CUSTOMER REPORT

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Criticality safety validation of Serpent for nuclear fuel wet storage calculations

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Contents

1. Introduction

The criticality safety of nuclear fuel storage and transfer configurations is typically demonstrated through extensive analysis relying on computational tools to predict the effective multiplication factor k_{eff} of the system in different configurations. Regulatory guides give upper limits to the k_{eff} of the storage and transfer configurations in different conditions. To assess the subcriticality of the system, the calculated multiplication factor $k_{\mathrm{calc.}}$ is compared to a pre-specified upper safety limit for the code system considering the uncertainty of $k_{\mathrm{calc.}}$. In order to determine the upper safety limit in such a way that, considering the inherent biases of the code system, $k_{\mathrm{calc.}}$ values lower than the upper safety limits can be considered to be indicative of a subcritical system, the inherent biases of the code system need to be determined systematically. This is the purpose of the criticality safety validation.

The criticality safety validation is conducted by simulating a large number of critical or near-critical experiments that hold the same key-parameters than the target system of the validation. The validation will thus have a specific *area of applicability*, in which the upper safety limits determined in the validation can be applied. From the calculated multiplication factors for the experimental configurations, the upper safety limit is derived through statistical means.

This report documents the validation of three officially distributed Serpent versions using ENDF/B-VII based cross sections for criticality safety calculations applied to nuclear fuel wet storage configurations with boron absorber. Section 2 describes the validated code systems, for which the upper safety limits calculated in this report are applicable. Section 3 describes the validation methodology followed in this validation alongside with the statistical treatments used in the analysis of the results. Section 4 details the process of choosing critical experiments to be modelled in the validation based on the target system and summarizes the included experiments. Section 5 shortly describes the execution of the calculations, while Section 6 describes the statistical analysis and trend analysis applied on the calculation results. The upper safety limits are determined in Section 7 and their area of applicability is stated in Section 8.

2. Code system

The validation was conducted for three officially distributed Serpent versions: 2.1.25, 2.1.27 and 2.1.28.

The publicly distributed version 2.1.28 contains a bug, which leads to some geometry transformations being handled incorrectly. In order to circumvent this bug, the PreTrans subroutine of Serpent 2.1.28 was disabled in the validation by adding a return statement on line 27 of pretrans.c. This validation is applicable for the code version 2.1.28 given that the PreTrans subroutine has been disabled in a similar fashion or if the bug in the subroutine can be shown to have no effect on the calculations conducted with the unmodified version 2.1.28.

The validation calculations used the ENDF/B-VII based cross section libraries that were distributed in the official distribution of Serpent 1 with the cross section data library file `sss_endfb7u.xsdata`.

The validation calculations were conducted on the potku2 cluster of VTT using a Serpent executable compiled with gcc 4.9.2. The source code was compiled with OpenMP calculation capabilities, but without MPI capabilities. The standard compiler flags included in the Serpent Makefile were used "-Wall -ansi -ffast-math -O3" and "-DOPEN_MP -fopenmp" and "-pedantic".

3. Validation methodology

The validation methodology applied in this validation is based on the Guide for Validation of Nuclear Criticality Safety Calculational Methodology [1].

The validation of a code system for nuclear criticality safety calculations quantifies the capability of the code system to calculate the multiplication factor of a critical or near-critical system. This quantification is based on the modelling of a number of critical experiments from various sources to estimate the correlation between the calculated and experimental multiplication factor. By conducting statistical analysis on the results of these validation calculations, a margin for the calculated k-effective is derived so that there is a 95 % confidence that future critical systems in the area of applicability of the validation will result in calculated k-effective values higher than the margin in 95 % of cases[1].

This margin is then used in calculation of the upper safety limit, which will be applied in any future criticality safety analyses to indicate systems that are subcritical with a high confidence.

3.1 Determination and use of the upper safety limit (USL)

In this validation we determine the safety limits to be used for the multiplication factor in criticality safety calculations based on the single sided lower tolerance limit as follows:

$$\text{USL} = K_L - \Delta_{\text{SM}} - \Delta_{\text{AoA}}, \tag{1}$$

where USL is the determined *upper safety limit* for the code system, K_L is the *single sided lower tolerance limit* for the k-effective, which is determined so that based on the critical experiments modeled in the validation there is a 95 % confidence that 95 % of future k-effective values calculated for critical configurations in the area of applicability of the validation will lie above K_L (see Section 3.3 for detailed information), Δ_{SM} is an additional safety margin determined by the regulator and Δ_{AoA} is an additional safety margin that will be used if the area of applicability of the validation needs to be extended to cover the system that will be studied using the code system. In applications where no extension is required to the area of applicability, Δ_{AoA} is set to zero.

The upper safety limit shall then be applied for future criticality safety calculation so that systems for which the calculated multiplication factor $k_{\text{calc.}}$ fulfills

$$k_{\text{calc.}} + 2\sigma_{\text{calc.}} < \text{USL} \tag{2}$$

can be considered to fulfill the requirement of subcriticality. $\sigma_{\text{calc.}}$ is the statistical uncertainty of the calculated multiplication factor.

The methodology for determining the K_L will be described in section 3.3 and it will be determined for the current validation in section 6.1.

The safety margin Δ_{SM} that shall be used when estimating the criticality safety of nuclear fuel is determined by the regulator. The Finnish Regulatory Guides on nuclear safety (YVL) state that (YVL-B.4, Nuclear Fuel and Reactor § 504) [2]:

"The storage locations and the handling and transfer systems shall be so designed that, when the storage is full of nuclear fuel, the effective multiplication factor k_{eff} will not exceed the value 0.95 under normal conditions or in anticipated operational occurrences and the value 0.98 in

[1] Other probability and confidence levels can be used if needed, but this validation will use the common 95/95 probability and confidence levels.

other design basis scenarios. In criticality safety analyses pertaining to dry storage, cases where water or other possible moderator enters the storage shall also be examined as an accident."

Two upper safety limits are therefore determined, one for normal conditions and anticipated operational occurrences and a second for other design basis scenarios. The safety margins in these cases are

$\Delta^{L1}_{SM} = 0.05$ Normal conditions and anticipated operational occurrences.
$\Delta^{L2}_{SM} = 0.02$ Other design basis scenarios.

The additional margin for extending the area of applicability Δ_{AoA} shall be determined whenever the code system is applied to criticality safety calculations based on the area of applicability and trend analyses described in this validation report possibly complemented with further analyses. The area of applicability of this validation is defined in Section 8 and the trend analyses are presented in Section 6.2.

3.2 Basic sample statistics derived from the results

This section describes the basic sample statistics that are calculated based on the experimental and calculated results and used in deriving the safety limits for criticality safety validation.

For the analysis of the results, the ratio between the calculated and the experimental multiplication factor of the system is used to indicate over- or underprediction of the system reactivity by the computer code. The ratio for experiment *i* is calculated simply as

$$k_{\text{rat},i} = \frac{k_{\text{eff,calc},i}}{k_{\text{eff,exp},i}}. \tag{3}$$

This ratio is used since the experimental multiplication factor is not necessarily exactly 1.0 in benchmark experiments[2].

The unweighted mean of the k-eff ratio is simply

$$\overline{k}^{\text{unweighted}}_{\text{eff}} = \frac{1}{N}\sum k_{\text{rat},i}, \tag{4}$$

where the summation is over all of the N modelled experiments.

The weighted mean value for the k-eff ratio is

$$\overline{k}_{\text{eff}} = \frac{\sum \frac{1}{\sigma_i^2} k_{\text{rat},i}}{\sum \frac{1}{\sigma_i^2}}, \tag{5}$$

where the summation is over all of the N modelled experiments and σ_i is the combined uncertainty of the calculation $\sigma_{\text{calc.},i}$ and the experiment $\sigma_{\text{exp.},i}$ for experiment i calculated by

$$\sigma_i^2 = \sigma^2_{\text{calc.},i} + \sigma^2_{\text{exp.},i}. \tag{6}$$

The computational uncertainty used in this analysis is the computational standard deviation of the calculated multiplication factor as given by Serpent, whereas the experimental uncertainties are taken directly from the evaluated experimental uncertainties included in the benchmark descriptions.

[2] The large majority of critical experiments typically does have a multiplication factor of 1.0.

The *average total uncertainty* is defined as

$$\overline{\sigma}^2 = \frac{N}{\sum \frac{1}{\sigma_i^2}}, \tag{7}$$

where the summation is over all of the N modelled experiments.

The *variance about the mean* for the weighted mean of the k-eff ratio is calculated by

$$s^2 = \frac{\left(\frac{1}{N-1}\right) \sum \frac{1}{\sigma_i^2} \left(k_{\mathrm{rat},i} - \overline{k}_{eff}\right)^2}{\frac{1}{N} \sum \frac{1}{\sigma_i^2}}. \tag{8}$$

The combination of the variance about the mean and the average total uncertainty is calculated as

$$S_p^2 = s^2 + \overline{\sigma}^2. \tag{9}$$

and called the *pooled variance*.

3.3 Single-sided lower tolerance limit

If the calculated k-eff ratios are considered to be normally distributed (see Section 3.4 for testing the normality of the k-eff ratios), the *single-sided lower tolerance limit* (K_L) can be calculated with

$$K_L = \begin{cases} \overline{k}_{\mathrm{eff}} - US_p & , \overline{k}_{\mathrm{eff}} \leq 1.0 \\ 1.0 - US_p & , \overline{k}_{\mathrm{eff}} > 1.0 \end{cases} \tag{10}$$

where the different terms are

$\overline{k}_{\mathrm{eff}}$	The weighted mean of the k-eff ratios.
U	Single-sided lower tolerance factor, based on the number of modelled experiments.
S_p	The square root of the pooled variance. (See Eq. 9)

The single-sided lower tolerance factor U indicates how many square roots of the pooled variance S_p should be subtracted from the weighted mean of the k-eff ratios to yield such a K_L that future simulations of critical systems will yield multiplication-factors higher than K_L in 95 % of the cases with a 95 % confidence. If the number of simulated experience is small, the confidence in the fact that the obtained values for $\overline{k}_{\mathrm{eff}}$ and S_p are truly representative for the code system for also future critical experiments is low and warrants the use of a larger value for U. The exact value to be used is read from Table 1, which is based on Table 2.1 of Ref. [1].

If the data can not be considered normally distributed, the tolerance limit K_L will be calculated based on the nonparametric statistical treatment:

$$K_L = \begin{cases} \min_i k_{\mathrm{rat},i} - \sigma_i - NPM & , \min_i k_{\mathrm{rat},i} \leq 1.0 \\ 1.0 - S_p - NPM & , \min_i k_{\mathrm{rat},i} > 1.0 \end{cases} \tag{11}$$

where the different terms are

$\min_i k_{\mathrm{rat},i}$	The minimum of the calculated k-eff ratios
σ_i	The combined uncertainty (Eq. 6) for the experiment with the smallest k-eff ratio.
S_p	The square root of the pooled variance. (See Eq. 9)
NPM	Nonparametric margin, based on the number of modelled experiments.

In order to determine the nonparametric margin, the confidence that 95 % of critical experiments will produce k-eff values larger than the smallest observed value is calculated with

$$\beta = 1 - 0.95^N, \tag{12}$$

where N is the number of critical experiments that have been modelled. Based on the confidence value β the nonparametric margin is obtained from Table 2, which is based on the recommendation by the validation methodology guide [1].

3.4 Testing the normality of data

By calculating the k-effective ratios between the calculated and experimental multiplication factors a distribution of $k_{\mathrm{rat},i}$ values is obtained. As the single sided lower tolerance limit determined in this validation is calculated with a 95 % confidence that 95 % of the data lies above the limit, the determination of the limit through statistical means depends on the underlying distribution of the $k_{\mathrm{rat},i}$ data. The choice of the statistical treatment depends on whether the $k_{\mathrm{rat},i}$ data can be considered to be normally distributed.

In this validation we use the Shapiro-Wilk test with Royston's extension described in [3] to determine, whether the data can be considered to be normally distributed or not. The null hypothesis of the test is that the calculated $k_{\mathrm{rat},i}$ is normally distributed with an unspecified mean and variance. The test first calculates the Shapiro-Wilk test statistic W, which is then normalized to obtain the normalized test statistic W_n. The normalized test statistic is then compared to the normal distribution with zero mean and unity variance ($\mathcal{N}(0,1)$).

Table 1. Single-sided lower tolerance factors

Number of experiments	U
10	2.911
11	2.815
12	2.736
13	2.670
14	2.614
15	2.566
16	2.523
17	2.486
18	2.453
19	2.423
20	2.396
21	2.371
22	2.350
23	2.329
24	2.309
25	2.292
30	2.220
35	2.166
40	2.126
45	2.092
50	2.065

Table 2. Non-parametric margin as a function of the confidence value β.

Confidence value (β beta 12)	non-parametric margin
> 90 %	0.00
> 80 %	0.01
> 70 %	0.02
> 60 %	0.03
> 50 %	0.04
> 40 %	0.05
$\leq$ 40 %	Not enough critical experiments

The p-value of the test, when applied as a two-tailed test will be

$$p = \begin{cases} 2(1 - \Phi(W_n)) & W_n > 0 \\ 2\Phi(W_n) & W_n < 0, \end{cases} \tag{13}$$

where $\Phi(x)$ is the cumulative distribution function for $\mathcal{N}(0, 1)$ at x. The test was applied at the significance level $\alpha = 0.05$, i.e. p values smaller than 0.05 will lead to the rejection of the null hypothesis.

3.5 Trend analysis

It is important to identify potential trends in the calculated k-eff ratios as a function of some important parameter of the target system. Trend analysis will be conducted for this validation in Section 6.2, but the calculation of the coefficients of the weighted linear fits and the linear-correlation coefficient are introduced in this section.

Considering a sample of k-eff ratios $y_i = k_{\mathrm{rat},i}$ with an associated combined uncertainty σ_i^2 and some independent parameter x_i (such as fuel enrichment) for a host of experimental configurations we can calculate coefficients a and b for a linear fit

$$y = ax + b \tag{14}$$

by using the weighted linear fit:

$$a = \frac{1}{\Delta}\left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2}\right) \tag{15}$$

$$b = \frac{1}{\Delta}\left(\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2}\right) \tag{16}$$

$$\Delta = \sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2}\right)^2 \tag{17}$$

We will use the (Pearson's) linear correlation coefficient r as an indication of the goodness of the fit. The linear correlation coefficient is calculated by

$$r = \frac{\sum \frac{1}{\sigma_i^2}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum \frac{1}{\sigma_i^2}(x_i - \overline{x})^2}\sqrt{\sum \frac{1}{\sigma_i^2}(y_i - \overline{y})^2}}, \tag{18}$$

where the weighted mean for the independent parameter is

$$\overline{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} \tag{19}$$

and $\overline{y}$ is equal to $\overline{k}_{\mathrm{eff}}$ from Eq. 5.

The linear correlation coefficient varies between -1 and 1 with large absolute values indicating strong linear correlation and values close to zero indicating no significant linear correlation.

4. Choosing critical experiments

The choice of the critical experiments for the validation is an essential step of the criticality safety validation and needs to be conducted systematically. The overall approach for determining suitable critical experiments and documenting the area of applicability for the validation is described in [1] as follows:

1. Identify the key parameters associated with the nominal and upset conditions of the system to be evaluated.
2. From the key parameters identified in the first step, establish a "screening" area of applicability for identifying potential critical experiments.
3. Identify criticality experiments that are within this screening area of applicability or have the same key physical parameter.
4. From the scope of selected criticality experiments, determine the detailed area of applicability that the experiments cover.
5. Show that the system to be evaluated is within the area of applicability provided by the critical experiments or provide justification for using the critical experiment parameters for the system in question.
6. Document the results for the area of applicability.

The key parameters to be considered for identifying similarity between the target system and the critical experiments are listed in Table 3, which is based on Table 2.3 of [1].

4.1 Target application

The target application of this validation were criticality safety analyses considering the Fennovoima interim spent fuel storage facility as described in [4]. The main characteristics of the storage geometry used in the criticality safety analyses are described in the following.

The target geometry is shown in Figure 1 as a two dimensional infinite lattice model. The geometry consists of an AES-2006 fuel assembly in a storage absorber tube in a repeated hexagonal lattice. The storage tube is filled with light water and the region between the adjacent storage tubes is also filled with light water.

We can assess the different key parameters of the target (parameters listed in Table 3) as follows:

Fissionable material: The fissionable material in the target system is low enriched uranium dioxide with an enrichment of approximately 5.0 wt.% ^{235}U. The density of the fuel will reflect typical fuel densities for uranium dioxide fuel pellets. The temperature of the fuel material as well as other materials will be room temperature.

Moderator material: The moderator material present in the target geometry will be light water at room temperature and nominal density (approximately 1.0 g/cm^3).

Reflector material: The geometry used for the criticality safety analyses is expected to be an infinite lattice geometry with no notable reflectors. The storage tube functions mainly as a neutron absorber and the moderator between the storage tubes functions as a neutron thermaliser, which will increase the absorption of neutrons by the absorber tube. However, the infinite lattice cannot be considered as an unreflected system either as the reflectors main purpose is to prevent neutron leakage, which is a non-issue in an infinite lattice geometry.

