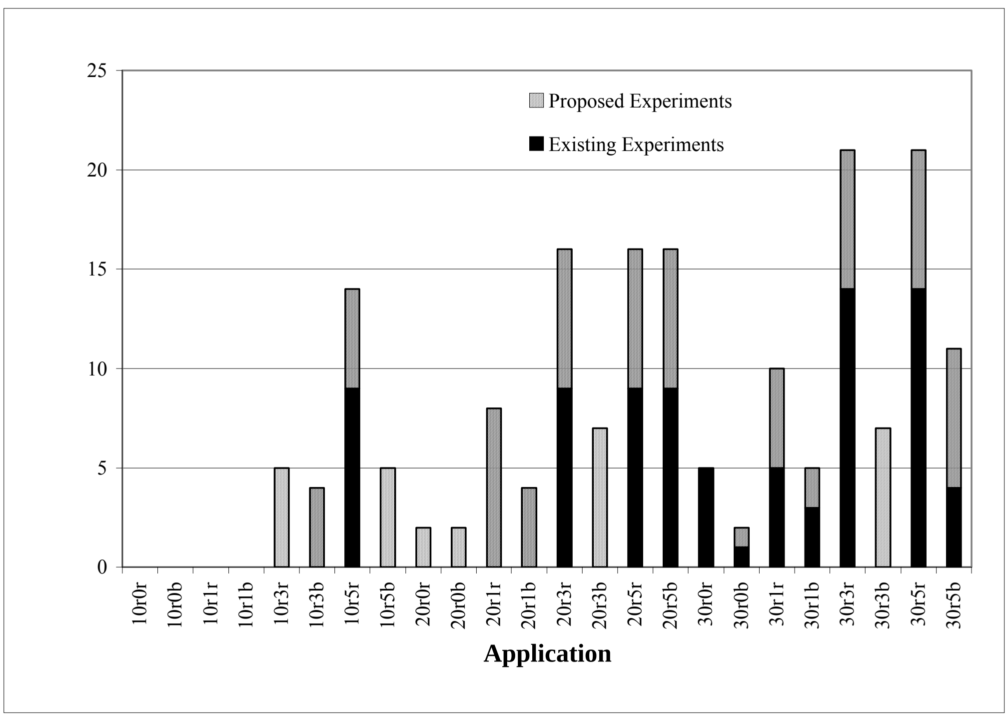

Fig. 2 Number of existing and proposed experiments with $c_k \geq 0.9$ relative to reactor-grade MOX applications.

8. Applicability of Proposed Experiments

The similarity of the nine proposed experiments to the MOX applications was assessed using the integral index c_k generated from the TSUNAMI-IP code. The c_k values for each of the proposed experiments relative to each weapons- and reactor-grade application are shown in Figures 3 and 4, respectively, and the number of proposed experiments with $c_k \geq 0.9$ for each weapons- and reactor-grade application are shown in Figures 1 and 2, respectively. Many of the proposed experiments exhibit c_k values $\geq$ 0.9 for both the weapons- and reactor-grade MOX applications, indicating that the experiments would provide useful data for code validation for these applications.

Further analysis of Figures 3 and 4 reveals that the two dry BFS experiments, configurations 1 and 2, are the most similar to the dry MOX applications, with 0 or 1 wt % water content, whereas the other two BFS experiments and the Valduc experiments are more similar to the 3 and 5 wt % water-content applications.

A more in-depth analysis of the reasons for the similarities of these systems is warranted but is not possible due to the brevity of this format.

