

Assessment of Existing Transportation Packages for Use with HALEU



Approved for public release.
Distribution is unlimited.

Robert Hall
B. J. Marshall
William A. Wieselquist

September 2020

DOCUMENT AVAILABILITY

Reports produced after January 1, 1996, are generally available free via US Department of Energy (DOE) SciTech Connect.

Website www.osti.gov

Reports produced before January 1, 1996, may be purchased by members of the public from the following source:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone 703-605-6000 (1-800-553-6847)
TDD 703-487-4639
Fax 703-605-6900
E-mail info@ntis.gov
Website <http://classic.ntis.gov/>

Reports are available to DOE employees, DOE contractors, Energy Technology Data Exchange representatives, and International Nuclear Information System representatives from the following source:

Office of Scientific and Technical Information
PO Box 62
Oak Ridge, TN 37831
Telephone 865-576-8401
Fax 865-576-5728
E-mail reports@osti.gov
Website <http://www.osti.gov/contact.html>

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Reactor and Nuclear Systems Division

**ASSESSMENT OF EXISTING TRANSPORTATION PACKAGES FOR USE WITH
HALEU**

Robert Hall, B. J. Marshall, William A. Wieselquist

Date Published: October 2020

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-BATTELLE, LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

CONTENTS

LIST OF FIGURES	iv
LIST OF TABLES	v
SUMMARY	6
1. INTRODUCTION	7
1.1 Criticality Calculations	8
1.2 TSUNAMI Calculations	8
2. FUEL RODS AND PWR FUEL ASSEMBLIES	9
2.1 Westinghouse Traveller Package Description	9
2.2 Traveller SCALE KENO-VI Models	9
2.3 Traveller Fuel Assembly Model Criticality Calculations	15
2.4 Traveller Fuel Assembly Model TSUNAMI-3D Calculations	18
2.5 Traveller Fuel Assembly Model TSUNAMI-IP Results	21
2.6 Traveller Rod Pipe Model Criticality Calculations	23
2.7 Traveller Rod Pipe Model TSUNAMI-3D Calculations	24
2.8 Traveller Rod Pipe Model TSUNAMI-IP Results	26
3. UO ₂ POWDER AND PELLETS	28
3.1 CHT-OP-TU Package Description	28
3.2 CHT-OP-TU Powder Model Criticality Calculations	31
3.3 CHT-OP-TU Pellet Model Criticality Calculations	32
3.4 CHT-OP-TU Powder Model TSUNAMI-3D Calculations	33
3.5 CHT-OP-TU UO ₂ Powder Model TSUNAMI-IP Results	35
3.6 CHT-OP-TU Pellet Model TSUNAMI-3D Calculations	37
3.7 CHT-OP-TU UO ₂ Pellet Model TSUNAMI-IP Results	38
4. U METAL AND ALLOYS	41
4.1 Versa-Pac Package Description	41
5. BWR FUEL RODS AND FUEL ASSEMBLIES	43
5.1 Framatome TN-B1 Package Description	43
5.2 TN-B1 SCALE KENO-VI Models	44
5.3 TN-B1 Criticality Calculations	45
5.4 TN-B1 TSUNAMI-3D Calculations	47
5.5 TN-B1 Model TSUNAMI-IP Results	49
6. UF ₆	52
6.1 Daher Nuclear Technologies DN-30 Description	52
6.2 DN-30 SCALE KENO-VI HAC Models	53
6.3 DN-30 Criticality Calculations	55
6.4 DN-30 TSUNAMI-3D Calculations	57
6.5 DN-30 Model TSUNAMI-IP Results	60
7. CONCLUSIONS	64
ACKNOWLEDGMENTS	66
REFERENCES	67
APPENDIX A. BENCHMARK EXPERIMENT SIMILARITY TABLE	A-1
APPENDIX B. TN-B1 WATER MODELING EFFECT ON BENCHMARK EXPERIMENT c_k	B-1
APPENDIX C. TN-B1 ARRAY SIZE MODELING EFFECT ON BENCHMARK EXPERIMENT c_k	C-1
APPENDIX D. COMPUTER INPUT AND OUTPUT FILES	D-1