Parameter	Critical Experiment Requirement
Fissionable material	Same fissionable element(s) as in target system
Uranium enrichment	Target system / Allowed variaton 0 – 2 wt.% / 1 wt.% 2 – 5 wt.% / 1.5 wt.% 5 – 10 wt.% / 2.5 wt.%
Physical form	Same as in target system
Concentration	No requirement
Temperature (also other materials)	Target system / Allowed variaton 80 – 273 K / 25 K 273 – 500 K / 50 K
Interstitial moderator material	Same moderating element(s) as in target system
Isotopic composition	For hydrogen, isotopic composition should be within 20 %
Physical form	Same as in target system
Density	Within ± 10 wt.%
Reflector material	Should be same as in target system.
Isotopic composition	Within ± 10 wt.% of target system.
Physical form	No requirement
Density	Within ± 25 %
Absorber material	Can be divided into 1/v absorbers and others. In 1/v-absorbers (He-3, B-10, Li-6) the isotopes are interchangeable given the same macroscopic absorption at 2200 m/s. In the case of other absorber elements, the elements should be the same as in target system.
Isotopic composition	No addition restriction for 1/v isotopes. For other isotopes the isotopic ratio should be within ± 5 %.
Ratio to fissile material	If the absorber is within the fuel, the atom ratio should be within 20 %.
Density	If the absorber is in a reflector and the absorber contributes greater than 1 % of the total absorption, then the atom ratio of absorber/scatterer and absorber/fissionable (if applicable) should be within 20 %.
Geometry	The geometry should be as close as possible to the actual case. Geometry is not considered as important as material specifications.
Shape	For non-reentrant bodies, ± 50 % variation on mean cord length. For internal reentrant bodies, ± 25 % variation on mean cord length. For external reentrant bodies, no tolerance in shape or size.
Reflection	Solid angle to within ± 10 %. Mean spacing between reflector and fuel within 10 %.
Relative material thickness	Physical thickness of all materials should agree within ± 50 %.
Neutron energy	The neutron energy spectra is to cover the same energy range, e.g., thermal (0 eV – 1 eV), intermediate (1 eV – 100 keV) or fast (100 keV – 20 MeV

Table 3. Key parameters that were considered in identifying suitable critical experiments for the validation and defining the area of applicability. Based on Table 2.3 of [1].

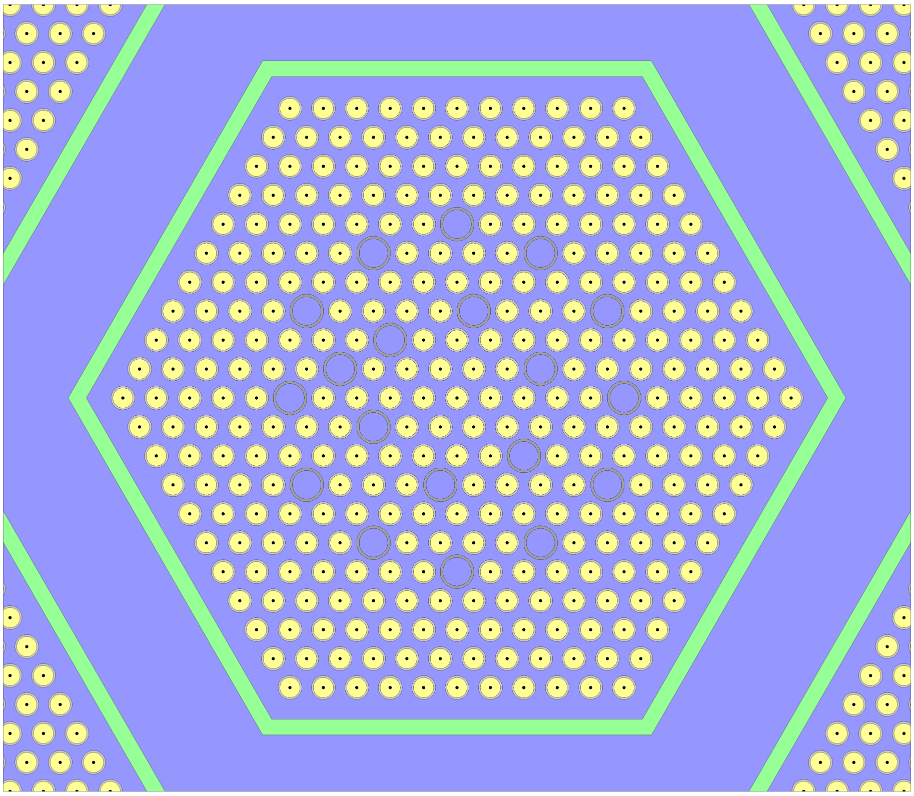

Figure 1. Geometry plot from the unit cell of the target geometry (infinite lattice 2 dimensional model). Yellow corresponds to fuel, blue to water, black to void regions, green to absorber tube and grey to cladding, guide tube and instrumentation tube materials.

Absorber material: The hexagonal storage tube surrounding the assembly consists of borated steel (boron content approximately 1.5 wt.%). The boron is expected to have a natural isotopic composition (80.1 at.% of ^{10}B and 19.9 at.% of ^{11}B).

Geometry: The unit cell of the target geometry consists of fuel rods in an assembly (hexagonal lattice) surrounded by an absorber tube and water. The hexagonal pitch in the fuel pin lattice is 1.275 cm. The assembly separation is approximately 30 cm. The fuel pellet inner and outer radii are 0.06 and 0.38 cm respectively.

Neutron energy: The target system is a thermal system. To measure the moderation in the target system, the energy corresponding to the average lethargy of neutrons causing fission (EALF) was calculated for the nominal conditions of the target geometry (Appendix 2 of reference [4]) with Serpent 2.1.28 using ENDF/B-VII based cross sections. The obtained EALF value was 0.35 eV.

4.2 General parameters for choosing critical experiments

Based on the parameters of the target system, general screening parameters for choosing critical experiments were derived:

Fissionable material: The fissionable material should be uranium dioxide with an enrichment in the range of 3.5 wt.% to 7.5 wt.% ^{235}U. The density of the fuel should reflect typical fuel densities for uranium dioxide fuel pellets. The temperature of the fuel material as well as other materials should be room temperature.

Moderator material: The moderator material should be light water at room temperature and nominal density (approximately 1.0 g/cm^3).

Reflector material: As the target system is neither reflected nor unreflected, there are no strict demands for the reflector material. As the gaps between the assemblies in the target system contain water and stainless steel, water and stainless steel reflectors would be preferred in the experiments.

Absorber material: The absorber material should be natural boron. Borated steel with boron content close to the target system is the preferred absorber material, but other borated materials may also be considered.

Geometry: The geometry should consist of fuel rods arranged in a lattice with interstitial water moderator. Geometries with a similar pin lattice as in the target system (hexagonal, similar pitch) should be favored. Other geometrical similarities to the target system should also be considered.

Neutron energy: Only thermal systems should be considered.

These screening parameters are collected into Table 4 for quick reference.

4.3 Experiments from existing collection

The first considered source for critical experiments was the library of inputs contained in the criticality safety validation package (CSVP) collected at VTT during the previous years [5]. All of the inputs found in this validation package have been created based on critical benchmark experiments taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [6] later referred to as *the Handbook*. As of the beginning of 2017, the validation package contained 234 inputs from six experimental series. The suitability of the various experiments for inclusion in this validation is evaluated in the following based on the screening parameters listed in Table 4.

All of the experimental series were from the LEU-COMP-THERM (LCT) part of the Handbook, which contains experiments using low-enriched uranium (LEU) in compound form (COMP) in thermal arrangements (THERM). As all of the experiments were from the thermal part of the handbook they fulfill the neutron energy screening parameter.

LCT-015

The title of the benchmark description was *The VVER Experiments: Regular and Perturbed Hexagonal Lattices of Low-Enriched UO_2 Fuel Rods in Light Water*.

This experimental series contained 165 critical or near-critical experiments of which 151 critical experiments have been modelled in the CSVP. The experimental program focused on experiments relevant to VVER-440 and VVER-1000 reactor types. The experiments contained regular or perturbed fuel rod configurations in hexagonal lattice geometry with variable pitch. The experiments were conducted in a water pool or tank, where criticality was achieved by adjusting the water level.

Fissionable material: The fuel material was 1.6, 3.6 or 4.4 wt.% enriched UO_2.

Moderator: The moderator was light water with or without boric acid,

Reflector: The experimental configurations were surrounded by water.

Parameter	Target system	Critical experiments
Fissionable material	Uranium with ^{235}U as the main fissioning isotope.	Same as in target.
Uranium enrichment	5.0 wt.%	3.5 – 7.5 wt.%
Physical form	Uranium dioxide	Same as in target.
Concentration	Density as fabricated	Density as fabricated
Temperature (also other materials)	Room temperature	Room temperature
Interstitial moderator material	Light water	Light water
Isotopic composition	Light water	Light water
Physical form	Liquid	Liquid
Density	1.0 g/cm^3	0.9–1.1 g/cm^3
Reflector material	Not applicable	Water, steel.
Absorber material	Borated steel	Materials with natural boron absorber.
Isotopic composition	Natural boron	Natural boron
Ratio to fissile material	Absorber not within fuel	N/A
Density	Absorber not within reflector	N/A
Geometry	Fuel pins in hexagonal assembly surrounded by storage tube of borated steel. Infinite lattice.	Fuel pins in lattice geometries. Preferably with absorber plates.
Shape	Mainly significant for deterministic solvers	Normal lattice geometry.
Reflection	Infinite lattice	N/A
Relative material thickness	Fuel rod geometry.	Similar fuel rod geometry if possible.
Neutron energy	Thermal system (0.35 eV EALF)	Thermal system

Table 4. Screening parameters that were considered in identifying suitable critical experiments for the validation and defining the area of applicability. Based on Table 2.3 of [1].

Absorber: The moderator contained boron (boric acid) as an absorber in a number of the experiments and additional absorber rods of borated zirconium, Boral, boron carbide and Europium oxide were used in a number of experiments.

Geometry: The geometry was fuel pins in a hexagonal lattice (1.1–1.9 cm pitch). The fuel rod geometry was reasonably similar to the one in the target system with the same outer radius of the fuel pellet but no central hole in the pellet.

The experiments with 1.6 wt. % enriched fuel were excluded based on the screening parameters. All experiments without boron absorber were excluded based on the screening parameters. The experiments with the Europium absorber were excluded based on the screening parameters.

In order to limit the number of cases from a single benchmark only 16 cases were included from LCT-015. All of the included cases contained boric acid in the moderator, no absorber rods and a fuel enrichment of 3.6 or 4.4 wt. %.

LCT-034

The title of the benchmark description was *Four 4.738-wt.%-enriched uranium dioxide rod assemblies contained in cadmium, borated stainless steel, or boral square canisters, water-moderated and -reflected*

The benchmark description contained 24 experiments with four fuel assemblies surrounded by absorber plates in a water tank, where criticality was achieved by adjusting the water level in the tank.

Fissionable material: The fuel material was 4.738 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The four assemblies were surrounded with a water reflector from sides and bottom.

Absorber: All of the experiments used absorbing plates of borated steel (1.1 wt.% boron), Boral or cadmium.

Geometry: The geometry was fuel pins in assemblies (square lattice 1.6 cm pitch) surrounded by absorber plates.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. The lattice geometry of the experiment was different from the target system (square lattice with larger pitch), but as Monte Carlo codes use the same solution routines for square and hexagonal lattices, this was not seen to warrant the exclusion of the experimental series. The 10 experiments with cadmium absorber were not included.

The 14 experiments with borated steel or Boral absorber plates were included in this validation.

LCT-040

The title of the benchmark description was *Four 4.738-wt.%-enriched uranium dioxide rod assemblies contained in borated stainless steel or boral square canisters, water moderated and reflected by lead or steel*

The benchmark description contained 10 experiments with four fuel assemblies surrounded by absorber plates and lead or steel reflector blocks in a water tank, where criticality was achieved by adjusting the water level in the tank.

Fissionable material: The fuel material was 4.738 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The four assemblies were surrounded with a lead or stainless steel reflector from sides and a water reflector from bottom.

Absorber: All of the experiments used absorbing plates of borated steel (1.1 wt.% boron) or Boral.

Geometry: The geometry was fuel pins in assemblies (square lattice 1.6 cm pitch) surrounded by absorber plates and reflector blocks.

The fissionable material, moderator and absorber fulfilled the screening parameters for all experiments. The lattice geometry of the experiment was same as in LCT-034 and while being different from the target system was not seen to warrant the exclusion of the experimental series. The system was reflected with lead or stainless steel in this setup instead of water as in LCT-034. As the reflector material was not a key parameter in the target system, this was not seen to warrant the exclusion of the experimental series.

All 10 experiments were included in this validation.

LCT-053

The title of the benchmark description was *VVER physics experiments: regular hexagonal (1.27 cm pitch) lattices of low-enriched U(4.4 wt.%* ^{235}U*)*O_2 *fuel rods in light water at different core critical dimensions*

The benchmark description contained 14 experiments with a variable number of fuel rods in a hexagonal lattice in a roughly circular shape. The experiments were conducted in a water tank, where criticality was achieved by adjusting the water level in the tank.

Fissionable material: The fuel material was 4.4 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The core formed by the fuel rods was surrounded with a water reflector from sides and bottom.

Absorber: None of the experiments contained neutron absorbers.

Geometry: The geometry was fuel pins in a hexagonal lattice with 1.27 cm pitch in a roughly circular shape.

As none of the experiments contained boron absorber, which was a key component of the target system, none of the experiments were included in this validation.

LCT-086

The title of the benchmark description was *VVER physics experiments: hexagonal lattices (1.275 cm pitch) of low-enriched U(3.6, 4.4 WT.%* ^{235}U*)*O_2 *fuel assemblies in light water with* H_3BO_3.

The benchmark description contained ten experiments with seven short VVER-1000 type fuel assemblies in a hexagonal configuration. The experiments were conducted in a water pool, where criticality was achieved by adjusting the water level in the pool.

Fissionable material: The fuel material of all assemblies was UO_2. The six driver assemblies had an enrichment of 3.6 or 4.4 wt.% and the enrichment of the central fuel assembly varied from 2.0 to 4.4 wt.%.

Moderator: The moderator was light water with boric acid.

Reflector: The core formed by the fuel assemblies was surrounded with a water reflector from sides and bottom.

Absorber: All of the experiments contained soluble boron absorber in the moderator.

Geometry: The fuel assemblies (hexagonal lattice 1.275 cm pitch) formed a hexagonal shape, where six driver assemblies surrounded a central assembly.

The fissionable material, moderator and reflector fulfilled the screening parameters. The neutron absorber in the experiments was not contained in plates but soluble in the moderator. The assembly geometry was notably similar to the target system.

The boron absorber was situated in the moderator rather than in plates as in the target system. However there is no restriction concerning the physical form of the absorber material (Ref. [1] Tbl 2.3). The assembly geometry was notably similar to the target system.

All of the 10 experiments were included in the validation.

LCT-087

The title of the benchmark description was *VVER physics experiments: hexagonal lattices (1.22-cm pitch) of low-enriched U(3.6, 4.4 WT.% U235)O_2 fuel assemblies in light water with variable fuel-assembly pitch*.

The benchmark description contained 25 experiments with 19 short VVER-440 type fuel assemblies in a hexagonal lattice configuration. The central assembly was surrounded by an absorber tube in some of the experiments. The experiments were conducted in a water pool, where criticality was achieved by adjusting the water level in the pool.

Fissionable material: The fuel material of the surrounding 18 fuel assemblies was 3.6 wt.% enriched UO_2. The fuel material of the central fuel assembly was either 3.6 or 4.4 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The core formed by the fuel assemblies was surrounded with a water reflector from sides and bottom.

Absorber: Some of the experiments contained an absorber tube (borated steel or iron with a small amount of boron).

Geometry: The fuel assemblies (hexagonal lattice 1.22 cm pitch) were situated in a hexagonal lattice with a variable pitch.

The fissionable material, moderator, reflector and geometry fulfilled the screening parameters for all experiments. Boron absorber was present only in part of the experiments, with the absorber being incorporated either in borated steel (0.76 or 1.04 wt.% boron) or an iron absorber (0.012 wt.% boron). The experiments with the iron absorber were excluded due to the low boron content of the absorber. The experiments with no absorber tube were also excluded.

The 7 experiments with borated steel absorbers were included in the validation.

4.4 Additional experiments

57 critical experiments fitting the screening criteria were identified from the existing criticality safety validation package. 19 experiments contained borated steel absorbers, 12 contained Boral plate absorbers and 26 contained boric acid in the moderator. In order to identify additional experiments with borated steel plate absorbers (similar to the target system), the Database for the International Criticality Safety Benchmark Evaluation Project (DICE) was searched with the following parameters:

```
Fissile material = Low Enriched Uranium
and Physical form = Compound
and Spectrum = Thermal
and Acceptable = Acceptable
and Fissile material = Uranium Oxide
and U isotope = U235
and Weight percent of U isotope >= 3.5 and  <= 7.5
and Moderator/coolant material = Water (Light Water)
and Solid = Borated Stainless Steel (B, Fe, Cr, Ni)
```

Three additional experimental series were identified with borated steel plates (LCT-009, LCT-013 and LCT-089).

The largest fuel enrichments in the included experiments and the additional experimental series were still below the target systems 5.0 wt.%. The included experiments should cover the target system from both sides so that any trends in the bias of the code system can be interpolated, rather than extrapolated, for the enrichment in the target system. This meant that additional experimental series with boron absorber and a higher fuel enrichment were required. A search with a fuel enrichment between 5.0 and 7.5 wt.% and any solid borated materials as neutron absorber resulted in two potential experimental series (LCT-075 and LCT-076). A search with a fuel enrichment between 5.0 and 7.5 wt.% and soluble boron in light water resulted in one potential experimental series (LCT-021).

All of the identified potential additional experimental series are evaluated against the screening parameters in the following. As all of the experiments were from the thermal part of the handbook they fulfill the neutron energy screening parameter.

LCT-009

The title of the benchmark description was *water-moderated rectangular clusters of U(4.31)O_2 fuel rods (2.54-cm pitch) separated by steel, Boral, copper, cadmium, aluminium or Zircaloy-4 plates*

The benchmark description contained 27 experiments in which rectangular clusters of fuel rods were separated by two absorbing or non-absorbing plates. The experiments were conducted in a water pool, where criticality was achieved by adjusting the separation of the fuel rod clusters.

Fissionable material: The fuel material was 4.31 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The three fuel rod clusters were surrounded with a water reflector from sides and top. The bottom reflector consisted of an acrylic support plate followed by water.