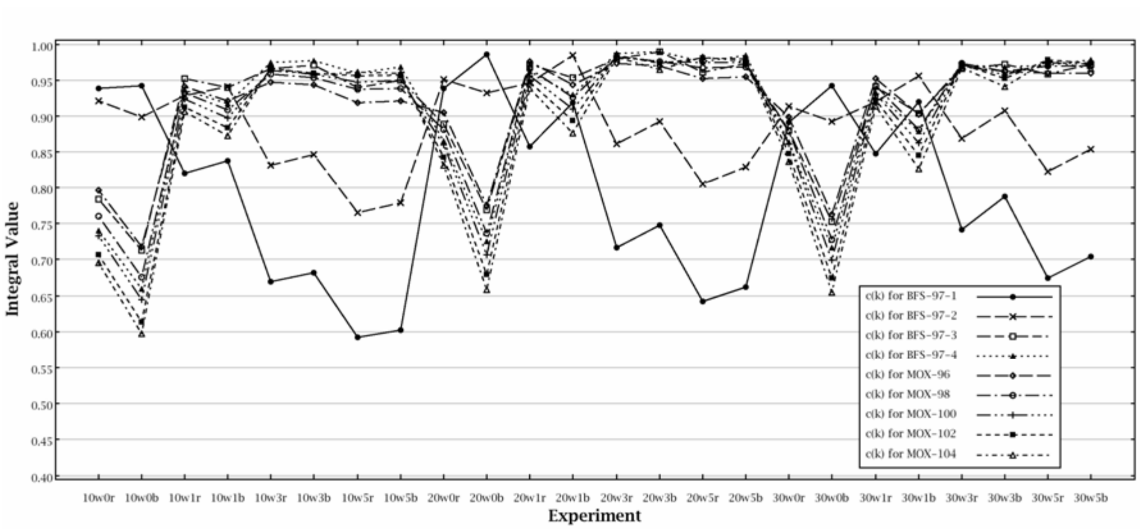

Fig. 3 Values of c_k for proposed experiments compared to weapons-grade applications.

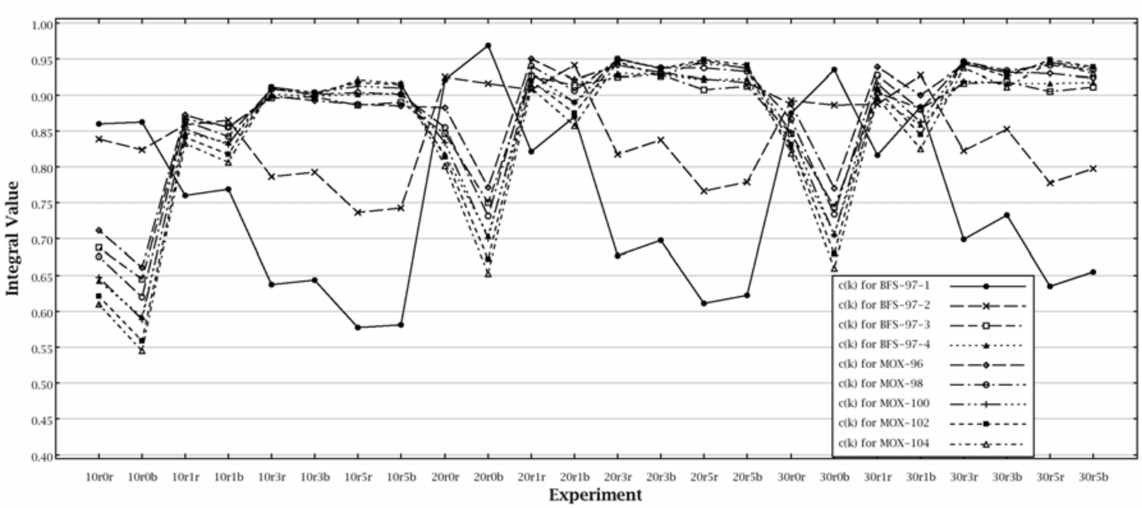

Fig. 4 Values of c_k for proposed experiments compared to reactor-grade applications.

9. Conclusions

The TSUNAMI techniques from SCALE 5 have been used to identify the need for additional benchmark data for the criticality code validation of weapons- and reactor-grade MOX applications. The TSUNAMI techniques have also confirmed that two series of proposed critical experiments both exhibit a high degree of similarity to the MOX applications and would provide useful new data for the criticality code validation of these proposed applications.

10. References

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