LIST OF FIGURES

Figure 1. Westinghouse Traveller Standard package.....	9
Figure 2. Traveller STD fuel assembly model.....	13
Figure 3. Traveller STD fuel assembly model moderator regions.....	14
Figure 4. Traveller STD rod pipe model.....	14
Figure 5. Sensitivity of the infinite array of packages with 5 wt.% fuel assemblies.	18
Figure 6. Sensitivity of the single package model with an 8 wt.% fuel assembly.	19
Figure 7. Sensitivity of the infinite array of packages with 8 wt.% 52 IFBA rod fuel assemblies.	19
Figure 8. Traveller c_k for the infinite array of packages with 5 wt.% fuel assemblies.....	21
Figure 9. Traveller c_k for a single package with an 8 wt.% fuel assembly.	22
Figure 10. Traveller c_k for the infinite array of packages with 8 wt.% 52 IFBA rod fuel assemblies.	22
Figure 11. Rod pipe model k_{eff} for fuel pellet diameter and rod pitch combinations for 5 wt.% UO ₂	23
Figure 12. Rod pipe model k_{eff} for fuel pellet diameter and rod pitch combinations for 10 wt.% UO ₂	24
Figure 13. Sensitivity of the infinite array of packages with 5 wt.% UO ₂ fuel rods.....	25
Figure 14. Sensitivity of the infinite array of packages with 10 wt.% UO ₂ fuel rods.....	25
Figure 15. Traveller c_k for the infinite array of packages with 5 wt.% UO ₂ fuel rods.	26
Figure 16. Traveller c_k for the infinite array of packages with 10 wt.% UO ₂ fuel rods.	27
Figure 17. CHT-OP-TU model UO ₂ powder model ($4 \times 4 \times 3$ package array).....	29
Figure 18. CHT-OP-TU UO ₂ powder model optimum moderation results.	30
Figure 19. CHT-OP-TU UO ₂ pellet model optimum moderation results.	31
Figure 20. CHT-OP-TU UO ₂ powder model sensitivity (48 packages, 5 wt.%, 8 in. OV).	34
Figure 21. CHT-OP-TU UO ₂ powder model sensitivity (18 packages, 8 wt.%, 7.5 in. OV).	34
Figure 22. CHT-OP-TU c_k for 5 wt.% UO ₂ powder (48 packages, 8 in. diameter OV).	35
Figure 23. CHT-OP-TU c_k for 8 wt.% UO ₂ powder (18 packages, 7.5 in. diameter OV).	36
Figure 24. CHT-OP-TU UO ₂ pellet model sensitivity (18 packages, 6.9 wt.%, 7.5 in. OV).	37
Figure 25. CHT-OP-TU UO ₂ pellet model sensitivity (48 packages, 16.5 wt.%, 6 in. OV).	38
Figure 26. CHT-OP-TU c_k for 6.9 wt.% UO ₂ pellets (18 packages, 7.5 in. diameter OV).....	39
Figure 27. CHT-OP-TU c_k for 16.5 wt.% UO ₂ pellets (48 packages, 6 in. diameter OV).....	39
Figure 28. Versa-Pac component illustration [9].	41
Figure 29. TN-B1 package assembly [11].	43
Figure 30. TN-B1 HAC package dimensions [11].....	44
Figure 31. TN-B1 $6 \times 1 \times 6$ package array top and front cutaway views.....	45
Figure 32. TN-B1 package array size vs. fuel assembly enrichment.....	46
Figure 33. TN-B1 $10 \times 1 \times 10$ package Gd rods required vs. fuel assembly enrichment.....	46
Figure 34. TN-B1 model sensitivity (100 packages, 5 wt.%, 13 Gd rods/fuel assembly).	48
Figure 35. TN-B1 model sensitivity (36 packages, 6.7 wt.%, 13 Gd rods/fuel assembly).	48
Figure 37. TN-B1 model sensitivity (100 packages, 8 wt.%, 24 Gd rods/fuel assembly).	48
Figure 37. TN-B1 c_k for 5 wt.% UO ₂ (100 packages, 13 Gd rods/fuel assembly).....	49
Figure 38. TN-B1 c_k for 6.7 wt.% UO ₂ (36 packages, 13 Gd rods/fuel assembly).	50
Figure 39. TN-B1 c_k for 8 wt.% UO ₂ (100 packages, 24 Gd rods/fuel assembly).	50
Figure 50. DN-30 c_k for 6.7 wt.% UF ₆ (3×2 HAC array).	61
Figure 51. DN-30 c_k for 12.5 wt.% UF ₆ (single package).....	61

