

APPLICATION OF VALIDATION METHODOLOGIES FOR A GENERIC VALIDATION PROBLEM

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ABSTRACT

A hypothetical operation problem was analyzed using several system parameters for code and data validation. The hypothetical problem is an array of 5-gal buckets with 2-ft edge-to-edge spacing. The buckets contain low-enriched uranium at or below 5 weight percent ^{235}U in the form of UO_2F_2 in waste material consisting of NaF or incinerator ash. The USLSTATS computer program is used to determine the upper subcritical limit (USL). System parameters are calculated using KENO V.a and the 238-group ENDF/B-V neutron cross-section library. In this study, energy of average lethargy causing fission (EALF), average energy group causing fission (AEGF), hydrogen-to-fissile ($\text{H}/^{235}\text{U}$) ratio, and the fissile isotope enrichment are used as the system parameters. In addition to this traditional approach to determining bias and uncertainty, a new approach that uses integral parameters based on sensitivity/uncertainty theory is used. The utility of the new integral parameters is demonstrated.

Key Words: criticality, validation, sensitivity, KENO V.a, SCALE

1 INTRODUCTION

This validation exercise was performed to follow the guidance of the Draft American National Standard ANSI/ANS-8.24, Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations. The purpose of the standard is to provide guidance on the process and methods that should be considered and/or used in the validation of neutron transport calculational methods for nuclear criticality safety analyses. When completed, the standard will provide guidance for establishing the area of applicability, estimating the bias and uncertainties, and selecting appropriate margins, both within and beyond the established area of applicability. The objective of the current study is to validate a code and the associated data set for a hypothetical problem. After identifying the pertinent parameters that should be considered for selecting appropriate benchmark experiments for potential trending of the data and for defining the area of applicability, analyses are performed to compare various validation methods.

* Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

2 PROBLEM DESCRIPTION

A hypothetical operation problem was defined by the working group of the American National Standard ANSI/ANS-8.24, which is currently being developed. It is comprised of an array of 5-gal buckets with 2-ft edge-to-edge spacing. The buckets contain low-enriched uranium at or below 5 weight percent ^{235}U in the form of UO_2F_2 in waste material consisting of NaF or incinerator ash. The uranium loading varies from small amounts of uranium to densities up to 3 g uranium per cubic centimeter. Under normal operating conditions, the material is dry at a H/U ratio of approximately 4. Upset conditions involve inclusion of water in the buckets as a moderator.

3 SYSTEM/PROCESS PARAMETER IDENTIFICATION

Since the sensitivity of the validation to the process parameters was not known, a set of parameters was selected that will sufficiently describe the process. These parameters and their associated data are presented in Table I.

Table I. Process parameters and data

Parameter	Process data
Fissile material	^{235}U in UO_2F_2
Fissile form	UO_2F_2 compound form (normal condition) UO_2F_2 solution (upset condition)
Moderation (H/X)	20 (normal condition) 600 (abnormal – estimated optimum moderation)
Enrichment (% U-235)	1–5% (analyzed at 5%)
Uranium concentration	Minimal to 3000 g/l
Moderating material	Water
Other materials	Predominant elements are Na, F, C
Reflecting material	Unreflected (light steel) – normal condition Water reflected – abnormal condition
Geometry	Cylinders and arrays
Heterogeneity/Homogeneity	Homogeneous system
Neutron energy	Unknown, estimated to be intermediate to thermal energy spectrum

The computational model of the problem included several assumptions that were made to arrive at a configuration that was representative of the hypothetical system. The model consisted of a 10×10 array of buckets filled with UO_2F_2 compound placed in a corner of a concrete room. The room was modeled as Magnuson concrete with 15-cm-thick walls and ceiling and 25-cm-thick floor. The room is 1096.3 cm square (wall-to-wall) and 500.0 cm high (inside). The Magnuson concrete was selected since it results in larger k_{eff} values when compared with other

types of concrete [1]. The system has a k_{eff} of less than 0.2 under normal conditions. Therefore, only the upset condition, which was flooding the buckets and the floor with water, was analyzed further. The buckets were modeled according to the specifications in American National Standard for 5-gal straight-side log-cover steel pails [2]. Although the final model represented a probable configuration corresponding to an abnormal condition, it was not necessarily the worst configuration. No attempt has been made to determine the worst configuration, as it was not the objective of this exercise.

4 SELECTION OF BENCHMARK EXPERIMENTS

Forty-three experiments were selected by the working group of the American National Standard ANSI/ANS-8.24. Of these 43 experiments, 15 are solution experiments. The remaining 28 experiments contain uranium in compound form as either UF_4 or $\text{UO}_2 - \text{UO}_2\text{F}_2$. A list of the experiments and their parameters is provided in Table II.

5 MODELING AND CALCULATED RESULTS OF THE BENCHMARK EXPERIMENTS

All of the benchmark experiments were modeled using the SCALE 5 code system [3] and the 238-group neutron cross-section library that is mainly based on the ENDF/B-V evaluations. The computational results are presented in Table III.

6 VALIDATION METHODOLOGY

The USLSTATS [4] computer program was used to determine the upper subcritical limit (USL). The USLSTATS program uses two methods—(1) confidence band with administrative margin and (2) single-sided uniform-width closed interval—to calculate the USL based on a common system parameter. In this study, energy of average lethargy causing fission (EALF), average energy group causing fission (AEGF), hydrogen-to-fissile ($\text{H}/^{235}\text{U}$) ratio, and the fissile isotope enrichment were used as the system parameters. In addition to this traditional approach to determining bias and uncertainty, a new approach that uses sensitivity/uncertainty theory as documented in Refs. 5-8 has been used.

Effective multiplication factors were calculated using the 3-D Monte Carlo code KENO V.a and the 238-group cross-section library of the SCALE code system. The sensitivities were calculated using TSUNAMI-3D sequence of SCALE.

Table II. Benchmark experiment parameters

Experiment	Fissile material	Fissile material form	Enrichment (%)	Fissile concentration (g U/l)	Interstitial moderator	Reflector material	H/X ratio	S/X ratio *	Geometry	Experimental uncertainty
1	UO ₂ , UO ₂ F ₂	Compound	4.9	300	None	None	1687	924	9x10 Array	0.01
2	UO ₂ , UO ₂ F ₂	Compound	4.9	300	None	None	1687	924	6x7 Array	0.01
3	UO ₂ , UO ₂ F ₂	Compound	4.9	300	None	None	1687	924	6x7 Array	0.01
4	UO ₂ , UO ₂ F ₂	Compound	4.9	300	None	None	1687	924	6x7 Array	0.01
5	UO ₂ , UO ₂ F ₂	Compound	4.9	300	None	None	1687	924	6x7 Array	0.01
6	UO ₂ F ₂	Solution	4.9	42.54	Water (solution)	None	524	344	Cylinder	0.005
7	UO ₂ F ₂	Solution	4.9	42.54	Water (solution)	None	524	344	Slab	0.005
8	UO ₂ F ₂	Solution	4.9	31.79	Water (solution)	None	735	448	Cylinder	0.005
9	UO ₂ F ₂	Solution	4.9	24.04	Water (solution)	None	1002	580	Sphere	0.005
10	UO ₂ F ₂	Solution	4.9	24.28	Water (solution)	None	991	575	Cylinder	0.005
11	UO ₂ F ₂	Solution	4.9	42.54	Water (solution)	Water	524	344	Cylinder	0.005
12	UO ₂ F ₂	Solution	4.9	42.54	Water (solution)	Water	524	344	Slab	0.005
13	UO ₂ F ₂	Solution	4.9	31.79	Water (solution)	Water	735	448	Cylinder	0.005
14	UO ₂ F ₂	Solution	4.9	22.11	Water (solution)	Water	1099	628	Sphere	0.005
15	UO ₂ F ₂	Solution	4.9	24.22	Water (solution)	Water	994	576	Cylinder	0.005
16	UF ₄	Compound	1.4	2490	Paraffin	None	422	478	Array	0.01
17	UF ₄	Compound	1.4	2490	Paraffin	None	422	478	Array	0.01
18	UF ₄	Compound	2.0	3640	Paraffin	Paraffin, Plexiglas	195	291	Array	0.01
19	UF ₄	Compound	2.0	3640	Paraffin	None	195	291	Array	0.01
20	UF ₄	Compound	2.0	2596	Paraffin	Paraffin	294	338	Array	0.01
21	UF ₄	Compound	2.0	2596	Paraffin	None	294	338	Array	0.01
22	UF ₄	Compound	2.0	2184	Paraffin	Paraffin, Plexiglas	406	293	Array	0.01
23	UF ₄	Compound	2.0	1936	Paraffin	Paraffin, Plexiglas	496	436	Array	0.01
24	UF ₄	Compound	2.0	1692	Paraffin	Polyethylene, Plexiglas	614	493	Array	0.01
25	UF ₄	Compound	2.0	1692	Paraffin	None	614	493	Array	0.01

*This is the number density ratio of light scattering elements ($Z < 26$) to the fissile nuclide (excluding H).