Absorber: All of the experiments contained separating plates, some of which contained absorbers. Four experiments used borated steel plates, one experiment used Boral plates, ten experiments used cadmium containing absorber plates and the rest of the experiments were conducted with plates that contained no notable concentrations of absorbers.

Geometry: The fuel clusters (15 by 8 rod square lattice 2.54 cm pitch) were situated in 3 by 1 cluster arrangement with a variable distance between the central cluster and the side clusters. The absorber plates were situated in the water gaps between the central cluster and the side clusters.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. Boron absorber was present only in part of the experiments, with the boron absorber being incorporated either in borated steel (1.1 or 1.67 wt.% boron) or Boral. The experiments without boron absorber were excluded. The pin-lattice geometry had a larger pitch than in the target system, but the aspect of "assemblies" separated with water and absorber plate was similar to the target system. Overall the geometry was judged to be similar enough to the target system not to warrant exclusion of the experimental series.

The 5 experiments containing borated steel or Boral absorber plates were included in the validation.

LCT-013

The title of the benchmark description was *Water-moderated rectangular clusters of U(4.31)O_2 fuel rods (1.892-cm pitch) separated by steel, Boral, Boroflex, cadmium, or copper plates, with steel reflecting walls*.

The experiments included in this benchmark are quite similar to those included in LCT-009. However, in this case stainless steel reflecting walls surrounded the clusters on two sides with two sides being still reflected by water. The central fuel cluster was again separated from the other two clusters with water and absorbing or non-absorbing plates.

Fissionable material: The fuel material was 4.31 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The three fuel rod clusters were surrounded with a water reflector from two sides and top. The reflector on two sides was stainless steel. The bottom reflector consisted of an acrylic support plate followed by water.

Absorber: All of the experiments contained separating plates, some of which contained absorbers. One experiments used borated steel plates, one experiment used Boral plates, one experiment used Boroflex plates and two experiments used cadmium containing absorber plates. The rest of the experiments were conducted with plates that contained no notable concentrations of absorbers.

Geometry: The fuel clusters (12 by 16 rod square lattice 1.892 cm pitch) were situated in 3 by 1 cluster arrangement with a variable distance between the central cluster and the side clusters. The absorber plates were situated in the water gaps between the central cluster and the side clusters.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. Boron absorber was present only in part of the experiments, with the boron absorber being incorporated either in borated steel (1.1 wt.% boron), Boral or Boroflex. The experiments without boron absorber were excluded. The pin-lattice geometry had a larger pitch than in the target system, but the aspect of "assemblies" separated with water and absorber plate was similar to the target system. As in LCT-009, the geometry was judged to be similar enough to the target system not to warrant exclusion of the experimental series.

The 3 experiments containing borated steel, Boral or Boroflex absorber plates were included in the validation.

LCT-021

The title of the benchmark description was *Hexagonally pitched partially flooded lattices of U(5%)O_2 zirconium clad fuel rods moderated by water with boric acid*.

The benchmark description contained 6 experiments with a variable number of fuel rods in a hexagonal lattice in a roughly circular shape. The experiments were conducted in a water pool, where criticality was achieved by adjusting the water level in the pool.

Fissionable material: The fuel material was 5.0 wt.% enriched UO_2.

Moderator: The moderator was light water with boric acid.

Reflector: The core formed by the fuel rods was surrounded with a water reflector from sides and bottom.

Absorber: All of the experiments contained soluble boron absorber in the moderator.

Geometry: The geometry was fuel pins in a hexagonal lattice with 1.0 or 1.3 cm pitch in a roughly circular shape.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. In these experiments, the boron absorber was present in the moderator rather than in solid structures, which is a minor issue in the benchmark. The geometry did not contain fuel assemblies or assembly imitators but the hexagonal lattice pitch was similar to the one in the target system.

As there is no restriction concerning the physical form of the absorber material (Ref. [1] Tbl 2.3) and the other key parameters were fulfilled well, all 6 experiments were included in the validation.

LCT-075

The title of the benchmark description was *VVER physics experiments: hexagonal (1.10 cm pitch) lattices of low-enriched U(6.5 WT.% ^{235}U)O_2 fuel rods in light water, perturbed by boron absorber rods and water holes*.

The benchmark description contained 6 experiments with VVER-type fuel rods in a hexagonal lattice forming a core with a roughly circular shape. The regular lattice was perturbed either by water holes or boron carbide absorber rods. The experiments were conducted in a water pool, where criticality was achieved by adjusting the water level in the pool.

Fissionable material: The fuel material was 6.5 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The core formed by the fuel rods was surrounded with a water reflector from sides and bottom.

Absorber: Three of the experiments contained six boron carbide absorber rods in the core.

Geometry: The geometry was fuel pins in a hexagonal lattice with 1.1 cm pitch in a roughly circular shape.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. The geometry did not contain fuel assemblies or assembly imitators but the hexagonal lattice pitch was reasonably close to the one in the target system. Three of the experiments contained no neutron absorber and were excluded. The other three experiments contained boron absorber in a small number of boron carbide rods.

The 3 experiments containing boron carbide rods were included in the validation.

LCT-076

The title of the benchmark description was *Light water moderated and reflected low enriched uranium (3 wt.% ^{235}U) dioxide rod lattices with ex-core detector feature*

The benchmark description contained 7 experiments that simulated a system of 12 PWR fuel assemblies at the periphery of a PWR core. The fuel assemblies were arranged into a cruciform shape. The experiments were conducted in a water tank, where criticality was achieved by adjusting the water level in the tank.

Fissionable material: The fuel was mostly 3.0 wt.% enriched UO_2 with three experiments using a number of fuel rods with 7.0 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The cruciform core was surrounded by a stainless steel baffle surrounded by water.

Absorber: Three experiments used 12 or 16 burnable absorber rods consisting of thick-walled hollow borosilicate glass cylinders.

Geometry: The fuel rods were arranged in a cruciform shape using a square lattice geometry with 1.2507 cm pitch.

Only one of the experiments (S06D/6) contained both 7.0 wt.% enriched fuel rods and boron absorbers. In this experiment the high enriched fuel rods made up less than ten percent of all fuel rods, the others being 3.0 wt.% enriched UO_2.

Due to the majority of fuel being of enrichment that is outside of the screening area, no experiments were included from this benchmark.

LCT-089

The title of the benchmark description was *Critical loading configurations of the IPEN/MB-01 reactor with UO_2 and borated stainless steel plates*.

The benchmark description contained 4 experiments, in which borated steel plates were inserted into a fuel rod lattice (core of the IPEN/MB-01 reactor) in different geometric configurations. The experiments were conducted in a water pool, where criticality was achieved by modifying the water temperature.

Fissionable material: The fuel was 4.34 wt.% enriched UO_2.

Moderator: The moderator was light water without additives.

Reflector: The core was surrounded by light water.

Absorber: All of the experiments contained two borated steel plates (1.787 wt.% boron) inside the fuel lattice. Additionally, the Ag-In-Cd (AIC) control rods situated in two quarters of the core were withdrawn from the active core, but their lower ends were still situated close to the top of the active core.

Geometry: The fuel rods were arranged in a square shape using a square lattice geometry with 1.5 cm pitch.

The fissionable material, moderator and reflector fulfilled the screening parameters for all experiments. The geometry did not contain fuel assemblies or assembly imitators and the square lattice pitch was larger the hexagonal pitch in the target system. The geometry did contain borated steel plates interacting with a fuel rod lattice similar to the lattice system. All of the experiments contained boron absorber in borated steel plates quite similar to the target system. The small effect of the AIC control rods on the neutron absorption near the top of the active core in two of the four quadrants was not seen to warrant the exclusion of the experimental series from the validation.

All 4 cases were included in the validation.

4.5 Summary of experiments included in the validation

The complete list of experiments included in the validation is given in Appendix A. The included experiments are summarized in Table 5 on benchmark level. The fuel enrichment of the target system (5.0 wt.%) is covered by the experiments, although only 9 experiments have fuel enrichments equal to or larger than the target system. However, 24 experiments have a fuel enrichment of 4.74 wt.% which is close to the target system. The enrichments in the other experiments are within the allowed range for variation (see Tbl. 3)[3].

All of the experiments used a light water moderator in room temperature like the target system. The target system was an infinite lattice system meaning that the neutron reflective properties of the included materials have a reduced impact on the multiplication factor. The experiments were finite systems with water, lead or stainless steel reflectors.

The absorber in the target system was natural (i.e. non-isotope enriched) boron in borated steel plates surrounding the fuel assemblies. All of the included experiments included natural boron absorbers: 28 experiments contained borated steel plates. 14 experiments contained Boral plates. 1 experiment contained Boroflex plates. 3 experiments contained boron carbide absorber rods. 32 experiments contained boric acid in the moderator. Although not all of the experiments contained borated steel plates like the target system, the collection of experiments should cover any biases resulting from the modelling of Boron absorbers (e.g. from uncertainties in the boron cross section data).

The key parameters of the target system are covered by the chosen experiments. The exact level of moderation in the experiments compared to the target system is estimated by calculating the energy corresponding to the average lethargy of neutrons causing fission (EALF) and comparing this value to the one obtained for the target system. This is done during the trend analyses in Section 6.2.

[3] In experiments 5 and 10 of the experimental series LCT-086 one of the fuel assemblies had a low enrichment of 2.0 %. However the driver fuel assemblies consisted of 4.4 % (case 5) or 3.6 % (case 10) enriched uranium oxide.

Table 5. Summary of the experimental series included in the validation. All of the experiments were moderated with light water.

Benchmark	Cases included (number)	Pellet radii inner/outer (cm)	Cladding outer radius (cm)	Enrichment (wt.%)	Reflector	Absorber
LCT-009	5	–/0.6325	0.7075	4.31	Water	Borated steel or Boral
LCT-013	3	–/0.6325	0.7075	4.31	Steel and water	Borated steel or Boral or Boroflex
LCT-015	16	–/0.3125	0.4525	3.6 or 4.4	Water	Boric acid in water
LCT-021	6	–/0.23	0.305	5.0	Water	Boric acid in water
LCT-034	14	–/0.395	0.47	4.74	Water	Borated steel or Boral
LCT-040	10	–/0.395	0.47	4.74	Lead or steel	Borated steel or Boral
LCT-075	3	0.06/0.38	0.455	6.5	Water	Boron carbide rods
LCT-086	10	0.07/0.3765	0.4575	2.0 – 4.4	Water	Boric acid in water
LCT-087	7	0.07/0.3765	0.4575	3.6 – 4.4	Water	Borated steel
LCT-089	4	–/0.42447	0.49037	4.34	Water	Borated steel (in core) and Ag-In-Cd (near core)
Summary	78	mixed	0.305 – 0.7075	2.0 – 6.5	Water, Steel, Lead	Borated materials
Target	—	0.06/0.38	0.455	5.0	N/A	Borated steel

5. Running calculations

The calculations were executed in the potku2 cluster of VTT (`espnr130.ad.vtt.fi`) using a perl script to create the inputs, run the calculations and collect the simulation results.

6. Analysis of the results

The experiment-by-experiment results of each code version are collected in Appendices B–D. Table 6 shows the basic sample statistics derived from the calculation results of each code version. The values are rounded for presentation in the table, but unrounded values were used to calculate the further derived parameters. The weighted mean of the k-eff ratios is greater than unity for all of the code versions. Overall, the statistics are very close to each other between the code versions suggesting that there are no notable differences in the applicability of the versions to criticality safety calculations.

Table 6. Basic sample statistics derived from the calculation results for each code version.

Statistical variable	How calculated?	Serpent 2.1.25	Serpent 2.1.27	Serpent 2.1.28
$\overline{k}_{\text{eff}}$	Eq. 5	1.00287	1.00293	1.00292
$\overline{\sigma}^2$	Eq. 7	5.861×10^{-6}	5.862×10^{-6}	5.863×10^{-6}
$\overline{\sigma}$	Square root of previous	0.002 42	0.002 42	0.002 42
s^2	Eq. 8	1.556×10^{-5}	1.525×10^{-5}	1.541×10^{-5}
s	Square root of previous	0.003 94	0.003 91	0.003 93
S_P^2	Eq. 9	2.141×10^{-5}	2.112×10^{-5}	2.128×10^{-5}
S_P	Square root of previous	0.004 63	0.004 60	0.004 61

The results from the normality test applied to the k-eff ratio distributions are collected in Table 7. The k-eff ratio distribution for each code version can be considered to be normal at the chosen significance level of α = 0.05. The single sided tolerance limit will therefore be calculated using Eq. 10.

Table 7. The results of the normality test applied to the results of the validation calculations.

Statistical variable	How calculated?	Serpent 2.1.25	Serpent 2.1.27	Serpent 2.1.28
W test parameter	Ref. [3]	0.971 270	0.971 117	0.971 390
W_n normalized test parameter	Ref. [3]	1.440 367	1.451 980	1.431 224
p-value for W_n	Eq. 13	0.149 764	0.146 508	0.152 366
Considered normal	$p > \alpha$?	Yes.	Yes.	Yes.

6.1 Single sided tolerance limit

As the weighted mean of the k-eff ratios exceeded unity for all of the code versions the lower variant of Eq. 10 was used to calculate the single sided tolerance limit K_L. This means that the K_L were calculated by

$$K_L = 1.0 - US_P \tag{20}$$

The parameter U was looked up from Table 1 based on the number of modelled experiments, which was 78. As the number of experiments exceeded the maximum tabulated value (50), the value of U corresponding to the maximum tabulated value was used (U = 2.065) as a conservative number as suggested in [1].

Table 8. The single sided tolerance limits (K_L) calculated for the different code versions based on the results of the validation calculations.

Statistical variable	How calculated?	Serpent 2.1.25	Serpent 2.1.27	Serpent 2.1.28
K_L	Eq. 20	0.990 444	0.990 511	0.990 475

The single sided tolerance limits were calculated for the three code versions using U equal to 2.065 and non-rounded values for the square root of the pooled variance S_P. The calculated values are tabulated in Table 8. The calculated single sided tolerance limits are used in Section 7 for the calculation of the upper safety limits.

6.2 Trend analyses

Identifying potential trends in the calculated k-eff ratios with respect to one of the important parameters in the experiments (enrichment, lattice pitch etc.) is an important part of the validation. This helps in either choosing the methodology for calculating the upper safety limit or in limiting the area of the applicability of the validation.

As the single sided tolerance limit was calculated based on the fact that the weighted mean of the k-effective ratio is larger than 1.0 we shall limit the area of applicability of this validation to the regions of the parameters, where the trends predict k-effective ratios larger than 1.0. An alternative approach would be to use the linear weighted tolerance band approach (described in [1]) for calculating a lower value for K_L based on the linear fit at the regions where the fit predicts k-effective ratios less than 1.0.

This idea is best illustrated visually. Figure 2 contains the calculated k-effective ratios as a function of fuel enrichment for Serpent 2.1.25. A weighted linear fit has been calculated based on the data and plotted in the figure with a black line. The Pearson linear-correlation coefficient for the fit is -0.274. Based on this coefficient and visual inspection of the data a linear correlation between the two variables (fuel enrichment and k-eff ratio) seems plausible. Based on the fit, fuel enrichments larger than 6.31 wt.% will produce (statistically speaking) k-effective ratios less than 1.0. This area is marked into the figure with a red tint in the background.

In order to provide a constant upper safety limit for easy application with a reduced risk of misuse, we shall exclude these "red tinted regions" from the area of the applicability.

The following parameters were considered in the trend analysis:

- Fuel enrichment. The value for the target system was 5.0 wt.%. The experiments containing multiple fuel enrichments in the same core were excluded from the trend analysis.
- The macroscopic absorption cross section of boron (sum of both isotopes) at 2200 m/s neutron energy in the boron containing material, which can be considered the "blackness" of the neutron absorbing material. The value for the target system was 4.92 1/cm.
- Pin pitch, which will affect the moderation in the fuel lattice. The value for the target system was 1.275 cm. Only experiments with hexagonal pin lattice geometry were included in the trend analysis.
- The energy corresponding to the average lethargy of neutrons that cause fission (EALF), which measures the fission inducing neutron energy spectrum in the system. The value for the target system was 0.35 eV.

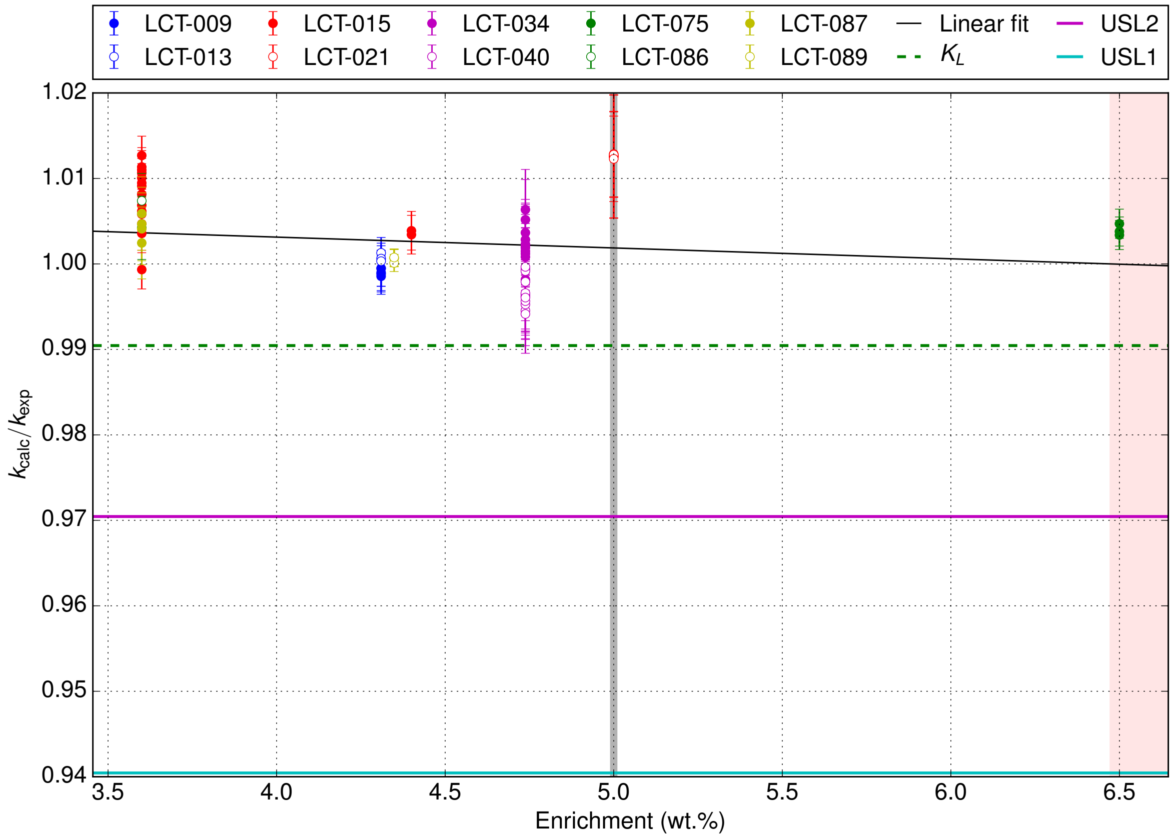

Figure 2. Trend analysis for a linear trend of k-effective ratio versus fuel enrichment for Serpent 2.1.25. The enrichment of the target system is indicated with a vertical grey line. The region where the linear fit predicts k-effective ratios below 1.0 is shown with red tinted background. The two upper safety limits calculated based on K_L are also shown: USL1 for normal conditions and anticipated operational occurrences and USL2 for other design basis scenarios.