LIST OF TABLES

Table 1. Traveller model 17×17 fuel assembly data.....	11
Table 2. Traveller design data.....	12
Table 3. Traveller fuel assembly k_{eff} cases.....	16
Table 4. Traveller enrichment and array size sensitivity cases.....	17
Table 5. Traveller fuel assembly model TSUNAMI-3D case data.....	18
Table 6. Traveller fuel assembly model sensitivity by mixture.....	20
Table 7. Traveller fuel assembly model TSUNAMI-IP similarity summary.....	23
Table 8. Traveller rod pipe model TSUNAMI-3D case data.....	24
Table 9. Traveller rod pipe model sensitivity by mixture.....	26
Table 10. Traveller rod pipe model TSUNAMI-IP similarity summary.....	27
Table 11. CHT-OP-TU model data.....	28
Table 12. CHT-OP-TU safety analysis bounding HAC results.....	29
Table 13. CHT-OP-TU UO_2 powder model criticality summary.....	32
Table 14. CHT-OP-TU UO_2 pellet model criticality summary.....	32
Table 15. CHT-OP-TU UO_2 powder model TSUNAMI-3D case data.....	33
Table 16. CHT-OP-TU UO_2 powder model sensitivity by mixture.....	35
Table 17. CHT-OP-TU UO_2 powder model TSUNAMI-IP similarity summary.....	36
Table 18. CHT-OP-TU UO_2 pellet model TSUNAMI-3D case data.....	37
Table 19. CHT-OP-TU UO_2 pellet model sensitivity by mixture.....	38
Table 20. CHT-OP-TU UO_2 pellet model TSUNAMI-IP similarity summary.....	40
Table 21. Versa-Pac maximum ^{235}U per package (ground/vessel transportation) [15].....	42
Table 22. TN-B1 HAC array criticality calculations.....	45
Table 23. TN-B1 HAC model TSUNAMI-3D case data.....	47
Table 24. TN-B1 model sensitivity by mixture.....	48
Table 25. TN-B1 model TSUNAMI-IP similarity summary.....	51
Table 28. DN-30 HAC model TSUNAMI-3D case data.....	58
Table 29. DN-30 model sensitivity by mixture.....	60

SUMMARY

Commercial light water reactor operators and fuel vendors in the United States are pursuing changes to fuel that include increased ^{235}U enrichment. Economic studies generally anticipate maximum near-term fuel assembly designs with up to 8 wt.% ^{235}U . Many next-generation nuclear reactor designs require high-assay low-enriched uranium (HALEU) (19.75 wt.% ^{235}U > 5 wt.%) fuel. One necessary element for the commercial-scale use of HALEU is the ability to safely transport large quantities of enriched fuel material in multiple forms. However, there is uncertainty as to whether subcriticality requirements can be satisfied with existing package designs and whether existing critical benchmark experiment data are sufficient to support criticality safety code validation for HALEU transportation applications.

This study assesses the potential to use currently licensed transportation packages for the transportation of increased enrichment unirradiated U fuel forms. The assessment uses selected package designs that represent the five categories of fuel form—boiling water reactor pins and assemblies, pressurized water reactor pins and assemblies, UF_6 , U-metal and tristructural isotropic (TRISO) particles, and UO_2 pellets or powder—and focuses on demonstrating subcriticality and identifying benchmark critical experiments appropriate for use in criticality computer code validation.