Table II. Benchmark experiment parameters (continued)

Experiment	Fissile material	Fissile material form	Enrichment (%)	Fissile concentration (g U/l)	Interstitial moderator	Reflector material	H/X ratio	S/X ratio *	Geometry	Experimental uncertainty
26	UF ₄	Compound	2.0	1214	Paraffin	Polyethylene, Plexiglas	972	665	Array	0.01
27	UF ₄	Compound	2.0	1214	Paraffin	None	972	665	Array	0.01
28	UF ₄	Compound	3.0	3056	Paraffin	Paraffin, Plexiglas	133	196	Array	0.01
29	UF ₄	Compound	3.0	3056	Paraffin	Paraffin, Plexiglas	133	196	Array	0.01
30	UF ₄	Compound	3.0	3056	Paraffin	Paraffin, Plexiglas	133	196	Array	0.01
31	UF ₄	Compound	3.0	3056	Paraffin	Paraffin, Plexiglas	133	196	Array	0.01
32	UF ₄	Compound	3.0	3056	Paraffin	Paraffin, Plexiglas	133	196	Array	0.01
33	UF ₄	Compound	3.0	3056	Paraffin	None	133	196	Array	0.01
34	UF ₄	Compound	3.0	3056	Paraffin	None	133	196	Array	0.01
35	UF ₄	Compound	3.0	3056	Paraffin	None	133	196	Array	0.01
36	UF ₄	Compound	3.0	2174	Paraffin	Polyethylene, Plexiglas	277	265	Array	0.01
37	UF ₄	Compound	3.0	2174	Paraffin	None	277	265	Array	0.01
38	UF ₄	Compound	3.0	2174	Paraffin	None	277	265	Array	0.01
39	UF ₄	Compound	3.0	2174	Paraffin	None	277	265	Array	0.01
40	UO ₂ F ₂	Solution	5.0	910.36	Water (solution)	Water	488	325	Cylinder	0.006
41	UO ₂ F ₂	Solution	5.0	910.36	Water (solution)	Water	488	325	Cylinder	0.006
42	UO ₂ F ₂	Solution	5.0	910.18	Water (solution)	None	490	325	Cylinder	0.006
43	UO ₂ F ₂	Solution	5.0	910.36	Water (solution)	None	490	325	Cylinder	0.006

*This is the number density ratio of light scattering elements ($Z < 26$) to the fissile nuclide (excluding H).

Table III. Calculation results for the benchmark experiments

Experiment	Calculated k_{eff}	Statistical uncertainty	Average energy group	Average lethargy energy (eV)
1	0.9912	0.0016	216.4	0.048
2	0.9972	0.0016	214.3	0.057
3	0.9937	0.0020	214.2	0.059
4	0.9925	0.0016	214.6	0.056
5	0.9947	0.0018	215.1	0.054
6	0.9912	0.0018	214.8	0.054
7	0.9961	0.0021	214.8	0.054
8	0.9952	0.0020	216.8	0.045
9	0.9939	0.0015	218.2	0.040
10	1.0010	0.0013	218.2	0.040
11	1.0032	0.0019	215.4	0.051
12	1.0043	0.0018	215.7	0.050
13	1.0015	0.0015	217.2	0.044
14	1.0001	0.0016	218.7	0.038
15	1.0042	0.0016	218.3	0.039
16	0.9929	0.0015	205.4	0.123
17	0.9910	0.0014	205.4	0.123
18	0.9967	0.0016	199.5	0.205
19	0.9989	0.0017	197.4	0.245
20	1.0032	0.0017	205.8	0.120
21	1.0000	0.0015	204.1	0.138
22	1.0024	0.0016	209.5	0.086
23	1.0001	0.0020	211.3	0.073
24	1.0000	0.0015	213.0	0.063
25	1.0004	0.0018	212.4	0.067
26	0.9952	0.0014	215.9	0.049
27	0.9972	0.0012	215.7	0.050
28	1.0112	0.0018	197.5	0.242
29	1.0070	0.0020	197.4	0.243
30	1.0114	0.0017	197.5	0.242
31	1.0108	0.0017	197.6	0.241
32	1.0096	0.0019	197.5	0.242
33	1.0088	0.0019	193.8	0.328
34	1.0119	0.0020	193.8	0.328
35	1.0136	0.0016	193.8	0.328
36	1.0122	0.0018	208.4	0.095
37	1.0139	0.0015	206.5	0.112
38	1.0189	0.0019	206.5	0.112
39	1.0105	0.0016	206.4	0.113
40	1.0049	0.0020	214.3	0.057
41	1.0006	0.0017	214.4	0.056
42	1.0045	0.0018	214.4	0.056
43	0.9953	0.0018	214.4	0.056

7 ANALYSIS

Analysis of the hypothetical system indicates that with the current edge-to-edge separation between the units, the largest k_{eff} for the upset conditions is around 0.8. When water is added to the powder, the water causes the powder to turn into slush, which was modeled as a homogeneous mixture of UO_2F_2 and water, where water fills the void space in the bucket that contains the powder. In this case, the largest k_{eff} , 0.85545 ± 0.00097 , is achieved with 1500 g U/l and a water volume fraction of 0.69. In addition, two other configurations with smaller edge-to-edge separations were selected for analysis. These cases were selected from a parametric study that resulted in k_{eff} values close to 1.0. The $\text{H}/^{235}\text{U}$, EALF, AEGF, and fuel density are given in Table IV.

Table IV. Parameter values for selected mixtures of UO_2F_2 and H_2O

Case	Case filename	k_{eff}	sigma	EALF (eV)	AEGF	$\text{H}/^{235}\text{U}$	g U/l
1	mix194-100u-069wat	0.8555	0.0010	0.091	209	240	1500
2	mix388-100u-039wat-s1*	1.0066	0.0009	0.345	193	68	3000
3	mix388-100u-039wat-s2**	0.9097	0.0004	0.343	193	68	3000

*Edge-to-edge separation of 1 cm.

**Edge-to-edge separation of 2 cm.

When water mixes with the UO_2F_2 powder, it could form a solution. Similar to the mixtures above, the configuration with uranyl fluoride solution that results in the largest k_{eff} and the configurations with an edge-to-edge spacing that yield k_{eff} values close to 1.0 were selected. The salt and water densities corresponding to various fuel densities were taken from Ref. 9. The parameter values for these configurations are listed in Table V.

Table V. Parameter values for selected solution configurations

Case	Case filename	k_{eff}	sigma	EALF (eV)	AEGF	$\text{H}/^{235}\text{U}$	g U/l
4	sol1776	0.8236	0.0010	0.088	209	300	1373
5	sol1776-s5*	1.0008	0.0010	0.083	210	300	1373
6	sol3760-s3**	0.9995	0.0011	0.376	192	100	2905

*Edge-to-edge separation of 5 cm.

**Edge-to-edge separation of 3 cm.

8 RESULTS

Using various procedures such as AEGF, EALF, H/X [4], c_k , E_{sum} , and GLLSM [5-8], the application systems were analyzed to determine the bias and associated standard deviation. The results are given in Table VI. The c_k and E_{sum} parameters, which give a measure of the system's similarity to the benchmarks that are being used in the validation, are listed in Table VII. A c_k value of 0.9 [10] or greater indicates similarity between the application system and the

benchmark. Likewise, an E_{sum} value of 0.9 [10] or greater indicates similarity between two systems. The c_k parameter is based on the cross-section uncertainty data as well as the sensitivities, whereas the E_{sum} parameter depends strictly on the sensitivities. These parameters indicate that 19 or more of a total of 43 benchmarks qualify as being very similar to the application problem.

The trend plots for EALF, AEGF, and $H/^{235}\text{U}$ are shown in Figs. 1 through 3, respectively. The AEGF method results in a maximum bias of 2.16% (bias + 2σ). Although AEGF indicates the similarity between systems based on the spectrum (group wise) of neutrons, it is easily skewed by some high-energy neutrons causing fission. Maximum bias calculated with the EALF method is 2.46%. Trending with the H/X method results in a maximum bias of 1.75%. In all three methods (AEGF, EALF, and H/X), cases 2, 3 and 6 fall outside the range of available benchmark values. The method based on the generalized linear least squares method (GLLSM)[6] has a maximum calculated bias of 1.6%.