The data for these four parameters in each experiment are given in Table H.1. The fuel enrichment and lattice pitch were obtained directly from the benchmark descriptions. The macroscopic absorption cross section of boron was calculated by taking the microscopic total absorption cross section of each isotope at 0.0253 eV (2200 m/s) from the cross section data, multiplying the cross sections with the atomic densities of each boron isotope in the boron containing material and summing up the two isotope-wise macroscopic absorption cross sections. The EALF values were calculated with Serpent 2.1.28 for each of the experiments using the same cross section library that was used in this validation.

The calculated coefficients for the weighted linear fits for each code version are listed in Tables 9–11. The differences in the fits between the code versions were small. Based on the linear-correlation coefficients *r* and visual inspection of the data (presented in Appendices E–G), the trends with respect to fuel enrichment and pin pitch were considered to be plausible trends and were treated as such. However, including the boron macroscopic cross section and the EALF to the plausible trends would not have resulted in further limitations to the area of applicability.

The limitations by the linear trends to the area of applicability are given in Table 12 for the two parameters and the different code versions. These limitations are used in Section 8 in conjunction with other data to define the area of applicability for this validation.

Table 9. Linear correlation coefficients for the linear fits ($y = ax+b$) against different parameters for Serpent 2.1.25.

	a	b	r	correlated?
Enrichment	-0.001262	1.008188	-0.233	Yes
Boron Σ_c	-0.000044	1.003305	-0.180	No
Pin pitch	0.020970	0.980503	0.455	Yes
EALF	0.002163	1.002175	0.197	No

Table 10. Linear correlation coefficients for the linear fits ($y = ax + b$) against different parameters for Serpent 2.1.27.

	a	b	r	correlated?
Enrichment	-0.001283	1.008334	-0.240	Yes
Boron Σ_c	-0.000045	1.003374	-0.186	No
Pin pitch	0.020935	0.980543	0.454	Yes
EALF	0.002058	1.002266	0.189	No

Table 11. Linear correlation coefficients for the linear fits ($y = ax + b$) against different parameters for Serpent 2.1.28.

	a	b	r	correlated?
Enrichment	-0.001267	1.008258	-0.235	Yes
Boron Σ_c	-0.000044	1.003355	-0.180	No
Pin pitch	0.020724	0.980834	0.449	Yes
EALF	0.002165	1.002223	0.198	No

Table 12. Limitations to the area of applicability resulting from the trend analysis.

	Serpent 2.1.25	Serpent 2.1.27	Serpent 2.1.28
Enrichment (maximum)	6.48 wt.%	6.49 wt.%	6.51 wt.%
Pin pitch (minimum)	0.93 cm	0.93 cm	0.93 cm

7. Determining safety limits

The upper safety limits are determined based on the single sided tolerance limits listed in Table 8 using Eq. 1. For analyses conducted for systems within the area of applicability (AoA) for this validation (see next section for determination of the AoA), the margin for extension of the area of applicability (Δ_{AoA}) is set to zero. The formula used for calculating the upper safety limits is then

$$\mathrm{USL} = K_L - \Delta_{\mathrm{SM}}, \tag{21}$$

where Δ_{SM} is the safety margin as was described in Section 3.1. To reiterate, two separate safety limits are given in the Finnish Regulatory Guides on nuclear safety that correspond to two separate safety margins. The first margin $\Delta^{\mathrm{L1}}_{\mathrm{SM}}$ is equal to 0.05 and is applied to normal conditions and anticipated operational occurrences. The second margin $\Delta^{\mathrm{L2}}_{\mathrm{SM}}$ is equal to 0.02 and is applied to other design basis scenarios. The single sided tolerance limits calculated in Section 6.1 were rounded down[4] to the fifth significant digit and the two safety margins were subtracted to obtain the upper safety limits listed in Table 13.

Table 13. Upper Safety Limits determined for the three code versions included in the validation.

Limit	Applied to	Serpent 2.1.25	Serpent 2.1.27	Serpent 2.1.28
USL1	Normal conditions and anticipated operational occurrences	0.94044	0.94051	0.94047
USL2	Other design basis scenarios	0.97044	0.97051	0.97047

The upper safety limits shall be applied for future criticality safety calculation so that systems for which the calculated multiplication factor $k_{\mathrm{calc.}}$ fulfills

$$k_{\mathrm{calc.}} + 2\sigma_{\mathrm{calc.}} < \mathrm{USL}. \tag{22}$$

can be considered to fulfill the requirement of subcriticality. $\sigma_{\mathrm{calc.}}$ is the statistical uncertainty of the calculated multiplication factor.

In applications that cannot be considered to lie in the area of applicability for this validation, a further margin for subcriticality Δ_{AoA} needs to be subtracted from the upper safety limits listed in Table 13. The margin should be based on the results of the sensitivity study (bias trends) as well as engineering judgement [1].

[4] Rounding down results in a stricter safety limit and is thus conservative.

8. Area of applicability

The fuel enrichment in the experiments varied between 3.6 and 6.5 wt.% ^{235}U. We will limit the area of applicability from the high enrichment direction based on the trend analysis results (Table 12) to 6.48 wt.% (the lowest limit among the three code versions). The fuel enrichment of the target system is covered by the area of applicability. The modelled experiments did not contain notable amounts of other fissile isotopes, especially the experiments contained no fuel with fissile plutonium.

The hexagonal lattice pitches in the experiments ranged from 1.0 to 1.3 cm. No further limitations to the area of applicability are needed based on the trend analysis results (Table 12). The lattice pitch of the target system is covered by the area of applicability.

The validation is applicable to systems where the neutron leakage is not controlled by reflection and to systems where water reflectors are used. Separate safety limits should be calculated for systems that contain solid reflectors that significantly reduce neutron leakage.

The validation is applicable for system containing boron absorber. Separate safety limits should be calculated for systems containing notable amounts of other absorbers.

The EALF of the systems ranged from 0.07 to 1.53 eV. The EALF of the target system is well covered by the area of applicability.

The average moderator density in the experiments was $0.9985\,\mathrm{g/cm^3}$ with slight variations (maximum density was $1.0012\,\mathrm{g/cm^3}$ and minimum $0.9973\,\mathrm{g/cm^3}$). The variations in moderator density followed from slight variations in room temperature and the concentration of the soluble absorber in the system. Based on the $\pm$ 10 % restriction given to the moderator density in Table 3 we define the area of applicability to be 0.9–1.1 $\mathrm{g/cm^3}$.

This validation is applicable to the code systems described in Section 2. If other versions of Serpent are to be used in criticality safety analyses, the lowest safety limit determined in this validation (Serpent 2.1.25) can be used provided that it can be shown that the code version to be used gives statistically similar results than the code versions used in this validation for the critical experiments included in this validation.

The area of applicability is collected into Table 14.

Table 14. The area of applicability for this validation. Analyses conducted for systems outside the area of application should use an additional margin for the extension of the upper safety limit Δ_{AoA} or consider executing a separate criticality safety validation for the system.

Parameter	Area of applicability
Fissionable material	Uranium dioxide with ^{235}U enrichment between 3.6 and 6.48 wt.% and no significant content of other fissile isotopes.
Fuel rod lattice pitch	Lattice pitches in the 1.0–1.3 cm range. Hexagonal lattice.
Reflectors	Systems with no significant reflectors and systems with water reflectors.
Absorber	Systems that contain natural boron absorber
Neutron energy	Thermal systems that have the energy corresponding to average lethargy of fission causing neutrons (EALF) in the range of 0.07–1.53 eV.
Moderator density	Moderator densities in the range of 0.9–1.1 g/cm^3

9. Summary

Three code versions of Serpent 2 were validated for criticality safety calculations for wet storage configurations of nuclear fuel in which boron absorber is present. The detailed description of the validated code systems is given in Section 2. The area of applicability for this validation is stated in Section 8. In the area of applicability, the upper safety limits for criticality safety calculations derived in Section 7 can be directly used. Outside the area of applicability, further safety margin Δ_{AoA} needs to be subtracted from the upper safety limits derived in Section 7 based on bias trends and engineering judgement.

References

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Appendices

A Experiments included in the validation

Table A.1. Experiments included in the validation.

Experimental series	Experiment	k_{exp}	σ_{exp}
LCT-009	Case05	1.00000	0.00210
LCT-009	Case06	1.00000	0.00210
LCT-009	Case07	1.00000	0.00210
LCT-009	Case08	1.00000	0.00210
LCT-009	Case09	1.00000	0.00210
LCT-013	Case02	1.00000	0.00180
LCT-013	Case03	1.00000	0.00180
LCT-013	Case04	1.00000	0.00180
LCT-015	100/100	1.00000	0.00226
LCT-015	111/110	1.00000	0.00226
LCT-015	112/112	1.00000	0.00226
LCT-015	12b/12	1.00000	0.00226
LCT-015	147/138	1.00000	0.00226
LCT-015	14b/14	1.00000	0.00226
LCT-015	161/161	1.00000	0.00226
LCT-015	162/161	1.00000	0.00226
LCT-015	163/161	1.00000	0.00226
LCT-015	18b/18	1.00000	0.00226
LCT-015	209/40	1.00000	0.00226
LCT-015	247/247	1.00000	0.00226
LCT-015	29/29	1.00000	0.00226
LCT-015	30/30	1.00000	0.00226
LCT-015	36/36	1.00000	0.00226
LCT-015	37/37	1.00000	0.00226
LCT-021	Case01	1.00000	0.00720
LCT-021	Case02	1.00000	0.00720
LCT-021	Case03	1.00000	0.00720
LCT-021	Case04	1.00000	0.00500
LCT-021	Case05	1.00000	0.00500
LCT-021	Case06	1.00000	0.00500

Table A.1. Experiments included in the validation (continued).

Experimental series	Experiment	k_{exp}	σ_{exp}
LCT-034	Case01	1.00000	0.00470
LCT-034	Case02	1.00000	0.00470
LCT-034	Case03	1.00000	0.00390
LCT-034	Case04	1.00000	0.00390
LCT-034	Case05	1.00000	0.00390
LCT-034	Case06	1.00000	0.00390
LCT-034	Case07	1.00000	0.00390
LCT-034	Case08	1.00000	0.00390
LCT-034	Case10	1.00000	0.00480
LCT-034	Case11	1.00000	0.00480
LCT-034	Case12	1.00000	0.00480
LCT-034	Case13	1.00000	0.00480
LCT-034	Case14	1.00000	0.00430
LCT-034	Case15	1.00000	0.00430
LCT-040	Case01	1.00000	0.00390
LCT-040	Case02	1.00000	0.00410
LCT-040	Case03	1.00000	0.00410
LCT-040	Case04	1.00000	0.00410
LCT-040	Case05	1.00000	0.00420
LCT-040	Case06	1.00000	0.00440
LCT-040	Case07	1.00000	0.00440
LCT-040	Case08	1.00000	0.00440
LCT-040	Case09	1.00000	0.00460
LCT-040	Case10	1.00000	0.00460
LCT-075	Case01	1.00030	0.00170
LCT-075	Case02	1.00030	0.00170
LCT-075	Case03	0.99810	0.00170
LCT-086	Case1	1.00000	0.00370
LCT-086	Case10	1.00000	0.00320
LCT-086	Case2	1.00000	0.00370
LCT-086	Case3	1.00000	0.00370
LCT-086	Case4	1.00000	0.00370
LCT-086	Case5	1.00000	0.00370
LCT-086	Case6	1.00000	0.00320
LCT-086	Case7	1.00000	0.00320
LCT-086	Case8	1.00000	0.00320
LCT-086	Case9	1.00000	0.00320

B Calculation results for Serpent 2.1.25

Table B.1. Results for Serpent 2.1.25.

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-009	Case05	0.99950	1.00000	0.00011	0.00210	0.99950	0.00210
LCT-009	Case06	0.99882	1.00000	0.00011	0.00210	0.99882	0.00210
LCT-009	Case07	0.99947	1.00000	0.00011	0.00210	0.99947	0.00210
LCT-009	Case08	0.99855	1.00000	0.00011	0.00210	0.99855	0.00210
LCT-009	Case09	0.99898	1.00000	0.00011	0.00210	0.99898	0.00210
LCT-013	Case02	1.00129	1.00000	0.00012	0.00180	1.00129	0.00180
LCT-013	Case03	1.00062	1.00000	0.00012	0.00180	1.00062	0.00180
LCT-013	Case04	1.00032	1.00000	0.00011	0.00180	1.00032	0.00180
LCT-015	100/100	1.00685	1.00000	0.00010	0.00226	1.00685	0.00226
LCT-015	111/110	1.00388	1.00000	0.00012	0.00226	1.00388	0.00226
LCT-015	112/112	1.00342	1.00000	0.00010	0.00226	1.00342	0.00226
LCT-015	12b/12	1.00910	1.00000	0.00011	0.00226	1.00910	0.00226
LCT-015	147/138	1.00469	1.00000	0.00011	0.00226	1.00469	0.00226
LCT-015	14b/14	1.01099	1.00000	0.00010	0.00226	1.01099	0.00226
LCT-015	161/161	1.00582	1.00000	0.00010	0.00226	1.00582	0.00226
LCT-015	162/161	1.00357	1.00000	0.00011	0.00226	1.00357	0.00226
LCT-015	163/161	1.00616	1.00000	0.00010	0.00226	1.00616	0.00226
LCT-015	18b/18	1.00947	1.00000	0.00010	0.00226	1.00947	0.00226
LCT-015	209/40	0.99934	1.00000	0.00011	0.00226	0.99934	0.00226
LCT-015	247/247	1.00815	1.00000	0.00010	0.00226	1.00815	0.00226
LCT-015	29/29	1.01268	1.00000	0.00010	0.00226	1.01268	0.00226
LCT-015	30/30	1.01134	1.00000	0.00010	0.00226	1.01134	0.00226
LCT-015	36/36	1.01007	1.00000	0.00010	0.00226	1.01007	0.00226
LCT-015	37/37	1.01065	1.00000	0.00010	0.00226	1.01065	0.00226
LCT-021	Case01	1.01254	1.00000	0.00011	0.00720	1.01254	0.00720
LCT-021	Case02	1.01256	1.00000	0.00010	0.00720	1.01256	0.00720
LCT-021	Case03	1.01259	1.00000	0.00010	0.00720	1.01259	0.00720
LCT-021	Case04	1.01285	1.00000	0.00009	0.00500	1.01285	0.00500
LCT-021	Case05	1.01278	1.00000	0.00010	0.00500	1.01278	0.00500
LCT-021	Case06	1.01229	1.00000	0.00009	0.00500	1.01229	0.00500

Table B.1. Results for Serpent 2.1.25 (continued).