Key quantities of interest that relate to subcriticality are limiting conditions (e.g., optimum moderation), package or package array k_{eff} , package capacity, and package transportation array size. The SCALE TSUNAMI-3D and TSUNAMI Indices and Parameters codes are used for sensitivity and uncertainty calculations and for identification of candidate critical benchmark experiments for code validation. The primary metric for identifying candidate benchmarks is the similarity coefficient, c_k .

For each fuel form category, a representative package is evaluated. Results provided for each package evaluation include enrichment and packaging limits (e.g., maximum transportation array size as a function of enrichment) and benchmark critical experiment similarity coefficients. Results indicate that there are viable means for increasing enrichments into the HALEU range across the spectrum of fuel forms with differing increase amounts available for different packages. Sources of subcriticality margin to offset increased enrichment reactivity include reduced transportation array size, reduced fissile mass, burnable absorber credit, and safety analysis margin harvesting. For all packages except the DN-30, numerous critical benchmark experiment candidates for validation were identified.

1. INTRODUCTION

Commercial light water reactor (LWR) operators and fuel vendors in the United States are pursuing changes to fuel that include increased ^{235}U enrichment. [1, 2]. Economic studies generally anticipate near-term fuel assembly average enrichment up to 8 wt.% ^{235}U , which is within the range of high-assay low-enriched uranium (HALEU) ($19.75\% > ^{235}\text{U} > 5\%$). Many next-generation nuclear reactor designs require HALEU fuel. One necessary element for the commercial-scale use of HALEU is the ability to safely transport large quantities of enriched fuel material in multiple forms. However, there is uncertainty as to whether subcriticality requirements can be satisfied with existing package designs and whether existing critical benchmark experiment data are sufficient to support criticality safety code validation for HALEU transportation applications.

To prepare for and support these potential changes, the potential use of currently licensed transportation packages for the transportation of EE and HALEU is being assessed. This assessment includes selected package designs that represent the five categories of fuel form—boiling water reactor (BWR) pins and assemblies, pressurized water reactor (PWR) pins and assemblies, UF_6 , U-metal and tristructural isotropic (TRISO), and UO_2 pellets or powder—and are limited to unirradiated U fuel forms. This assessment focuses on modeling the limiting packaging conditions with current enrichment limits and modifying those models to include potential HALEU enrichments to identify criticality and validation effects.

The primary focus of this study is to determine whether existing package designs can be used to transport increased HALEU LWR fuel materials, what transportation limitations might be required, and whether sufficient applicable benchmark critical experiments can be identified for computer code validation. The SCALE KENO-VI code is used for criticality calculations [3]. Key quantities of interest relating to subcriticality are limiting conditions (e.g., optimum moderation), package or package array k_{eff} , package capacity, and package transportation array size. The SCALE TSUNAMI-3D and TSUNAMI Indices and Parameters (TSUNAMI-IP) codes are used for sensitivity and uncertainty calculations and for identification of candidate critical benchmark experiments for code validation. [3, 4.] The primary metric for identifying candidate benchmarks is the similarity coefficient, c_k .

For each category of fuel form, a representative package is evaluated.

- 1) Traveller (PWR fuel assemblies, PWR and BWR fuel pins) [5, 6].
- 2) CHT-OP-TU (UO_2 powder and pellets) [7, 8].
- 3) VersaPac (U-metal/TRISO) [9, 10].
- 4) TN-B1 (BWR fuel assemblies) [11, 12].
- 5) DN-30 (UF_6) [13, 14].

Results provided for each package evaluation include the enrichment and packaging limits (e.g., maximum transportation array size as a function of enrichment) and identification of benchmark critical experiments that are appropriate for use in computer code validation (determination of k_{eff} bias and bias uncertainty for the application).

1.1 Criticality Calculations

For each package, KENO-VI criticality calculations are performed by using the following process.