Table VI. Predicted bias and its standard deviation for various methods

	Case 1			Case 2			Case 3		
Method	Application value	% bias	% std dev	Application value	% bias	% std dev	Application value	% bias	% std dev
AEGF	209	0.11	0.60	193	0.89	0.60	193	0.89	0.60
EALF	0.091	-0.01	0.60	0.343	1.12	0.60	0.343	1.11	0.60
H/X	240	0.41	0.60	68	0.55	0.60	68	0.55	0.60
c_k	0.9845*	-0.01	0.73	0.9753	0.90	0.62	0.9804	0.85	0.61
E_{sum}	0.9847*	-0.03	0.73	0.9471	0.90	0.71	0.9530	-0.63	0.71
GLLSM**	--	0.12	0.23	--	0.34	0.28	--	0.34	0.63
	Case 4			Case 5			Case 6		
Method	Application value	% bias	% std dev	Application value	% bias	% std dev	Application value	% bias	% std dev
AEGF	209	0.09	0.60	210	0.05	0.60	192	0.96	0.60
EALF	0.088	-0.03	0.60	0.082	-0.05	0.60	0.375	1.26	0.60
H/X	300	0.36	0.60	300	0.36	0.60	100	0.53	0.60
c_k	0.9883	-0.02	0.72	0.9909	-0.08	0.72	0.9799	0.87	0.59
E_{sum}	0.9888	-0.20	0.71	0.9885	-0.08	0.72	0.9737	0.90	0.57
GLLSM**	--	0.08	0.24	--	0.07	0.14	--	0.47	0.31

* The c_k and E_{sum} values are the largest calculated values for the application against all benchmarks.

** The GLLSM bias is the predicted Δk bias, and the standard deviations are the standard deviations of biased k_{eff} due to cross-section uncertainties.

Table VII. System correlation parameter values

	Case 1	Case 2	Case 3
$c_k > 0.9$	33	27	30
$E_{sum} > 0.9$	43	43	37
	Case 4	Case 5	Case 6
$c_k > 0.9$	28	42	23
$E_{sum} > 0.9$	43	43	19