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-034	Case01	1.00517	1.00000	0.00011	0.00470	1.00517	0.00470
LCT-034	Case02	1.00635	1.00000	0.00011	0.00470	1.00635	0.00470
LCT-034	Case03	1.00365	1.00000	0.00011	0.00390	1.00365	0.00390
LCT-034	Case04	1.00189	1.00000	0.00011	0.00390	1.00189	0.00390
LCT-034	Case05	1.00149	1.00000	0.00011	0.00390	1.00149	0.00390
LCT-034	Case06	1.00283	1.00000	0.00011	0.00390	1.00283	0.00390
LCT-034	Case07	1.00119	1.00000	0.00011	0.00390	1.00119	0.00390
LCT-034	Case08	1.00082	1.00000	0.00011	0.00390	1.00082	0.00390
LCT-034	Case10	1.00231	1.00000	0.00011	0.00480	1.00231	0.00480
LCT-034	Case11	1.00214	1.00000	0.00011	0.00480	1.00214	0.00480
LCT-034	Case12	0.99816	1.00000	0.00011	0.00480	0.99816	0.00480
LCT-034	Case13	0.99939	1.00000	0.00011	0.00480	0.99939	0.00480
LCT-034	Case14	0.99644	1.00000	0.00011	0.00430	0.99644	0.00430
LCT-034	Case15	0.99622	1.00000	0.00011	0.00430	0.99622	0.00430
LCT-040	Case01	0.99790	1.00000	0.00011	0.00390	0.99790	0.00390
LCT-040	Case02	0.99453	1.00000	0.00011	0.00410	0.99453	0.00410
LCT-040	Case03	0.99526	1.00000	0.00011	0.00410	0.99526	0.00410
LCT-040	Case04	0.99618	1.00000	0.00012	0.00410	0.99618	0.00410
LCT-040	Case05	0.99659	1.00000	0.00011	0.00420	0.99659	0.00420
LCT-040	Case06	0.99916	1.00000	0.00011	0.00440	0.99916	0.00440
LCT-040	Case07	0.99564	1.00000	0.00011	0.00440	0.99564	0.00440
LCT-040	Case08	0.99606	1.00000	0.00011	0.00440	0.99606	0.00440
LCT-040	Case09	0.99965	1.00000	0.00011	0.00460	0.99965	0.00460
LCT-040	Case10	0.99414	1.00000	0.00011	0.00460	0.99414	0.00460
LCT-075	Case01	1.00500	1.00030	0.00011	0.00170	1.00470	0.00170
LCT-075	Case02	1.00409	1.00030	0.00011	0.00170	1.00379	0.00170
LCT-075	Case03	1.00147	0.99810	0.00011	0.00170	1.00338	0.00170
LCT-086	Case1	1.00422	1.00000	0.00010	0.00370	1.00422	0.00370
LCT-086	Case10	1.00713	1.00000	0.00009	0.00320	1.00713	0.00320
LCT-086	Case2	1.00528	1.00000	0.00010	0.00370	1.00528	0.00370
LCT-086	Case3	1.00532	1.00000	0.00010	0.00370	1.00532	0.00370
LCT-086	Case4	1.00548	1.00000	0.00010	0.00370	1.00548	0.00370
LCT-086	Case5	1.00528	1.00000	0.00010	0.00370	1.00528	0.00370
LCT-086	Case6	1.00738	1.00000	0.00010	0.00320	1.00738	0.00320
LCT-086	Case7	1.00506	1.00000	0.00010	0.00320	1.00506	0.00320
LCT-086	Case8	1.00721	1.00000	0.00010	0.00320	1.00721	0.00320
LCT-086	Case9	1.00746	1.00000	0.00009	0.00320	1.00746	0.00320
LCT-087	Case10	1.00245	1.00000	0.00010	0.00420	1.00245	0.00420
LCT-087	Case11	1.00230	1.00000	0.00010	0.00230	1.00230	0.00230
LCT-087	Case3	1.00589	1.00000	0.00010	0.00430	1.00589	0.00430
LCT-087	Case4	1.00576	1.00000	0.00010	0.00230	1.00576	0.00230
LCT-087	Case5	1.00411	1.00000	0.00010	0.00420	1.00411	0.00420
LCT-087	Case6	1.00307	1.00000	0.00010	0.00230	1.00307	0.00230
LCT-087	Case9	1.00467	1.00000	0.00010	0.00430	1.00467	0.00430
LCT-089	Case01	1.00100	1.00030	0.00010	0.00100	1.00070	0.00100
LCT-089	Case02	1.00117	1.00050	0.00010	0.00100	1.00067	0.00100
LCT-089	Case03	1.00041	1.00030	0.00010	0.00100	1.00011	0.00100
LCT-089	Case04	1.00105	1.00030	0.00010	0.00100	1.00075	0.00100

C Calculation results for Serpent 2.1.27

Table C.1. Results for Serpent 2.1.27.

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-009	Case05	0.99960	1.00000	0.00011	0.00210	0.99960	0.00210
LCT-009	Case06	0.99897	1.00000	0.00011	0.00210	0.99897	0.00210
LCT-009	Case07	0.99964	1.00000	0.00011	0.00210	0.99964	0.00210
LCT-009	Case08	0.99868	1.00000	0.00011	0.00210	0.99868	0.00210
LCT-009	Case09	0.99913	1.00000	0.00011	0.00210	0.99913	0.00210
LCT-013	Case02	1.00106	1.00000	0.00011	0.00180	1.00106	0.00180
LCT-013	Case03	1.00062	1.00000	0.00011	0.00180	1.00062	0.00180
LCT-013	Case04	1.00054	1.00000	0.00011	0.00180	1.00054	0.00180
LCT-015	100/100	1.00671	1.00000	0.00010	0.00226	1.00671	0.00226
LCT-015	111/110	1.00403	1.00000	0.00011	0.00226	1.00403	0.00226
LCT-015	112/112	1.00297	1.00000	0.00010	0.00226	1.00297	0.00226
LCT-015	12b/12	1.00882	1.00000	0.00011	0.00226	1.00882	0.00226
LCT-015	147/138	1.00494	1.00000	0.00010	0.00226	1.00494	0.00226
LCT-015	14b/14	1.01071	1.00000	0.00010	0.00226	1.01071	0.00226
LCT-015	161/161	1.00593	1.00000	0.00010	0.00226	1.00593	0.00226
LCT-015	162/161	1.00340	1.00000	0.00011	0.00226	1.00340	0.00226
LCT-015	163/161	1.00608	1.00000	0.00010	0.00226	1.00608	0.00226
LCT-015	18b/18	1.00941	1.00000	0.00010	0.00226	1.00941	0.00226
LCT-015	209/40	0.99950	1.00000	0.00011	0.00226	0.99950	0.00226
LCT-015	247/247	1.00829	1.00000	0.00011	0.00226	1.00829	0.00226
LCT-015	29/29	1.01274	1.00000	0.00010	0.00226	1.01274	0.00226
LCT-015	30/30	1.01142	1.00000	0.00010	0.00226	1.01142	0.00226
LCT-015	36/36	1.01020	1.00000	0.00010	0.00226	1.01020	0.00226
LCT-015	37/37	1.01084	1.00000	0.00009	0.00226	1.01084	0.00226
LCT-021	Case01	1.01275	1.00000	0.00010	0.00720	1.01275	0.00720
LCT-021	Case02	1.01243	1.00000	0.00010	0.00720	1.01243	0.00720
LCT-021	Case03	1.01249	1.00000	0.00010	0.00720	1.01249	0.00720
LCT-021	Case04	1.01261	1.00000	0.00009	0.00500	1.01261	0.00500
LCT-021	Case05	1.01263	1.00000	0.00009	0.00500	1.01263	0.00500
LCT-021	Case06	1.01236	1.00000	0.00009	0.00500	1.01236	0.00500

Table C.1. Results for Serpent 2.1.27 (continued).

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-034	Case01	1.00533	1.00000	0.00011	0.00470	1.00533	0.00470
LCT-034	Case02	1.00665	1.00000	0.00011	0.00470	1.00665	0.00470
LCT-034	Case03	1.00368	1.00000	0.00011	0.00390	1.00368	0.00390
LCT-034	Case04	1.00211	1.00000	0.00011	0.00390	1.00211	0.00390
LCT-034	Case05	1.00125	1.00000	0.00011	0.00390	1.00125	0.00390
LCT-034	Case06	1.00294	1.00000	0.00011	0.00390	1.00294	0.00390
LCT-034	Case07	1.00114	1.00000	0.00011	0.00390	1.00114	0.00390
LCT-034	Case08	1.00088	1.00000	0.00011	0.00390	1.00088	0.00390
LCT-034	Case10	1.00228	1.00000	0.00011	0.00480	1.00228	0.00480
LCT-034	Case11	1.00228	1.00000	0.00011	0.00480	1.00228	0.00480
LCT-034	Case12	0.99785	1.00000	0.00011	0.00480	0.99785	0.00480
LCT-034	Case13	0.99949	1.00000	0.00011	0.00480	0.99949	0.00480
LCT-034	Case14	0.99651	1.00000	0.00011	0.00430	0.99651	0.00430
LCT-034	Case15	0.99614	1.00000	0.00011	0.00430	0.99614	0.00430
LCT-040	Case01	0.99772	1.00000	0.00011	0.00390	0.99772	0.00390
LCT-040	Case02	0.99454	1.00000	0.00011	0.00410	0.99454	0.00410
LCT-040	Case03	0.99545	1.00000	0.00011	0.00410	0.99545	0.00410
LCT-040	Case04	0.99643	1.00000	0.00011	0.00410	0.99643	0.00410
LCT-040	Case05	0.99661	1.00000	0.00011	0.00420	0.99661	0.00420
LCT-040	Case06	0.99920	1.00000	0.00011	0.00440	0.99920	0.00440
LCT-040	Case07	0.99535	1.00000	0.00011	0.00440	0.99535	0.00440
LCT-040	Case08	0.99578	1.00000	0.00011	0.00440	0.99578	0.00440
LCT-040	Case09	0.99977	1.00000	0.00011	0.00460	0.99977	0.00460
LCT-040	Case10	0.99422	1.00000	0.00011	0.00460	0.99422	0.00460
LCT-075	Case01	1.00489	1.00030	0.00012	0.00170	1.00459	0.00170
LCT-075	Case02	1.00418	1.00030	0.00011	0.00170	1.00388	0.00170
LCT-075	Case03	1.00136	0.99810	0.00012	0.00170	1.00327	0.00170
LCT-086	Case1	1.00432	1.00000	0.00010	0.00370	1.00432	0.00370
LCT-086	Case10	1.00723	1.00000	0.00010	0.00320	1.00723	0.00320
LCT-086	Case2	1.00529	1.00000	0.00010	0.00370	1.00529	0.00370
LCT-086	Case3	1.00526	1.00000	0.00010	0.00370	1.00526	0.00370
LCT-086	Case4	1.00548	1.00000	0.00010	0.00370	1.00548	0.00370
LCT-086	Case5	1.00522	1.00000	0.00010	0.00370	1.00522	0.00370
LCT-086	Case6	1.00717	1.00000	0.00010	0.00320	1.00717	0.00320
LCT-086	Case7	1.00509	1.00000	0.00010	0.00320	1.00509	0.00320
LCT-086	Case8	1.00738	1.00000	0.00010	0.00320	1.00738	0.00320
LCT-086	Case9	1.00767	1.00000	0.00010	0.00320	1.00767	0.00320
LCT-087	Case10	1.00240	1.00000	0.00010	0.00420	1.00240	0.00420
LCT-087	Case11	1.00223	1.00000	0.00010	0.00230	1.00223	0.00230
LCT-087	Case3	1.00608	1.00000	0.00010	0.00430	1.00608	0.00430
LCT-087	Case4	1.00576	1.00000	0.00010	0.00230	1.00576	0.00230
LCT-087	Case5	1.00393	1.00000	0.00010	0.00420	1.00393	0.00420
LCT-087	Case6	1.00342	1.00000	0.00010	0.00230	1.00342	0.00230
LCT-087	Case9	1.00475	1.00000	0.00010	0.00430	1.00475	0.00430
LCT-089	Case01	1.00117	1.00030	0.00010	0.00100	1.00087	0.00100
LCT-089	Case02	1.00124	1.00050	0.00011	0.00100	1.00074	0.00101
LCT-089	Case03	1.00066	1.00030	0.00010	0.00100	1.00036	0.00100
LCT-089	Case04	1.00116	1.00030	0.00010	0.00100	1.00086	0.00100

D Calculation results for Serpent 2.1.28

Table D.1. Results for Serpent 2.1.28.

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-009	Case05	0.99957	1.00000	0.00011	0.00210	0.99957	0.00210
LCT-009	Case06	0.99880	1.00000	0.00011	0.00210	0.99880	0.00210
LCT-009	Case07	0.99976	1.00000	0.00011	0.00210	0.99976	0.00210
LCT-009	Case08	0.99865	1.00000	0.00011	0.00210	0.99865	0.00210
LCT-009	Case09	0.99906	1.00000	0.00011	0.00210	0.99906	0.00210
LCT-013	Case02	1.00138	1.00000	0.00011	0.00180	1.00138	0.00180
LCT-013	Case03	1.00059	1.00000	0.00012	0.00180	1.00059	0.00180
LCT-013	Case04	1.00053	1.00000	0.00012	0.00180	1.00053	0.00180
LCT-015	100/100	1.00668	1.00000	0.00010	0.00226	1.00668	0.00226
LCT-015	111/110	1.00390	1.00000	0.00011	0.00226	1.00390	0.00226
LCT-015	112/112	1.00335	1.00000	0.00010	0.00226	1.00335	0.00226
LCT-015	12b/12	1.00896	1.00000	0.00010	0.00226	1.00896	0.00226
LCT-015	147/138	1.00457	1.00000	0.00011	0.00226	1.00457	0.00226
LCT-015	14b/14	1.01080	1.00000	0.00010	0.00226	1.01080	0.00226
LCT-015	161/161	1.00601	1.00000	0.00010	0.00226	1.00601	0.00226
LCT-015	162/161	1.00367	1.00000	0.00010	0.00226	1.00367	0.00226
LCT-015	163/161	1.00624	1.00000	0.00010	0.00226	1.00624	0.00226
LCT-015	18b/18	1.00948	1.00000	0.00010	0.00226	1.00948	0.00226
LCT-015	209/40	0.99939	1.00000	0.00011	0.00226	0.99939	0.00226
LCT-015	247/247	1.00822	1.00000	0.00010	0.00226	1.00822	0.00226
LCT-015	29/29	1.01274	1.00000	0.00010	0.00226	1.01274	0.00226
LCT-015	30/30	1.01148	1.00000	0.00011	0.00226	1.01148	0.00226
LCT-015	36/36	1.01005	1.00000	0.00010	0.00226	1.01005	0.00226
LCT-015	37/37	1.01063	1.00000	0.00010	0.00226	1.01063	0.00226
LCT-021	Case01	1.01260	1.00000	0.00010	0.00720	1.01260	0.00720
LCT-021	Case02	1.01228	1.00000	0.00011	0.00720	1.01228	0.00720
LCT-021	Case03	1.01244	1.00000	0.00010	0.00720	1.01244	0.00720
LCT-021	Case04	1.01251	1.00000	0.00009	0.00500	1.01251	0.00500
LCT-021	Case05	1.01264	1.00000	0.00009	0.00500	1.01264	0.00500
LCT-021	Case06	1.01204	1.00000	0.00009	0.00500	1.01204	0.00500

Table D.1. Results for Serpent 2.1.28 (continued).

Experimental series	Experiment	k_{calc}	k_{exp}	σ_{calc}	σ_{exp}	k_{calc}/k_{exp}	σ_i
LCT-034	Case01	1.00526	1.00000	0.00011	0.00470	1.00526	0.00470
LCT-034	Case02	1.00678	1.00000	0.00011	0.00470	1.00678	0.00470
LCT-034	Case03	1.00387	1.00000	0.00011	0.00390	1.00387	0.00390
LCT-034	Case04	1.00213	1.00000	0.00011	0.00390	1.00213	0.00390
LCT-034	Case05	1.00126	1.00000	0.00011	0.00390	1.00126	0.00390
LCT-034	Case06	1.00275	1.00000	0.00011	0.00390	1.00275	0.00390
LCT-034	Case07	1.00075	1.00000	0.00011	0.00390	1.00075	0.00390
LCT-034	Case08	1.00103	1.00000	0.00011	0.00390	1.00103	0.00390
LCT-034	Case10	1.00229	1.00000	0.00011	0.00480	1.00229	0.00480
LCT-034	Case11	1.00227	1.00000	0.00011	0.00480	1.00227	0.00480
LCT-034	Case12	0.99805	1.00000	0.00011	0.00480	0.99805	0.00480
LCT-034	Case13	0.99952	1.00000	0.00011	0.00480	0.99952	0.00480
LCT-034	Case14	0.99671	1.00000	0.00011	0.00430	0.99671	0.00430
LCT-034	Case15	0.99603	1.00000	0.00011	0.00430	0.99603	0.00430
LCT-040	Case01	0.99813	1.00000	0.00011	0.00390	0.99813	0.00390
LCT-040	Case02	0.99468	1.00000	0.00011	0.00410	0.99468	0.00410
LCT-040	Case03	0.99528	1.00000	0.00011	0.00410	0.99528	0.00410
LCT-040	Case04	0.99646	1.00000	0.00011	0.00410	0.99646	0.00410
LCT-040	Case05	0.99657	1.00000	0.00011	0.00420	0.99657	0.00420
LCT-040	Case06	0.99937	1.00000	0.00011	0.00440	0.99937	0.00440
LCT-040	Case07	0.99569	1.00000	0.00011	0.00440	0.99569	0.00440
LCT-040	Case08	0.99590	1.00000	0.00011	0.00440	0.99590	0.00440
LCT-040	Case09	0.99966	1.00000	0.00011	0.00460	0.99966	0.00460
LCT-040	Case10	0.99421	1.00000	0.00011	0.00460	0.99421	0.00460
LCT-075	Case01	1.00477	1.00030	0.00012	0.00170	1.00447	0.00170
LCT-075	Case02	1.00404	1.00030	0.00011	0.00170	1.00374	0.00170
LCT-075	Case03	1.00142	0.99810	0.00011	0.00170	1.00333	0.00170
LCT-086	Case1	1.00420	1.00000	0.00010	0.00370	1.00420	0.00370
LCT-086	Case10	1.00744	1.00000	0.00009	0.00320	1.00744	0.00320
LCT-086	Case2	1.00529	1.00000	0.00010	0.00370	1.00529	0.00370
LCT-086	Case3	1.00528	1.00000	0.00010	0.00370	1.00528	0.00370
LCT-086	Case4	1.00559	1.00000	0.00010	0.00370	1.00559	0.00370
LCT-086	Case5	1.00536	1.00000	0.00010	0.00370	1.00536	0.00370
LCT-086	Case6	1.00735	1.00000	0.00010	0.00320	1.00735	0.00320
LCT-086	Case7	1.00496	1.00000	0.00010	0.00320	1.00496	0.00320
LCT-086	Case8	1.00743	1.00000	0.00010	0.00320	1.00743	0.00320
LCT-086	Case9	1.00751	1.00000	0.00010	0.00320	1.00751	0.00320