- 1) Construct package and package array models by using Certificate of Compliance (CoC) and safety analysis report (SAR) information.
 - a. The hypothetical accident condition (HAC) array model is typically limiting.
- 2) Confirm limiting conditions and establish maximum target k_{eff} .
 - a. Target k_{eff} is chosen to preserve margin to the upper subcritical limit from the safety analysis with current package enrichment limit (e.g., 5 wt.% ^{235}U).
- 3) Calculate k_{eff} varying enrichment and package array size.
 - a. Burnable absorbers, fuel rod pitch, optimum moderation, and package capacity might also be varied, as applicable.
 - b. Determine model variations with k_{eff} close to the target.
- 4) Select representative enrichment, array size, and other acceptable increased enrichment packaging variations for TSUNAMI analysis.

KENO k_{eff} convergence is typically set for scoping-level results (i.e., k_{eff} standard deviation of 0.001) for these calculations. Optimum moderation searches are automated by using the SCALE SAMPLER stochastic sampling sequence. Criticality calculations use KENO-VI in SCALE version 6.3 pre-release beta 11 with the 252 group ENDF/B-VII.1 cross section library.

1.2 TSUNAMI Calculations

The SCALE TSUNAMI suite of tools performs sensitivity and uncertainty (S/U) calculations [4]. TSUNAMI-3D uses adjoint-based perturbation theory to calculate the energy and reaction-dependent sensitivity of a system k_{eff} to changes in cross section data. A sensitivity data file (SDF) that contains the calculated sensitivity coefficients is produced for the application of interest and as a set of benchmark critical experiments. TSUNAMI-IP combines sensitivity data with nuclear data uncertainty information to produce a correlation coefficient, c_k , for each application experiment pair. The c_k value indicates the degree to which the k_{eff} of an application and the k_{eff} of an experiment are correlated in sensitivity to cross section perturbation or to cross section data uncertainty.

A c_k value of 1.0 indicates perfectly correlated models, and a value of zero indicates that the two models share no neutronic similarity. For the purpose of computer code validation to establish criticality safety k_{eff} bias and bias uncertainty, experiments and applications are considered similar for c_k values ≥ 0.9 and marginally similar for c_k values ≥ 0.8 [15, 16].

A suite of 1,584 critical experiments with LEU or intermediate-enriched uranium (IEU) is used with TSUNAMI-IP to identify potentially applicable experiments for k_{eff} validation. Within the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [17], IEU is defined as uranium enriched to 10–60 wt.% ^{235}U . SDFs for these systems are distributed with the ICSBEP Handbook. One-hundred and eleven SDFs were drawn from the VALID library maintained at ORNL [18]. The ICSBEP SDFs are considered sufficiently accurate for experiment selection [19]. The ICSBEP experiment naming convention indicates the enrichment range, material form, and energy spectrum (i.e., LCT represents LEU, compound form, and thermal energy spectrum).

SCALE version 6.3 pre-release beta 11 was used for all calculations.

2. FUEL RODS AND PWR FUEL ASSEMBLIES

2.1 Westinghouse Traveller Package Description

The Westinghouse Traveller package is the representative design chosen to assess the transportation of PWR fuel pins and fuel assemblies [5, 6]. There are several versions of the Traveller: Standard (STD), XL, and VVER. For this analysis, the Standard version was used because it can carry the most common length of PWR fuel (12 ft of active fuel).

The Traveller is designed to transport one commercial-grade unirradiated U PWR fuel assembly with enrichment up to 5.0 wt.% ^{235}U and unirradiated BWR and PWR fuel rods in a rod pipe. The primary packaging components are an Outerpack and a hinged Al Clamshell that can accommodate one fuel assembly or one rod pipe. The Clamshell includes Boral neutron absorber plates, and the Outerpack contains polyethylene moderator blocks. The combination of moderator blocks and absorber plates provides criticality control across a range of dry and flooded conditions. PWR assembly packing materials are limited to ≤ 2.0 kg per package. A representation of an empty Traveller package is shown in Figure 1.