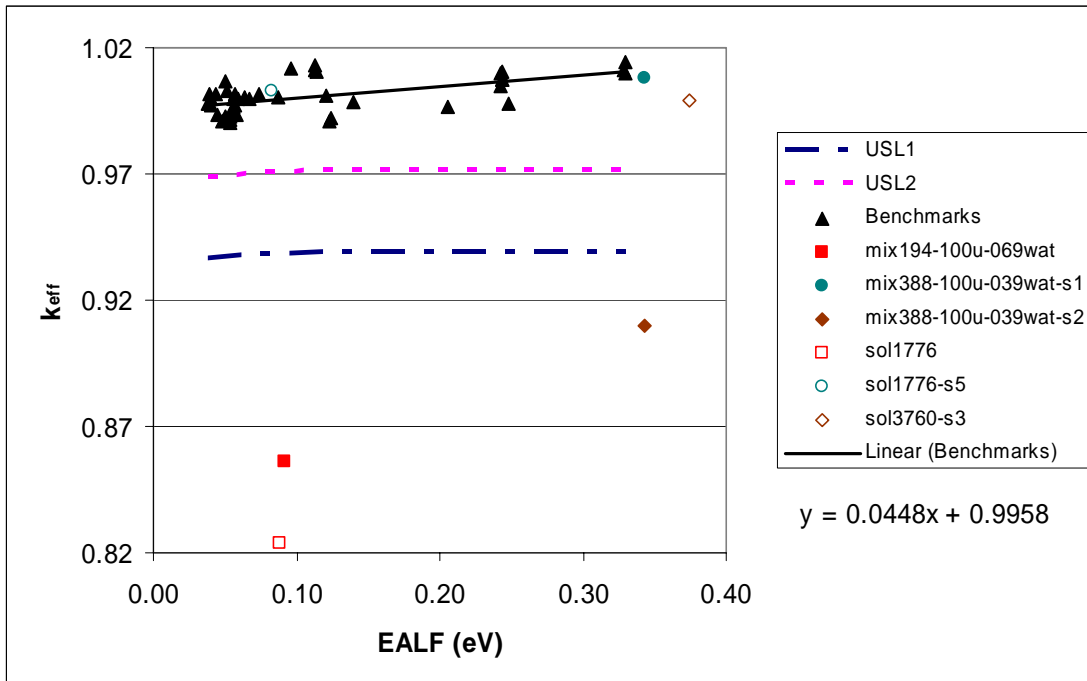


Figure 1. Values for k_{eff} vs EALF

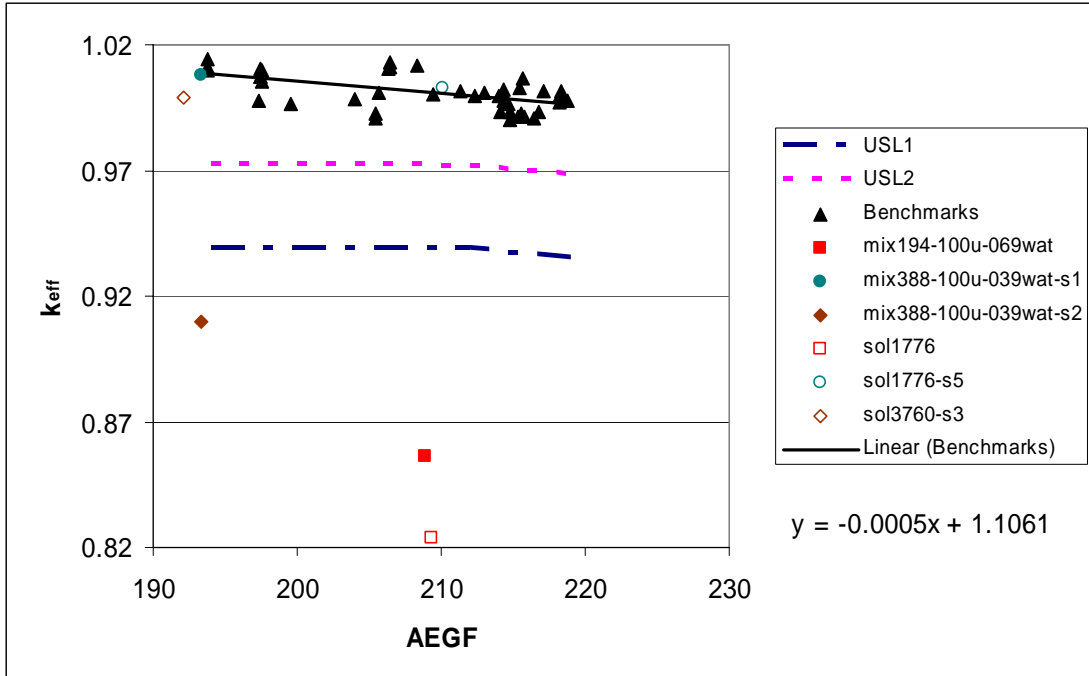


Figure 2. Values for k_{eff} vs $AEGF$

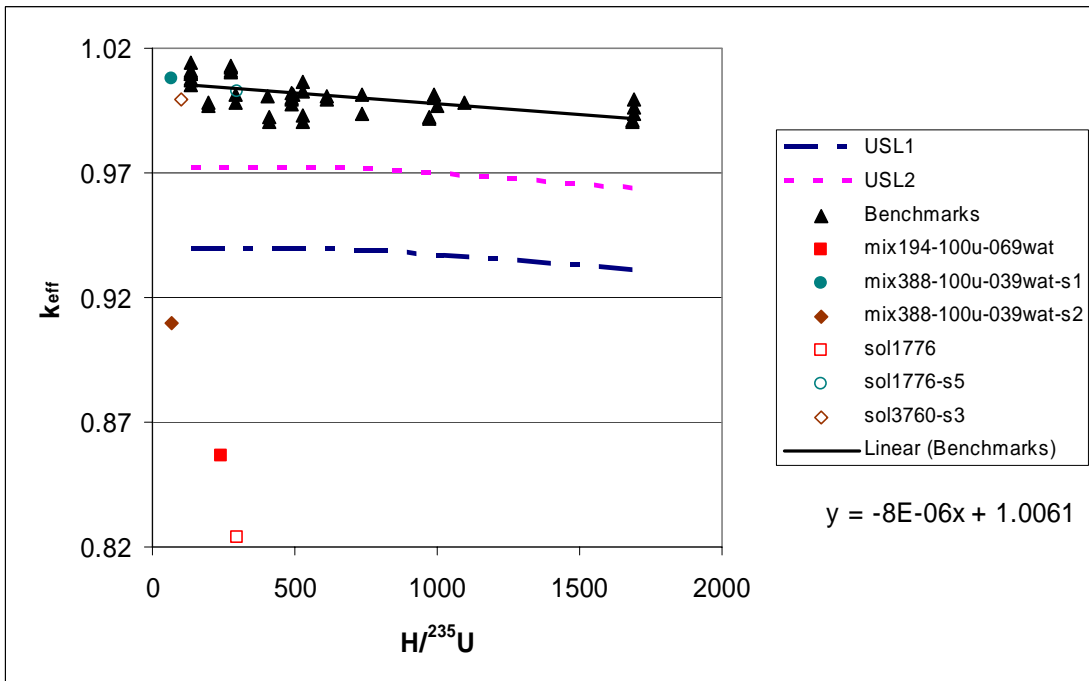


Figure 3. Values for k_{eff} vs $H/^{235}\text{U}$

The trend plots for c_k and E_{sum} for all six configurations are shown in Figs. 4 through 15. The c_k and E_{sum} parameters for the six application configurations are plotted against the benchmark problems and shown in Figs. 16 and 17, respectively. Analyses of the c_k and E_{sum} values indicate that some of the benchmarks that are included in the analysis have small c_k or E_{sum} values (less than 0.9) and therefore skew the calculation of the bias. Further analysis indicates that these benchmarks, despite being similar to the application configurations, have very low fuel concentration, which renders the systems less similar. Hence, the application configurations have been analyzed with different subsets of the benchmark problems: one set that includes all benchmarks, one set that includes only the benchmarks that yield a c_k value of 0.9 or greater, and another set with benchmarks that yield an E_{sum} value of 0.9 or greater. Analysis results with these three sets are listed in Table VIII for Case 3. For this case, the c_k set includes 30 benchmarks, and the E_{sum} set includes 37 benchmarks. The c_k and E_{sum} parameters for Case 3 are plotted against the similar set of benchmark problems and shown in Figs. 18 and 19, respectively. Analysis of the three sets for normality using the Shapiro-Wilk test indicates that the sets based on c_k and E_{sum} values ≥ 0.9 are normal whereas the complete set is not normal.

Using the set based on c_k values generally causes an increase in the calculated bias among different methods, including the method based on the c_k parameter. The E_{sum} set results in even greater bias values from all methods except for the E_{sum} method.

9 SUMMARY

Although the greatest bias is calculated using the EALF method using the E_{sum} set, due to inclusion of cross-section uncertainty data in the calculation of bias, the c_k method has been selected to determine the final bias because it utilizes the cross-section uncertainties. In addition, since the set based on c_k values ≥ 0.9 form a normal distribution, only the benchmarks that comprise this smaller set was included in the final bias calculation. Hence, the bias for application Case 3 is 1.2% with a percent standard deviation of 0.60, which results in a calculated bias of 2.4% (bias + 2σ). The sensitivity/uncertainty-based approach yields a comparable bias to the traditional approaches but addresses the issue of applicability of the benchmarks for the assessment of bias and uncertainty.

Table VIII. Predicted bias and its standard deviation for various methods using similar set of benchmarks

Procedure	Case3						
	Application value	Complete set		Similar set (c_k)		Similar set (E_{sum})	
		% bias	% std dev	% bias	% std dev	% bias	% std dev
AEGF	193	0.89	0.60	0.92	0.65	1.27	0.53
EALF	0.343	1.11	0.60	1.07	0.65	1.59	0.56
H/X	68	0.55	0.60	0.64	0.63	0.66	0.51
GLLSM	--	0.34	0.26	0.36	0.27	0.37	0.30
c_k	0.980	0.85	0.61	1.20	0.60	--	--
E_{sum}	0.953	-0.63	0.71	--	--	-0.48	0.67