E Trend analysis plots for Serpent 2.1.25

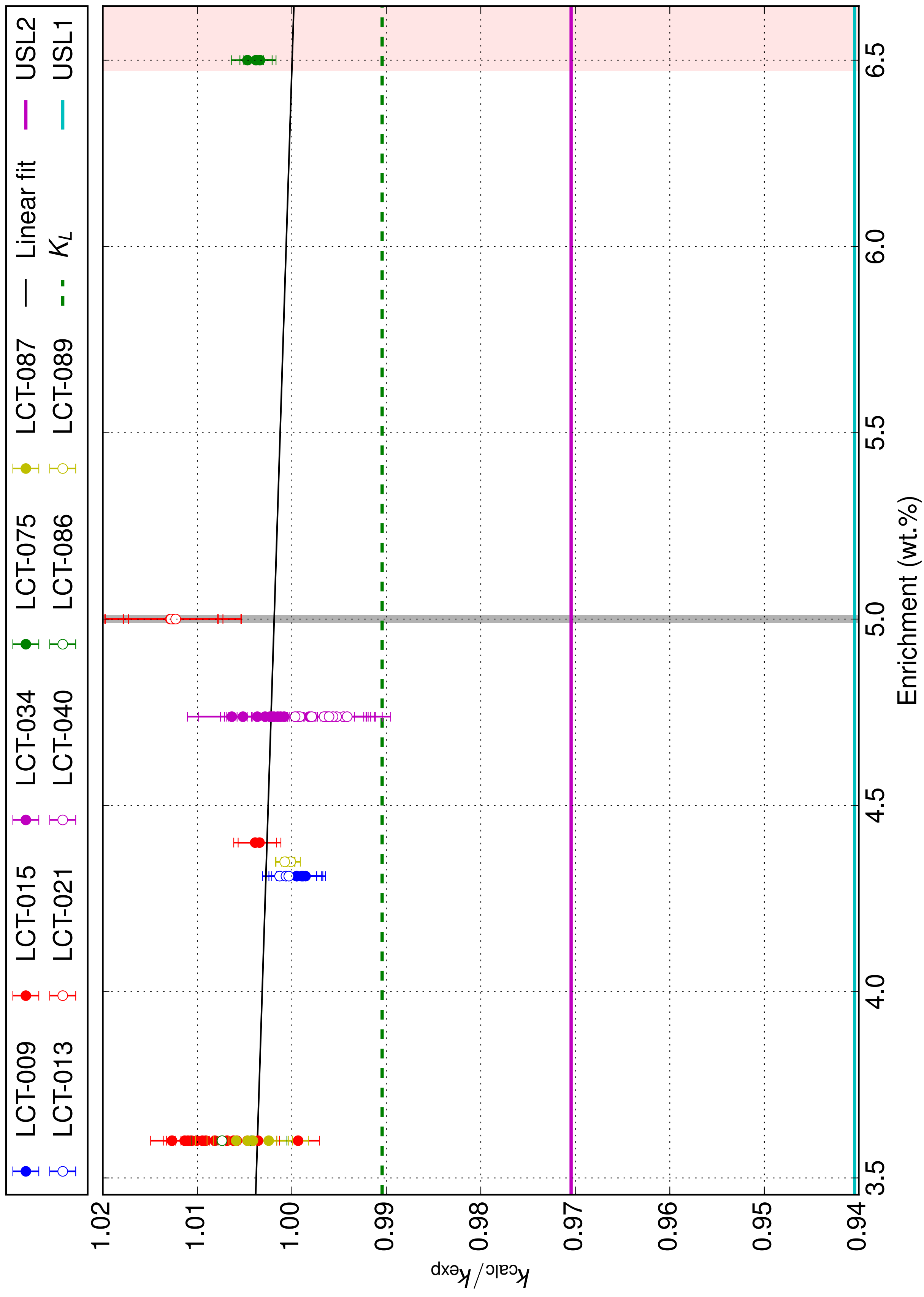

Figure E.1. Trend analysis for a linear trend of k-effective ratio versus fuel enrichment for Serpent 2.1.25. The enrichment of the target system is indicated with a vertical grey line. The region where the linear fit predicts k-effective ratios below 1.0 is shown with red tinted background. The correlation was deemed statistically significant.

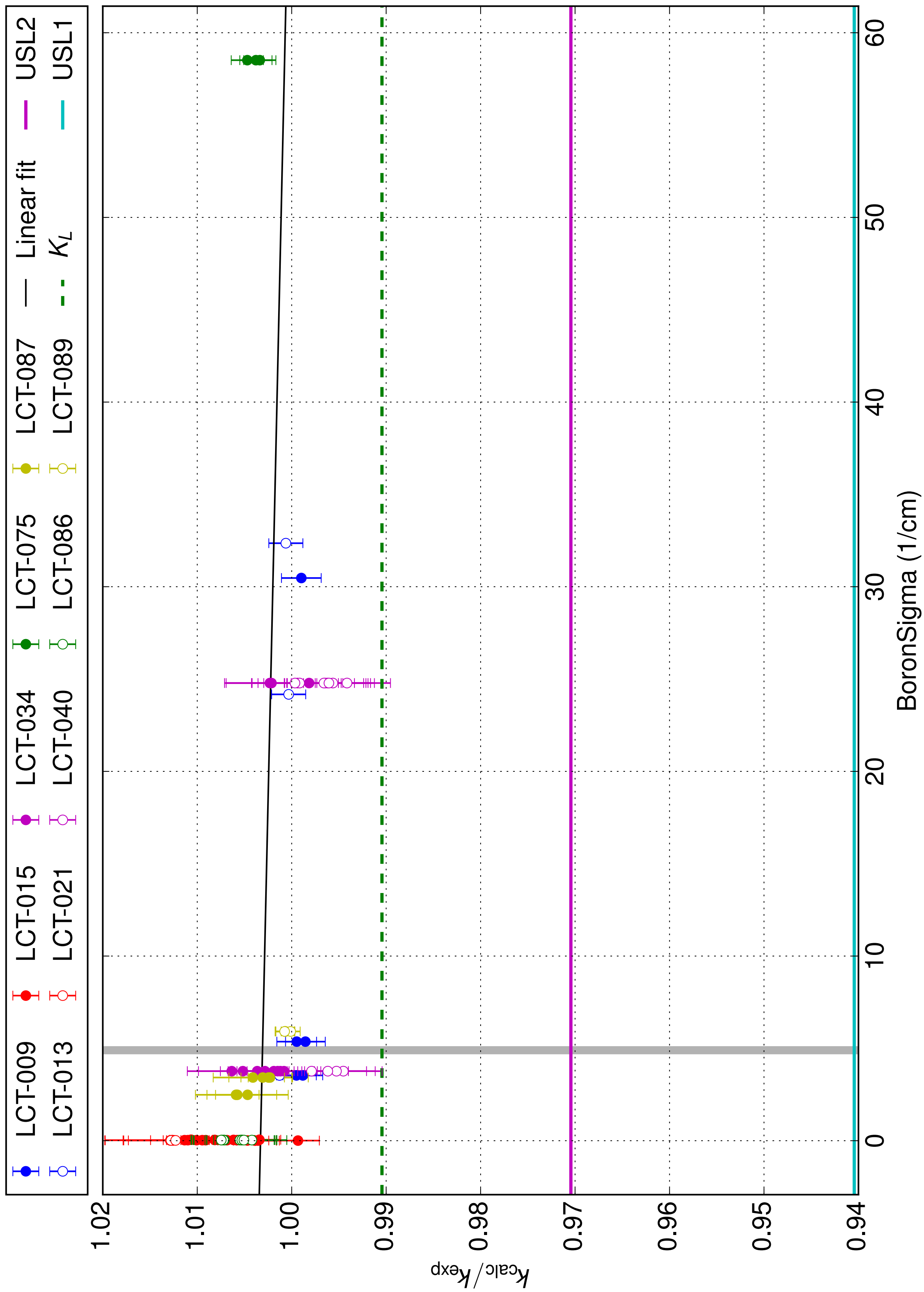

Figure E.2. Trend analysis for a linear trend of k-effective ratio versus boron macroscopic capture cross section in borated material for Serpent 2.1.25. The boron macroscopic capture cross section in the borated steel plates of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

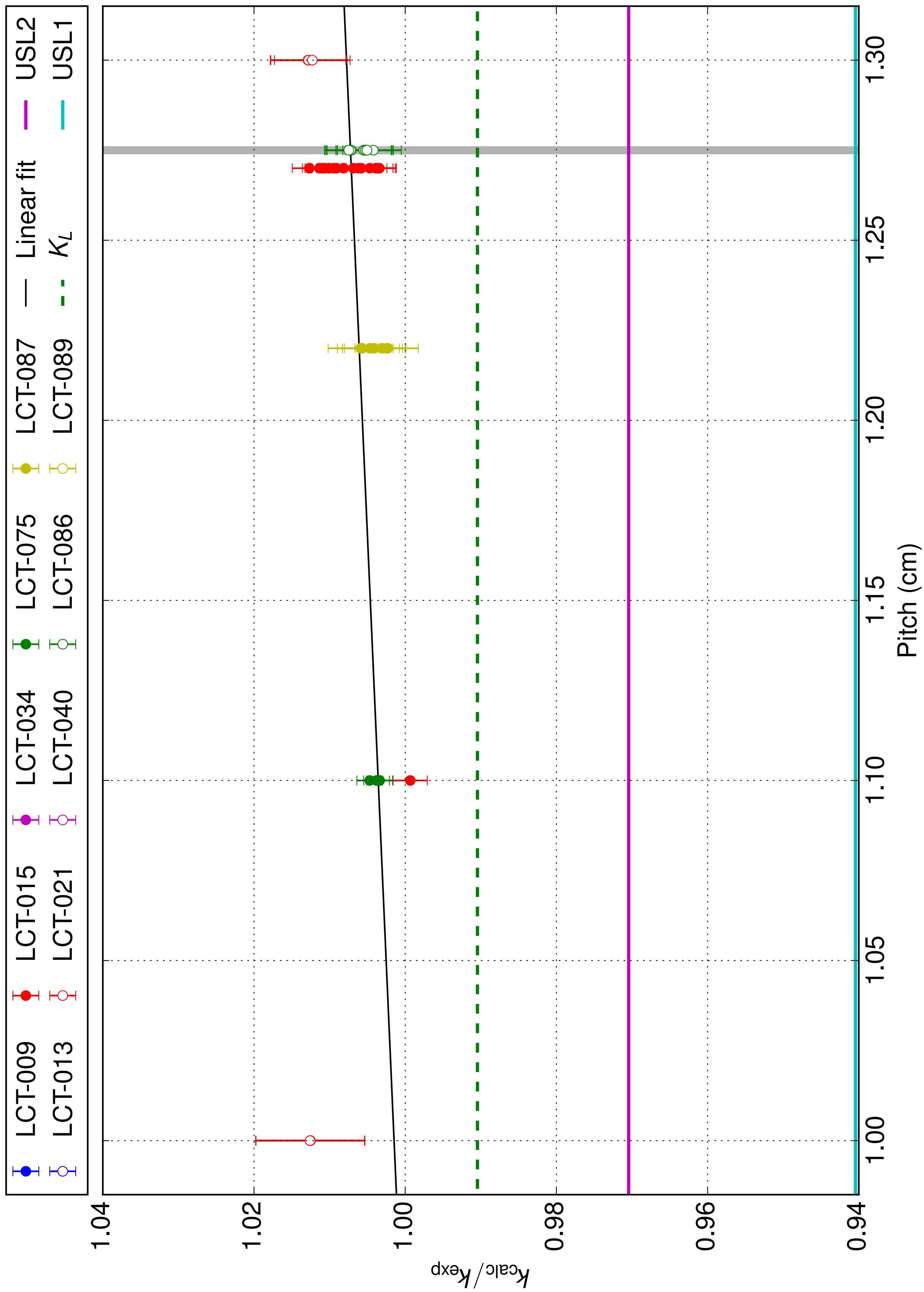

Figure E.3. Trend analysis for a linear trend of k-effective ratio versus pin pitch for Serpent 2.1.25. The pin pitch of the target system is indicated with a vertical grey line. The correlation was deemed statistically significant.

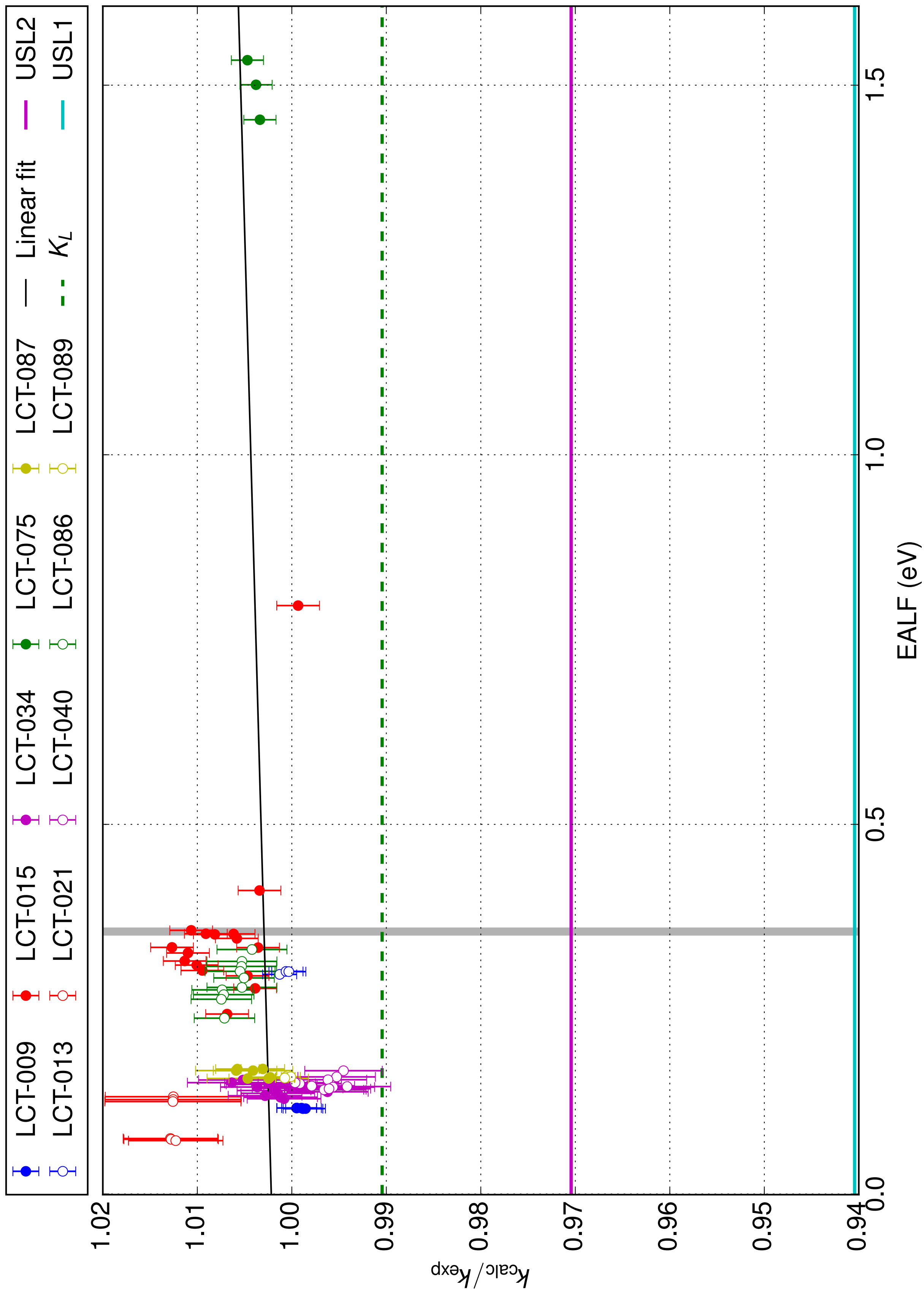

Figure E.4. Trend analysis for a linear trend of k-effective ratio versus EALF for Serpent 2.1.25. The EALF of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

F Trend analysis plots for Serpent 2.1.27

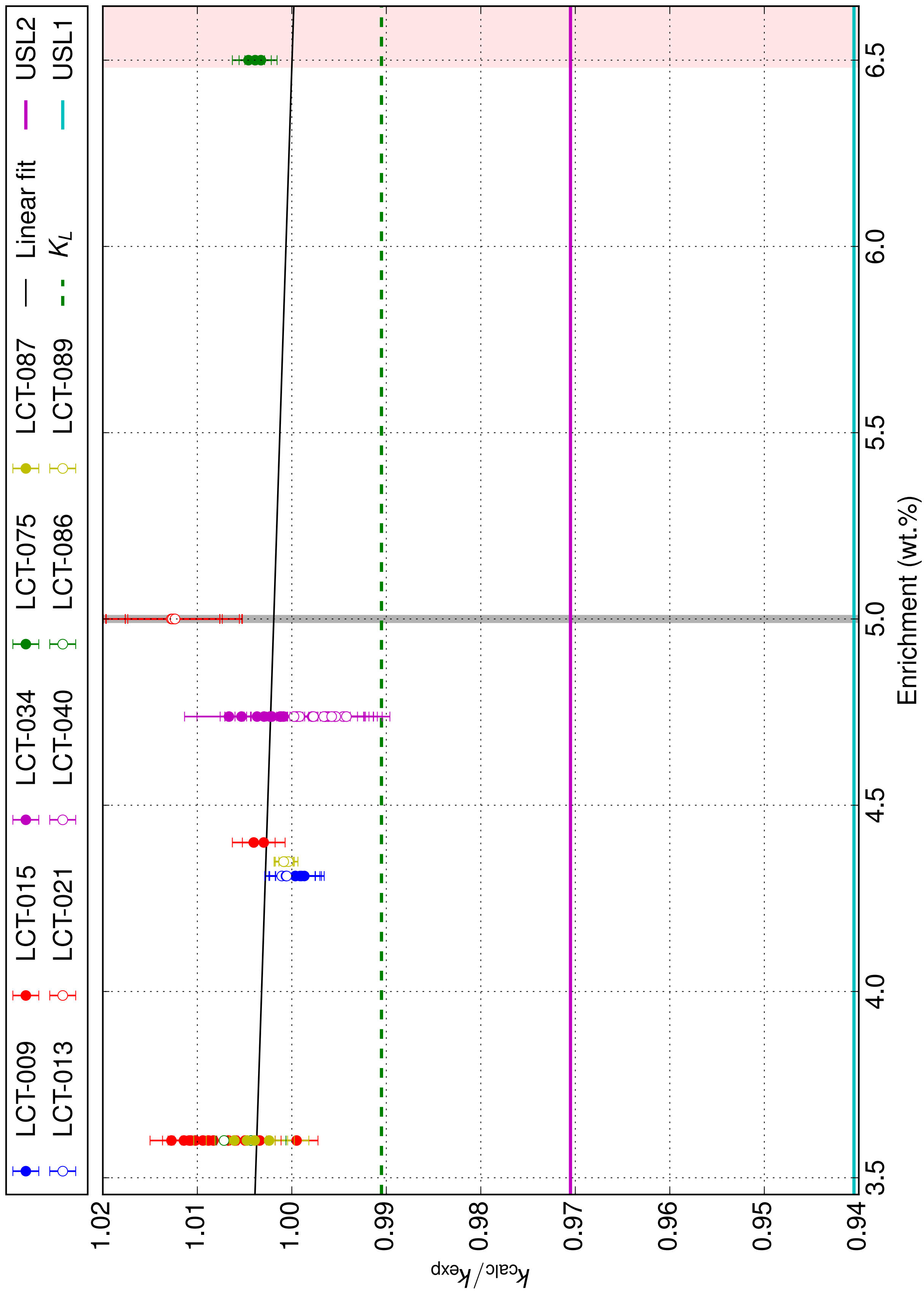

Figure F.1. Trend analysis for a linear trend of k-effective ratio versus fuel enrichment for Serpent 2.1.27. The enrichment of the target system is indicated with a vertical grey line. The region where the linear fit predicts k-effective ratios below 1.0 is shown with red tinted background. The correlation was deemed statistically significant.