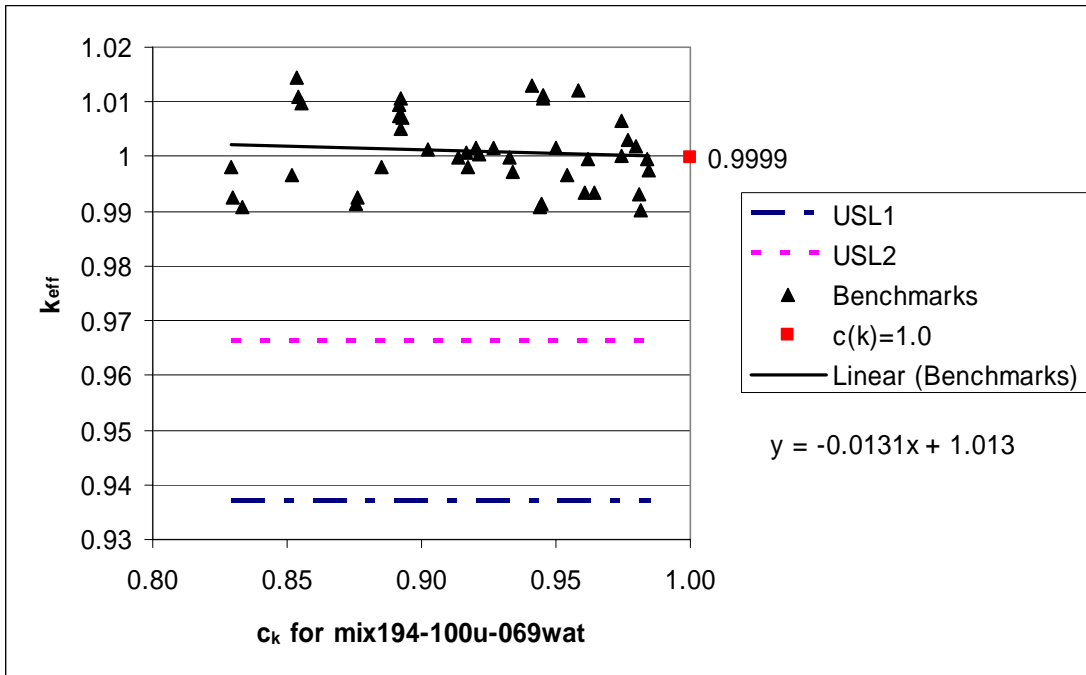


Figure 4. Values for k_{eff} vs c_k for Case 1

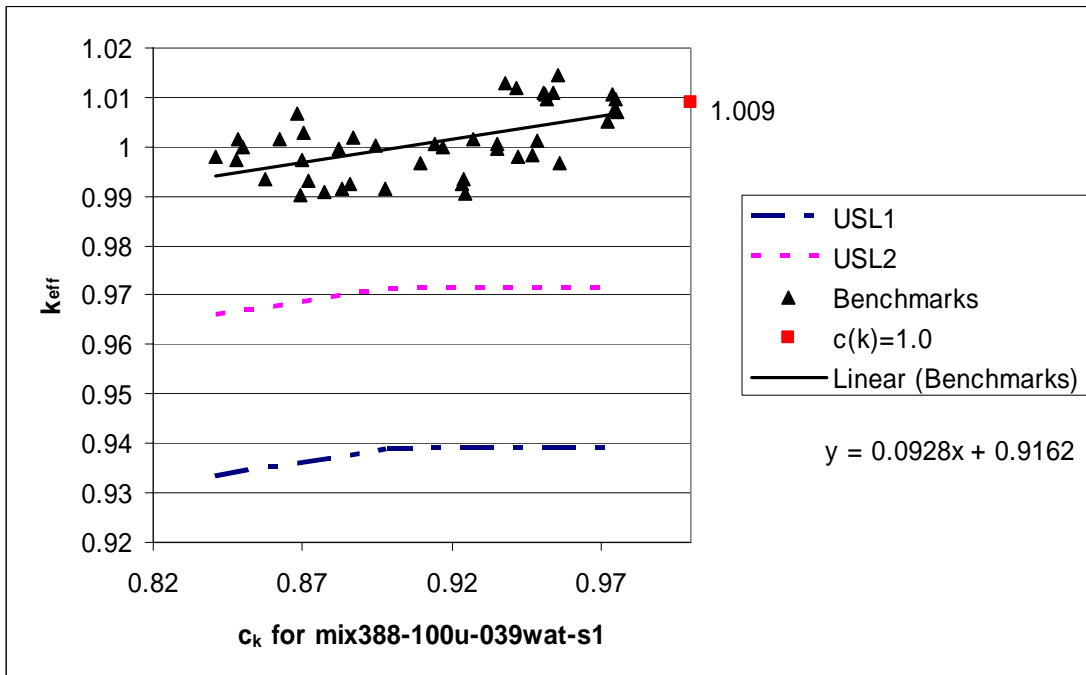


Figure 5. Values for k_{eff} vs c_k for Case 2

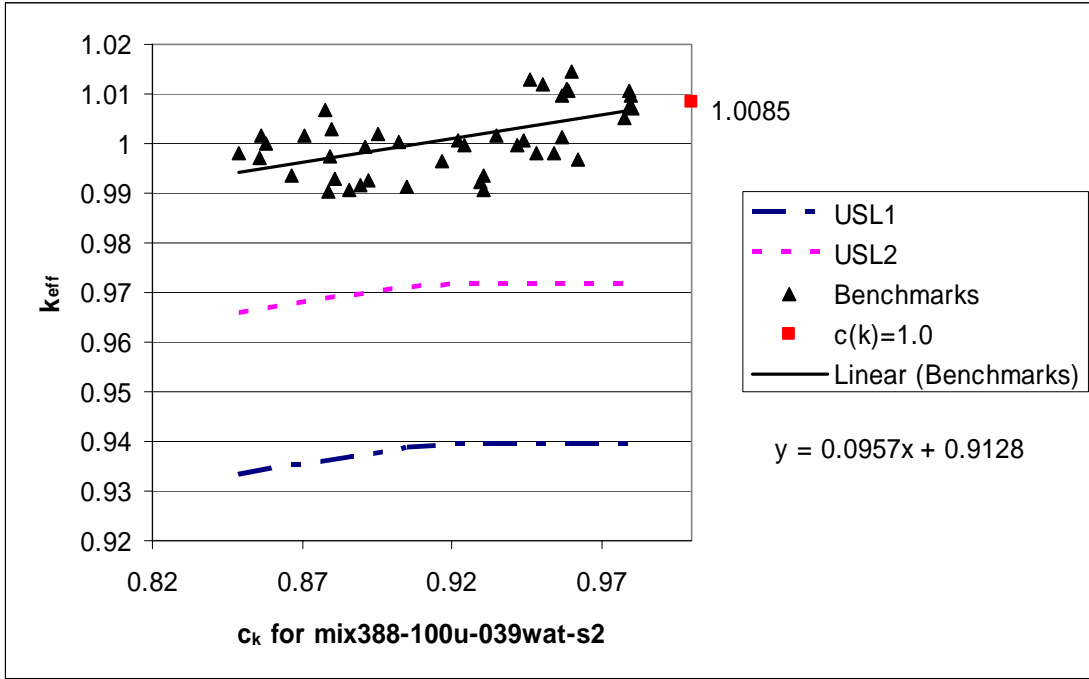


Figure 6. Values for k_{eff} vs c_k for Case 3

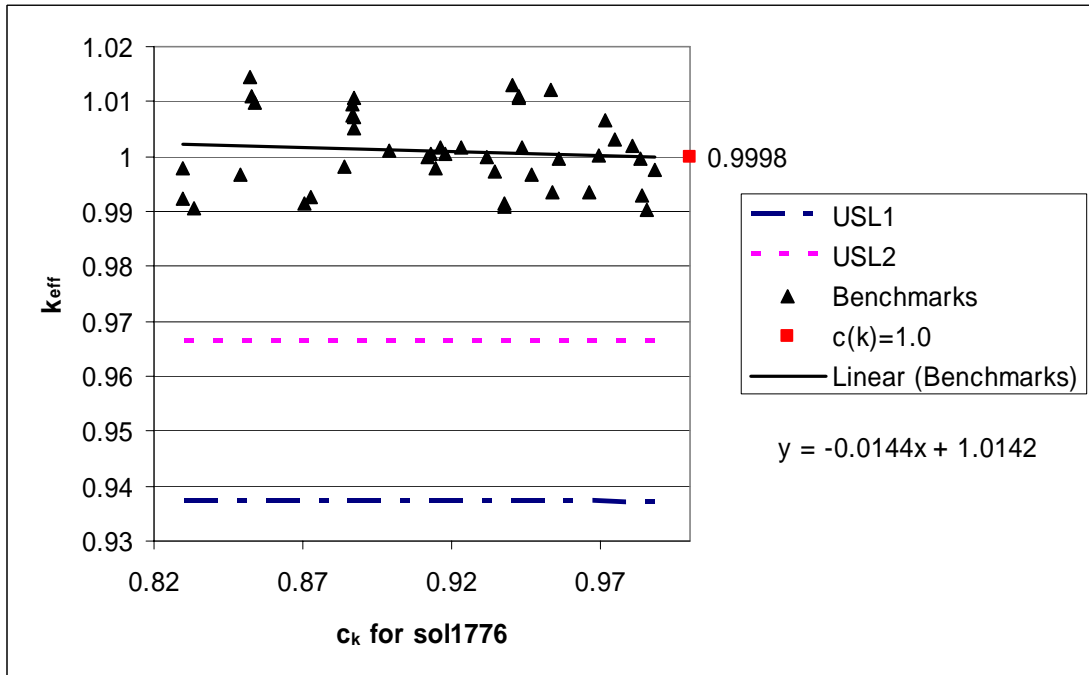


Figure 7. Values for k_{eff} vs c_k for Case 4

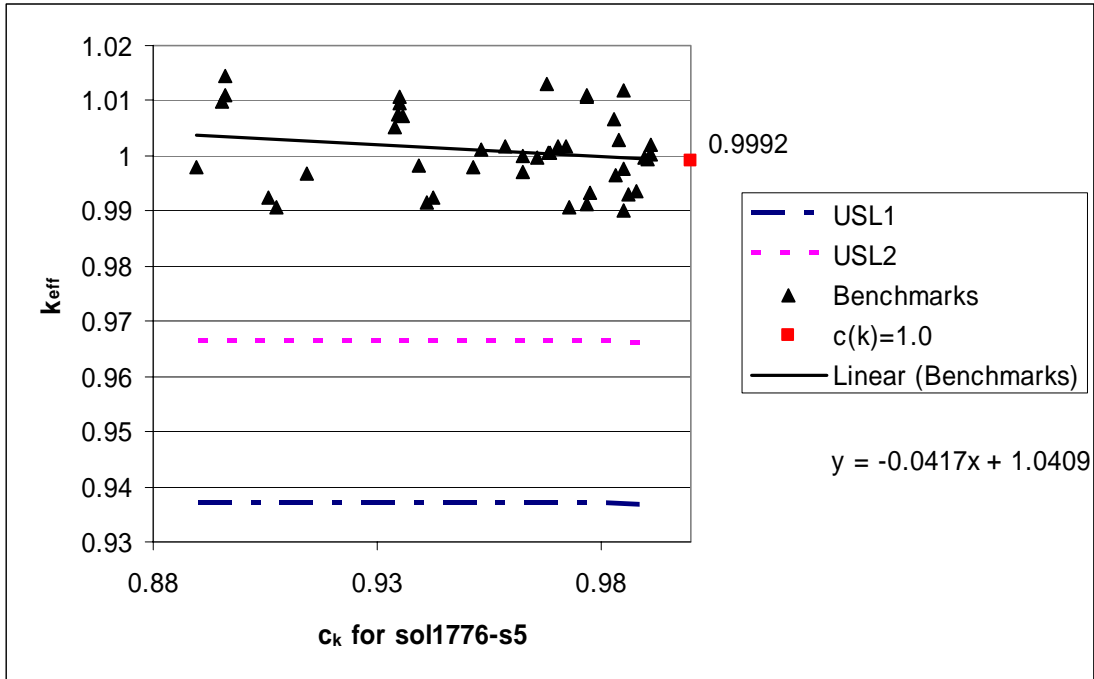


Figure 8. Values for k_{eff} vs c_k for Case 5

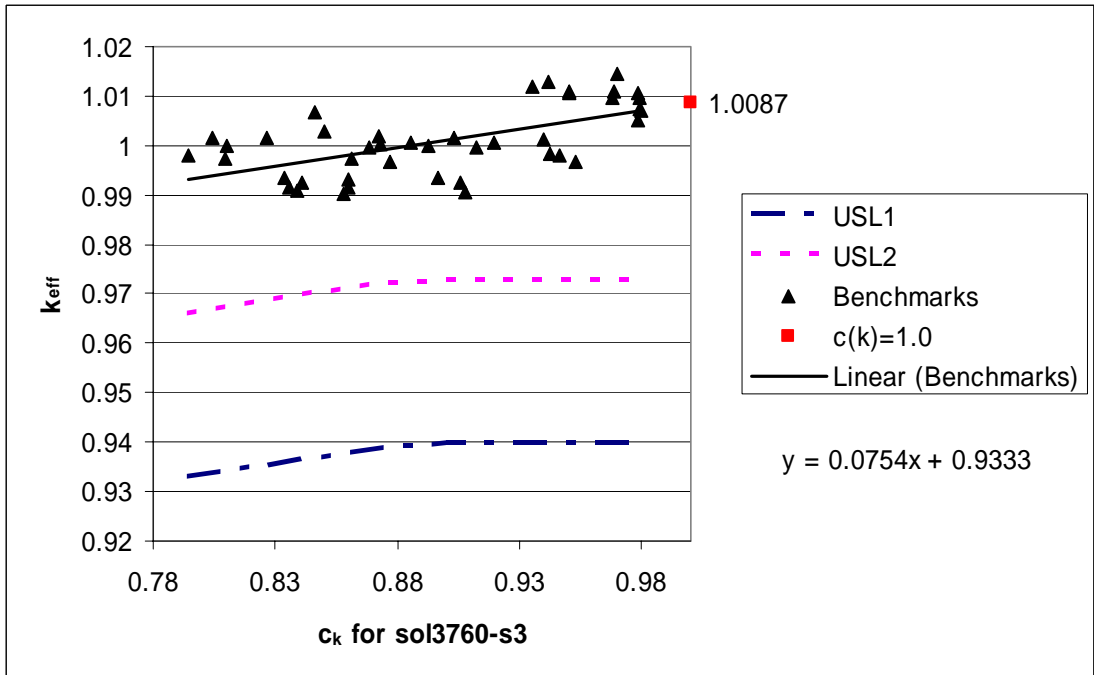


Figure 9. Values for k_{eff} vs c_k for Case 6

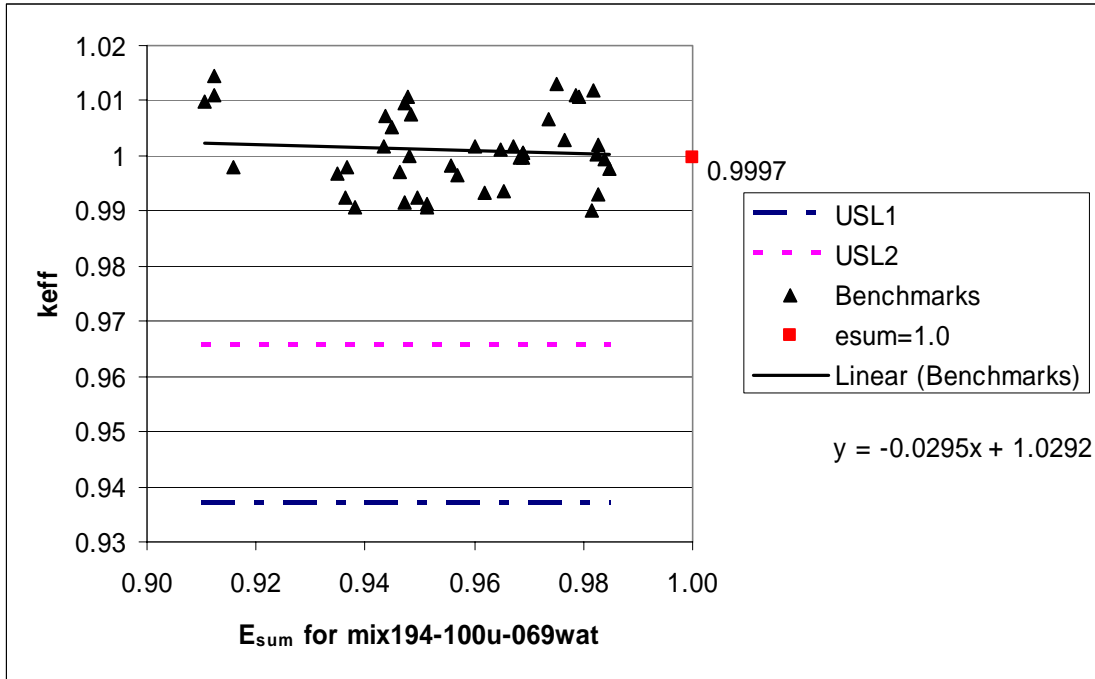


Figure 10. Values for k_{eff} vs E_{sum} for Case 1

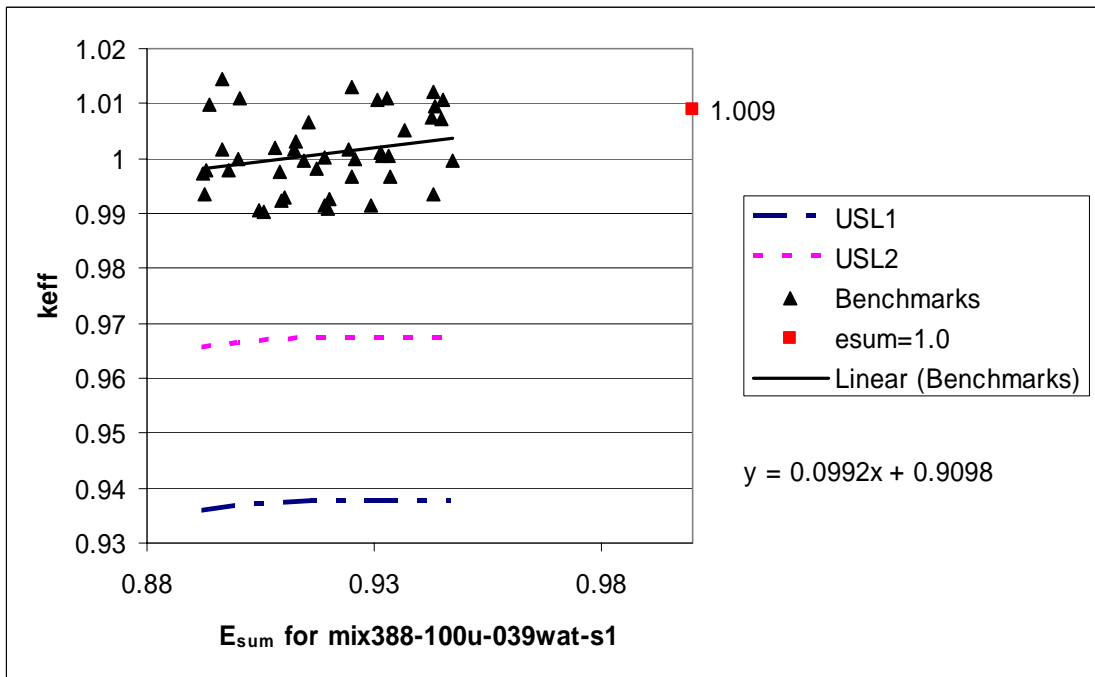


Figure 11. Values for k_{eff} vs E_{sum} for Case 2

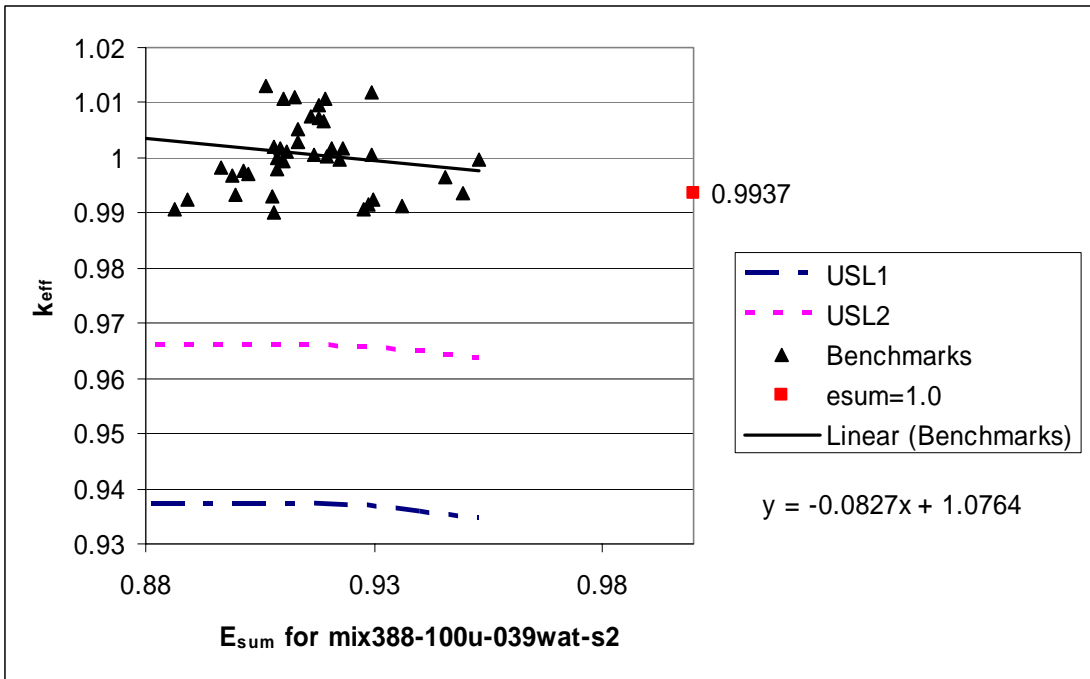