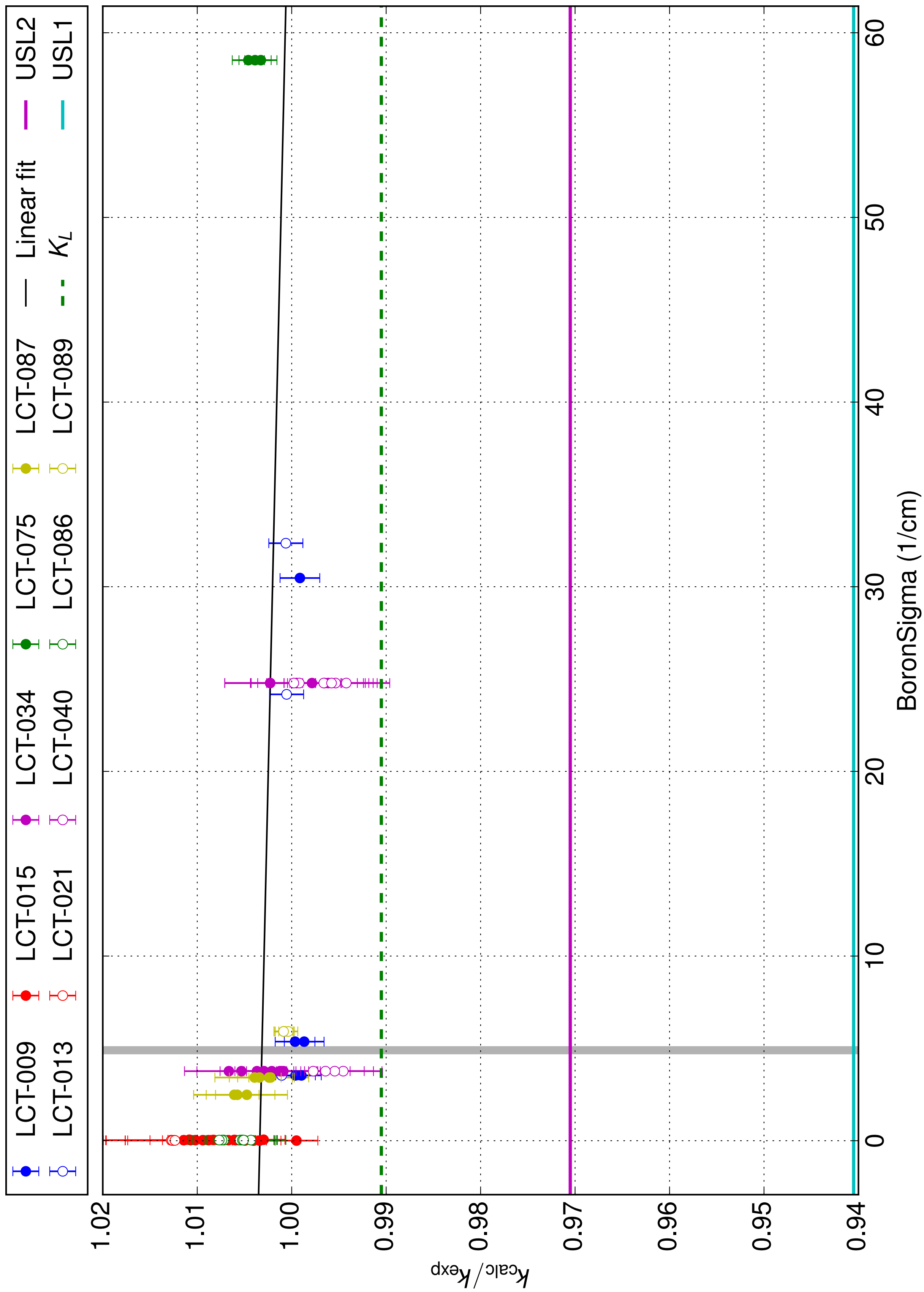

Figure F.2. Trend analysis for a linear trend of k-effective ratio versus boron macroscopic capture cross section in borated material for Serpent 2.1.27. The boron macroscopic capture cross section in the borated steel plates of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

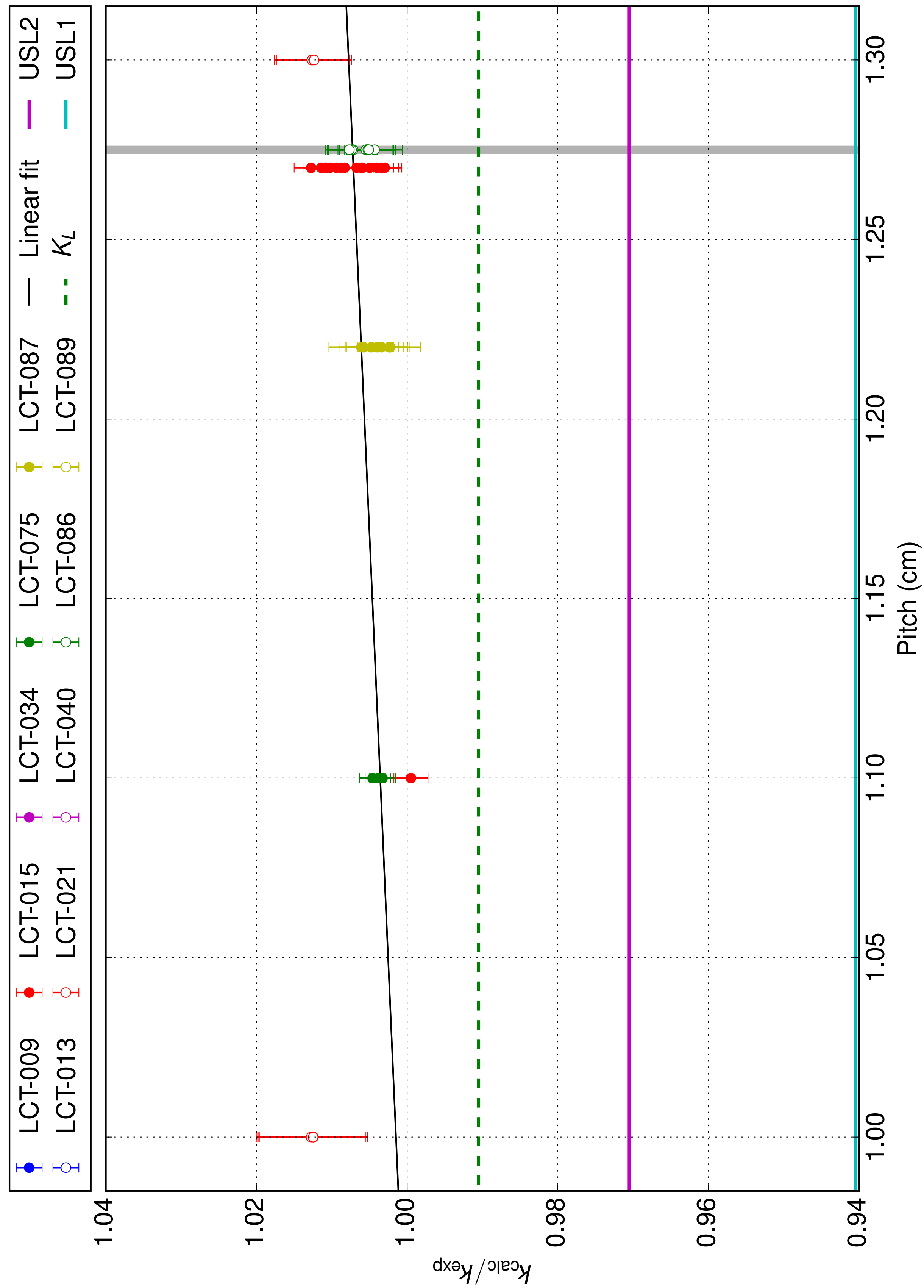

Figure F.3. Trend analysis for a linear trend of k-effective ratio versus pin pitch for Serpent 2.1.27. The pin pitch of the target system is indicated with a vertical grey line. The correlation was deemed statistically significant.

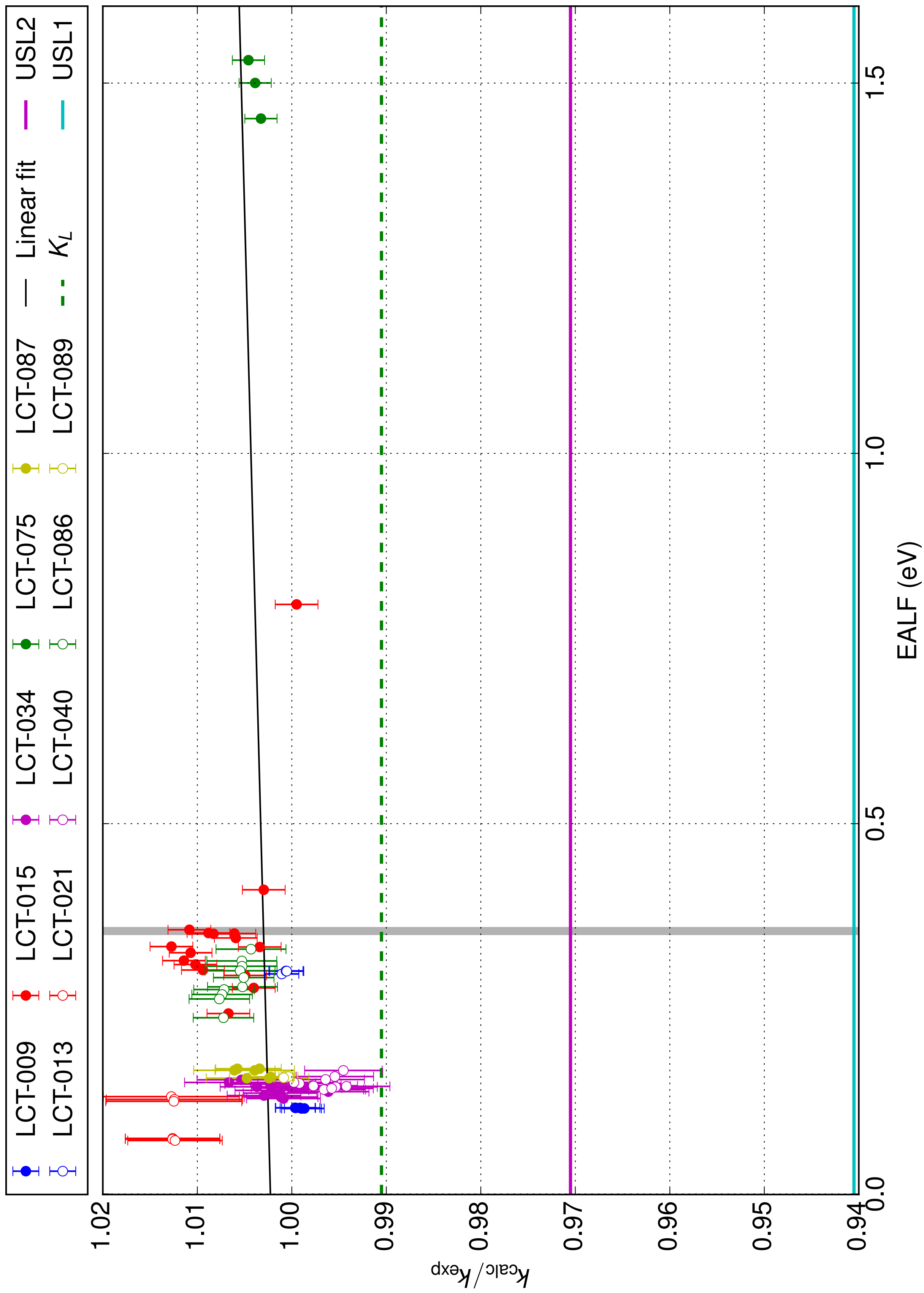

Figure F.4. Trend analysis for a linear trend of k-effective ratio versus EALF for Serpent 2.1.27. The EALF of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

G Trend analysis plots for Serpent 2.1.28

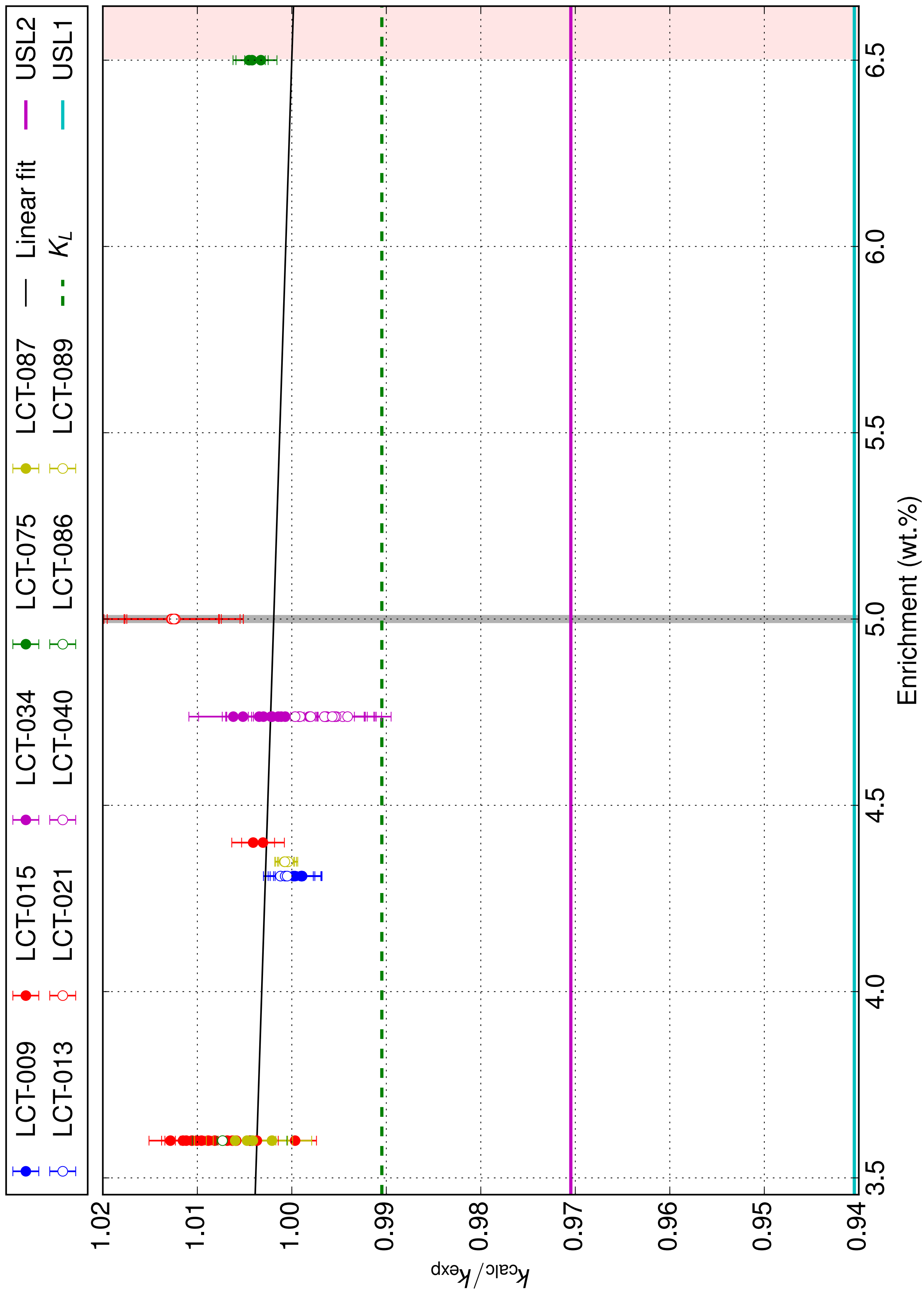

Figure G.1. Trend analysis for a linear trend of k-effective ratio versus fuel enrichment for Serpent 2.1.28. The enrichment of the target system is indicated with a vertical grey line. The region where the linear fit predicts k-effective ratios below 1.0 is shown with red tinted background. The correlation was deemed statistically significant.