Figure 12. Values for k_{eff} vs E_{sum} for Case 3

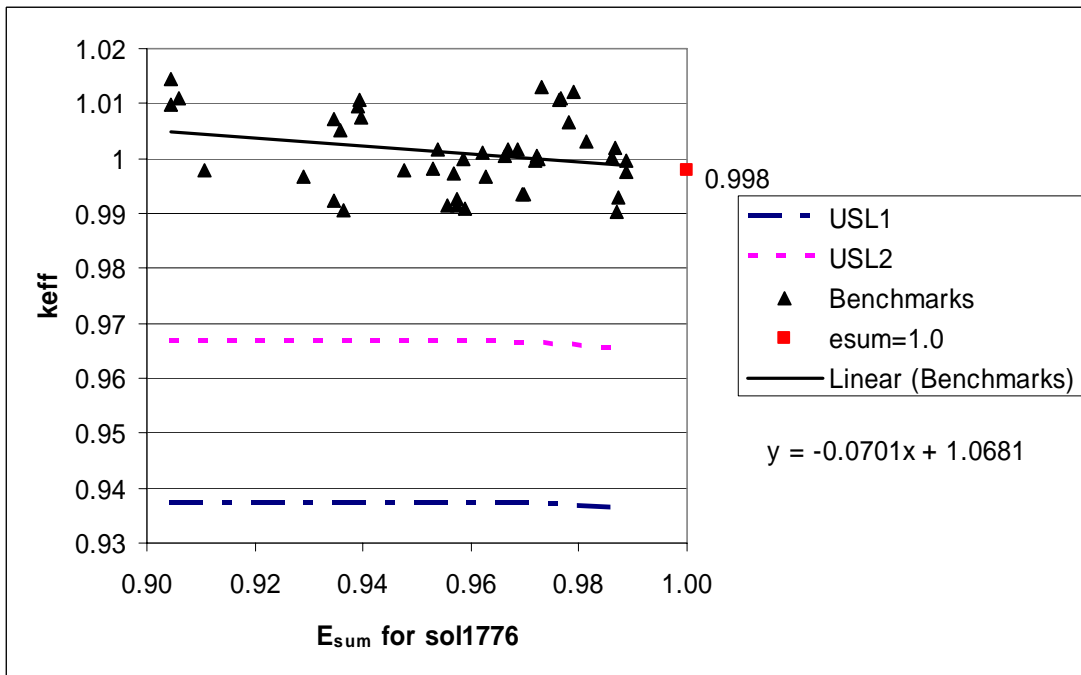


Figure 13. Values for k_{eff} vs E_{sum} for Case 4

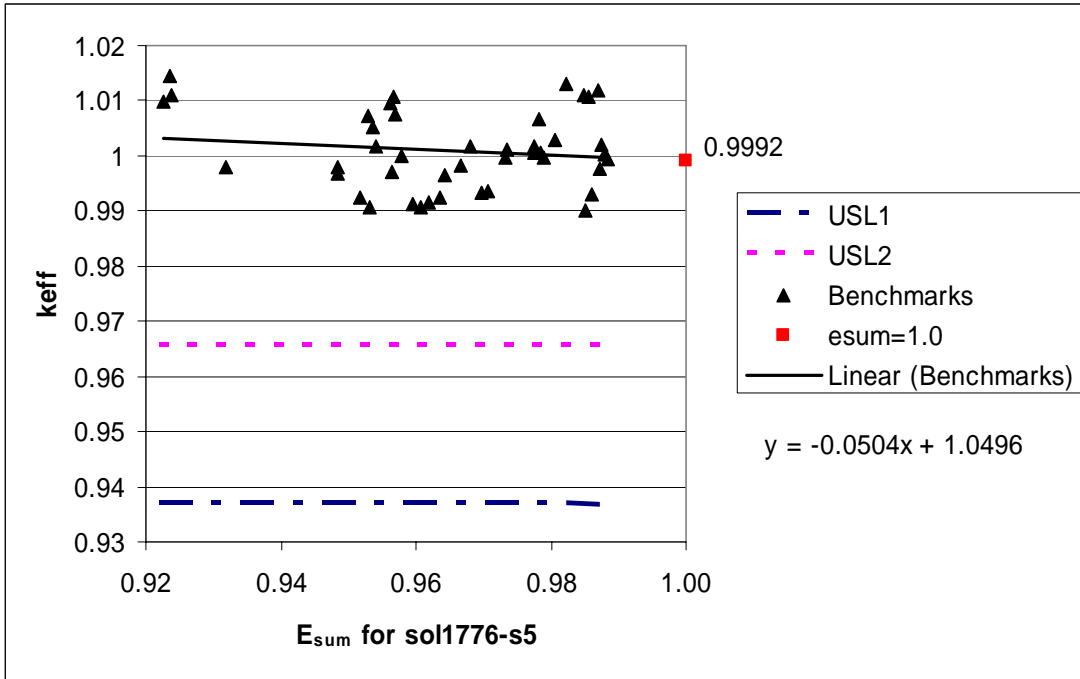


Figure 14. Values for k_{eff} vs E_{sum} for Case 5

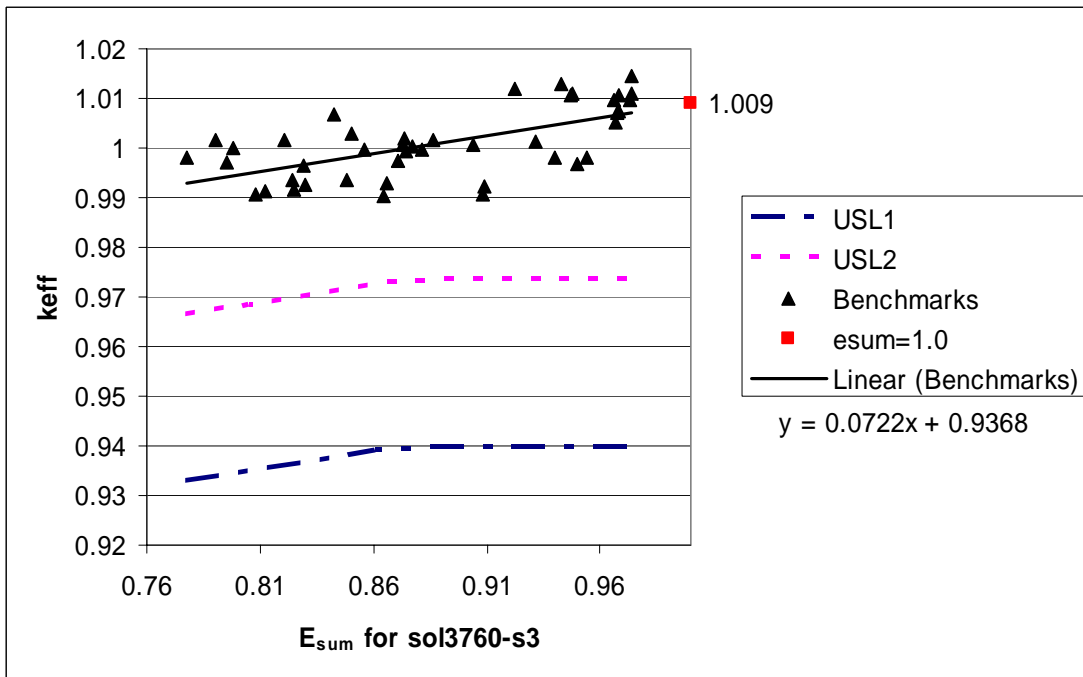


Figure 15. Values for k_{eff} vs E_{sum} for Case 6

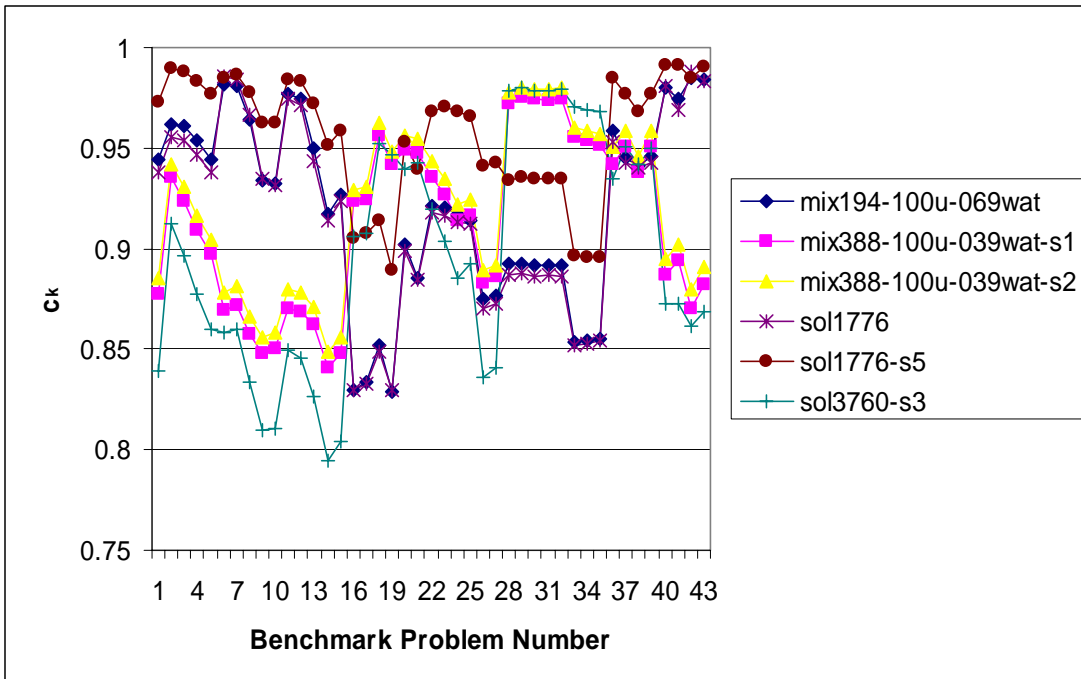