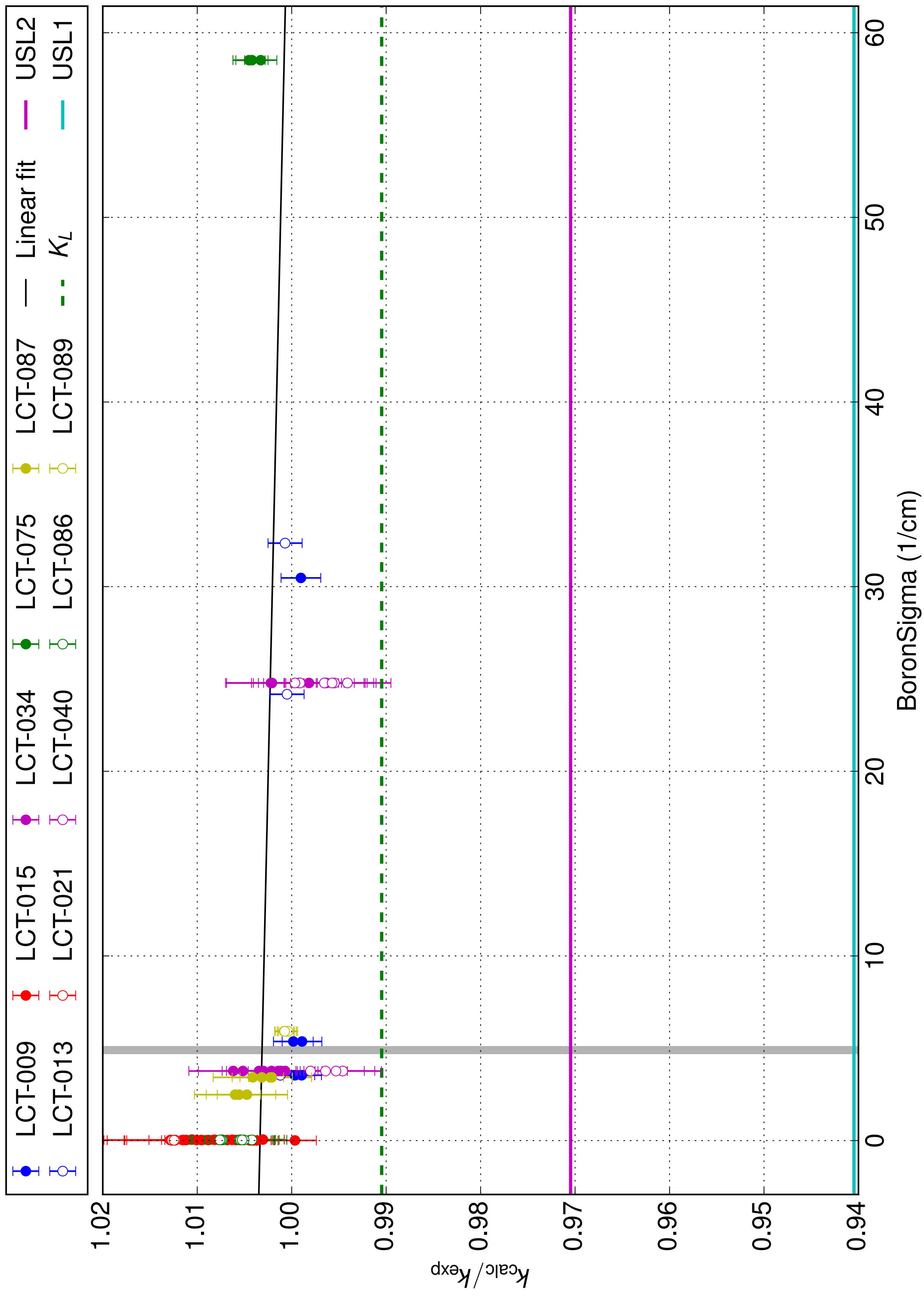

Figure G.2. Trend analysis for a linear trend of k-effective ratio versus boron macroscopic capture cross section in borated material for Serpent 2.1.28. The boron macroscopic capture cross section in the borated steel plates of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

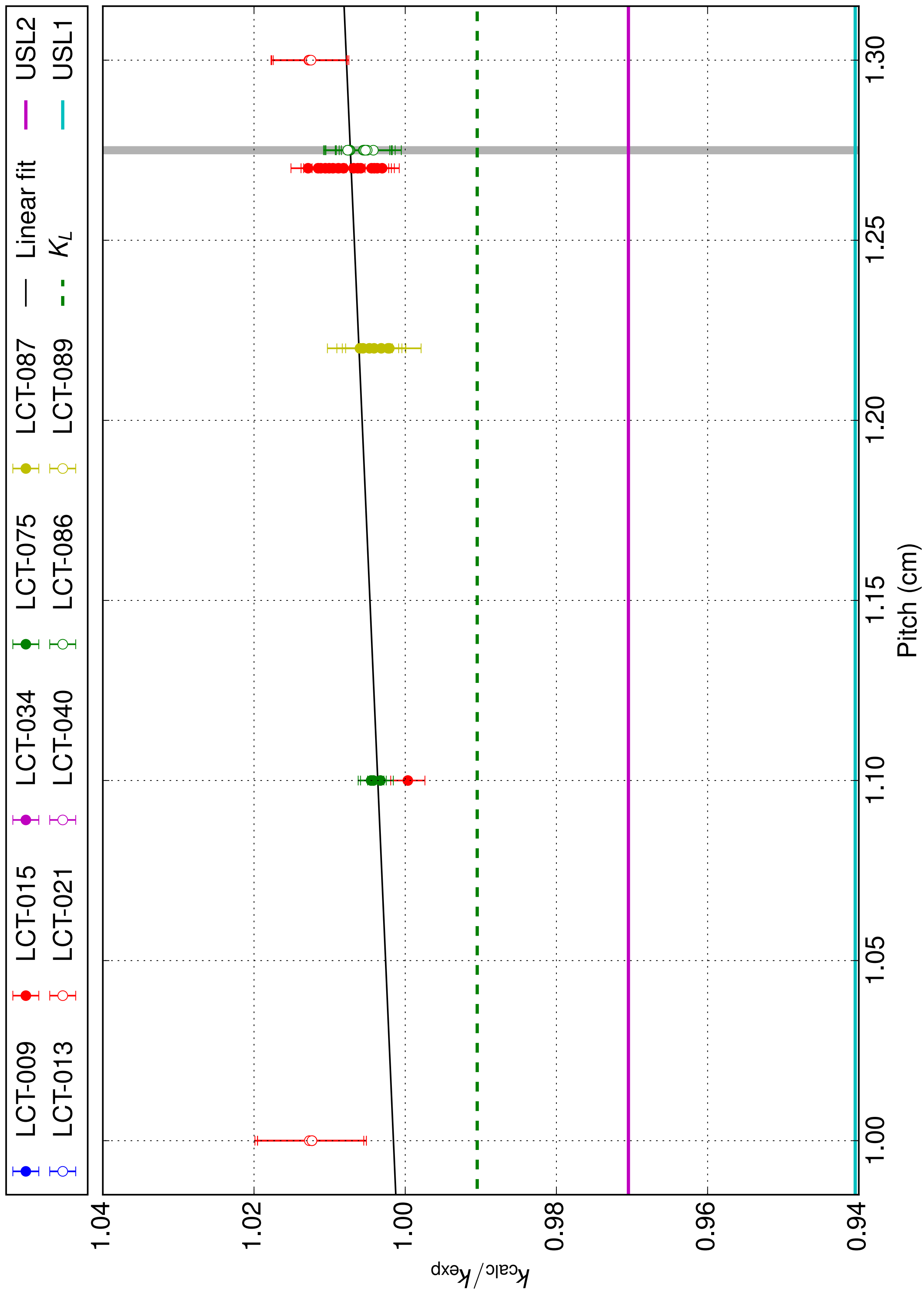

Figure G.3. Trend analysis for a linear trend of k-effective ratio versus pin pitch for Serpent 2.1.28. The pin pitch of the target system is indicated with a vertical grey line. The correlation was deemed statistically significant.

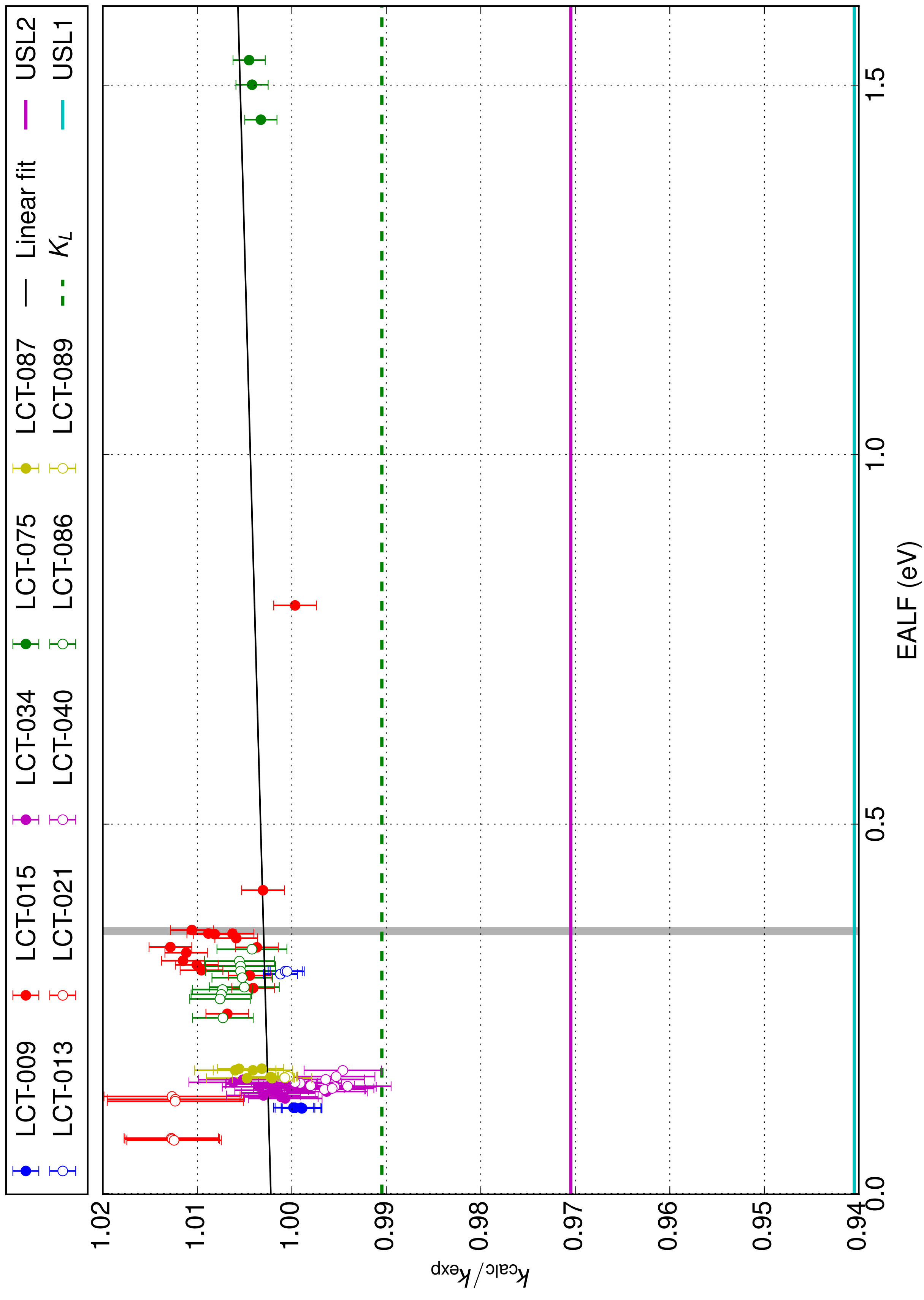

Figure G.4. Trend analysis for a linear trend of k-effective ratio versus EALF for Serpent 2.1.28. The EALF of the target system is indicated with a vertical grey line. The correlation was not deemed statistically significant.

H Data used for trend fitting

Table H.1. Data used for trend fitting. Square lattice pitches and mixed enrichments were excluded from trend fitting.

Experimental series	Experiment	Enrichment wt.%	Boron Σ_c at 2200 m/s. 1/cm	Lattice pitch cm	EALF eV
lct-009	Case05	4.31	3.54	2.54 (square)	0.12
lct-009	Case06	4.31	3.54	2.54 (square)	0.12
lct-009	Case07	4.31	5.37	2.54 (square)	0.12
lct-009	Case08	4.31	5.37	2.54 (square)	0.12
lct-009	Case09	4.31	30.47	2.54 (square)	0.12
lct-013	Case02	4.31	3.54	1.89 (square)	0.30
lct-013	Case03	4.31	32.36	1.89 (square)	0.30
lct-013	Case04	4.31	24.17	1.89 (square)	0.30
lct-015	100/100	3.6	0.03	1.27	0.24
lct-015	111/110	4.4	0.00	1.27	0.28
lct-015	112/112	4.4	0.05	1.27	0.41
lct-015	12b/12	3.6	0.03	1.27	0.35
lct-015	147/138	3.6	0.01	1.27	0.30
lct-015	14b/14	3.6	0.03	1.27	0.33
lct-015	161/161	3.6	0.03	1.27	0.35
lct-015	162/161	3.6	0.01	1.27	0.33
lct-015	163/161	3.6	0.04	1.27	0.35
lct-015	18b/18	3.6	0.03	1.27	0.30
lct-015	209/40	3.6	0.01	1.10	0.80
lct-015	247/247	3.6	0.04	1.27	0.35
lct-015	29/29	3.6	0.03	1.27	0.33
lct-015	30/30	3.6	0.03	1.27	0.32
lct-015	36/36	3.6	0.03	1.27	0.31
lct-015	37/37	3.6	0.05	1.27	0.36
lct-021	Case01	5.0	0.02	1.00	0.13
lct-021	Case02	5.0	0.02	1.00	0.13
lct-021	Case03	5.0	0.02	1.00	0.13
lct-021	Case04	5.0	0.02	1.30	0.08
lct-021	Case05	5.0	0.02	1.30	0.07
lct-021	Case06	5.0	0.02	1.30	0.07

Table H.1. Data used for trend fitting (continues). Square lattice pitches and mixed enrichments were excluded from trend fitting.

Experimental series	Experiment	Enrichment wt.%	Boron Σ_c at 2200 m/s. 1/cm	Lattice pitch cm	EALF eV
lct-034	Case01	4.74	3.77	1.60 (square)	0.15
lct-034	Case02	4.74	3.77	1.60 (square)	0.15
lct-034	Case03	4.74	3.77	1.60 (square)	0.14
lct-034	Case04	4.74	3.77	1.60 (square)	0.14
lct-034	Case05	4.74	3.77	1.60 (square)	0.14
lct-034	Case06	4.74	3.77	1.60 (square)	0.13
lct-034	Case07	4.74	3.77	1.60 (square)	0.13
lct-034	Case08	4.74	3.77	1.60 (square)	0.13
lct-034	Case10	4.74	24.78	1.60 (square)	0.15
lct-034	Case11	4.74	24.78	1.60 (square)	0.15
lct-034	Case12	4.74	24.78	1.60 (square)	0.15
lct-034	Case13	4.74	24.78	1.60 (square)	0.14
lct-034	Case14	4.74	24.78	1.60 (square)	0.14
lct-034	Case15	4.74	24.78	1.60 (square)	0.14
lct-040	Case01	4.74	3.77	1.60 (square)	0.15
lct-040	Case02	4.74	3.77	1.60 (square)	0.17
lct-040	Case03	4.74	3.77	1.60 (square)	0.16
lct-040	Case04	4.74	3.77	1.60 (square)	0.15
lct-040	Case05	4.74	24.78	1.60 (square)	0.14
lct-040	Case06	4.74	24.78	1.60 (square)	0.15
lct-040	Case07	4.74	24.78	1.60 (square)	0.14
lct-040	Case08	4.74	24.78	1.60 (square)	0.14
lct-040	Case09	4.74	24.78	1.60 (square)	0.15
lct-040	Case10	4.74	24.78	1.60 (square)	0.15
lct-075	Case01	6.5	58.51	1.10	1.53
lct-075	Case02	6.5	58.51	1.10	1.50
lct-075	Case03	6.5	58.51	1.10	1.45
lct-086	Case1	4.4	0.03	1.27	0.33
lct-086	Case2	3.6–4.4 (mixed)	0.03	1.27	0.31
lct-086	Case3	3.3–4.4 (mixed)	0.03	1.27	0.31
lct-086	Case4	3.0–4.4 (mixed)	0.03	1.27	0.30
lct-086	Case5	2.0–4.4 (mixed)	0.03	1.27	0.28
lct-086	Case6	3.6	0.03	1.27	0.28
lct-086	Case7	3.6–4.4 (mixed)	0.03	1.27	0.29
lct-086	Case8	3.3–3.6 (mixed)	0.03	1.27	0.27
lct-086	Case9	3.0–3.6 (mixed)	0.03	1.27	0.26
lct-086	Case10	2.0–3.6 (mixed)	0.03	1.27	0.24
lct-087	Case3	3.6	2.49	1.22	0.17
lct-087	Case4	3.6–4.4 (mixed)	2.49	1.22	0.17
lct-087	Case5	3.6	3.42	1.22	0.17
lct-087	Case6	3.6–4.4 (mixed)	3.42	1.22	0.17
lct-087	Case9	3.6	2.49	1.22	0.16
lct-087	Case10	3.6	3.42	1.22	0.16
lct-087	Case11	3.6–4.4 (mixed)	3.42	1.22	0.16
lct-089	Case01	4.35	5.92	1.50 (square)	0.16
lct-089	Case02	4.35	5.92	1.50 (square)	0.16
lct-089	Case03	4.35	5.92	1.50 (square)	0.16
lct-089	Case04	4.35	5.92	1.50 (square)	0.16