Figure 16. Values for c_k vs benchmark number

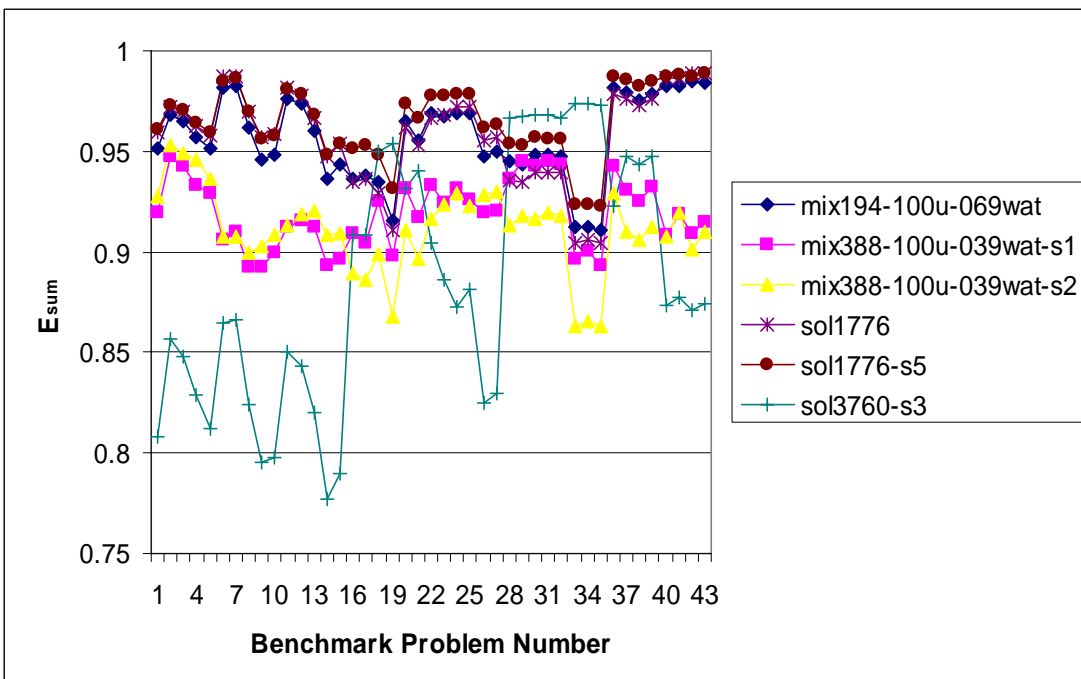


Figure 17. Values for E_{sum} vs benchmark number

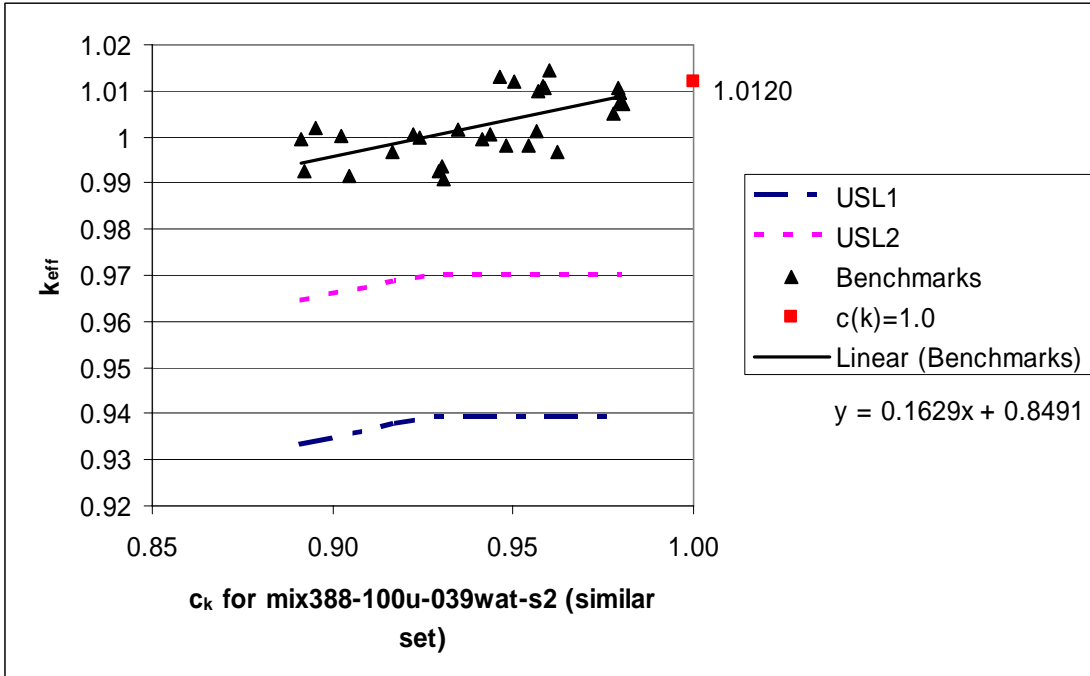


Figure 18. Values for c_k vs benchmark number for Case 3

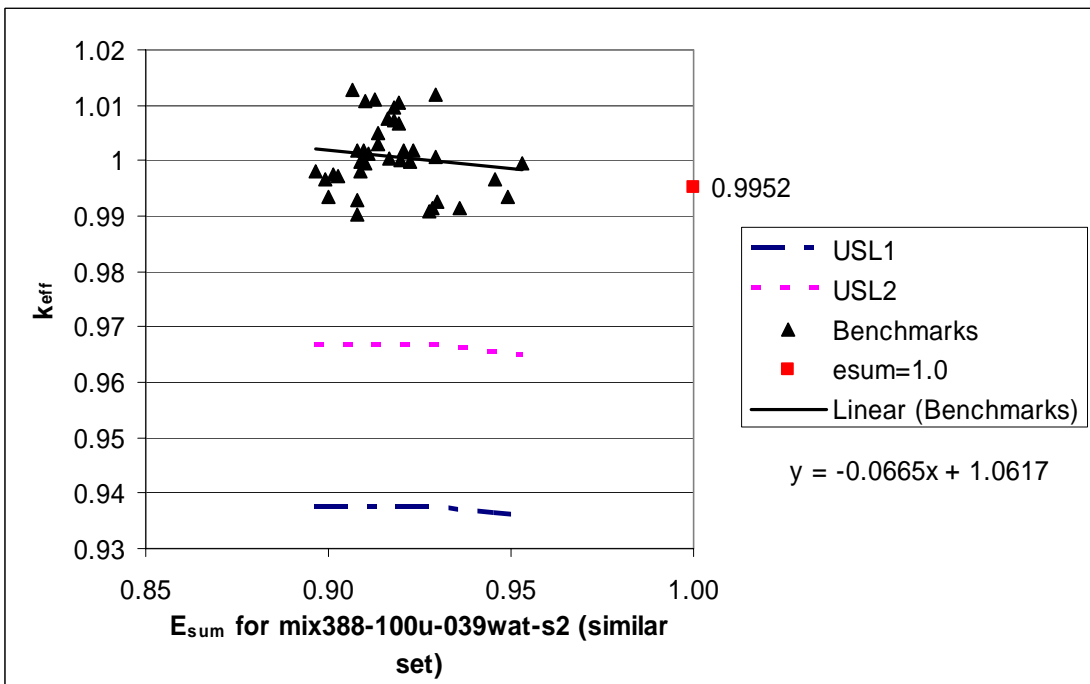


Figure 19. Values for E_{sum} vs benchmark number for Case 3

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