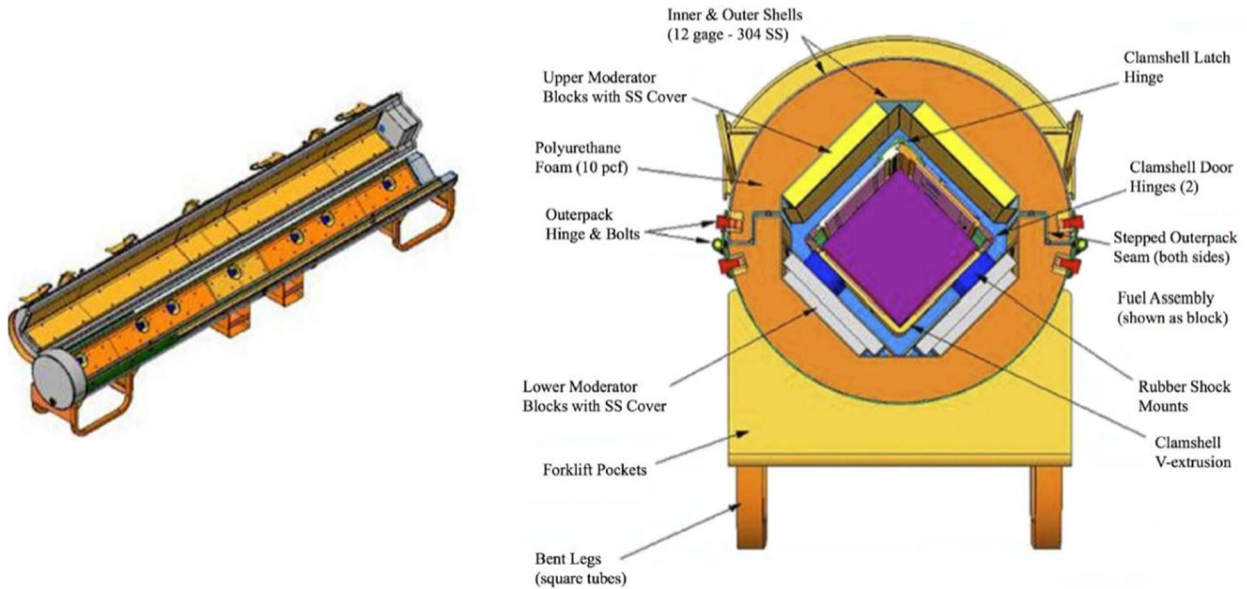


Figure 1. Westinghouse Traveller Standard package. [5]

The rod pipe is a 6 in. Schedule 40 304 stainless-steel (SS) pipe with SS closures at each end. Within the rod pipe, UO_2 or U_3Si_2 fuel rods are wrapped in polyethylene sleeves with a H density of ≤ 0.1325 g/cm³. Loose fuel rod packing material is unlimited in the rod pipe.

2.2 Traveller SCALE KENO-VI Models

Two models were used: one with a 17×17 Westinghouse fuel assembly centered in the Clamshell and one with UO_2 rods in a rod pipe centered in the Clamshell. Only one fuel design was used because the objective of this calculation was to assess the effect of increased enrichment. This objective can be met with a representative fuel assembly. Determining a bounding assembly design for all conditions is complex and was outside the scope of this analysis.

Many Traveller design features unrelated to criticality control are neglected in the KENO models. The elements of the package considered important to criticality that are included in the models are:

- Clamshell shell,
- Boral plates,
- polyethylene blocks,
- Outerpack SS covers,
- rod pipe,
- polyethylene packing in the rod pipe,
- preferential water flooding, and
- HAC fuel assembly damage (rod pitch increase).

The current Traveller SAR indicates that the most reactive flooding configuration is full-density water in the Clamshell, which includes within the fuel pin lattice, in the fuel-clad gap space, and in place of guide tube and instrument tube material. Void in all other regions maximizes reactivity, which indirectly supports modeling foam in the Outerpack as void.

The Traveller SAR evaluates multiple fuel assembly designs and numerous tolerance perturbations to the nominal package and fuel design (e.g., clad thickness, polyethylene block density, fuel rod pitch, axial positioning in the Clamshell, annular pellet region length) to obtain bounding penalties that do not necessarily apply to any single fuel assembly design. Because attempting to replicate the SAR approach is complex, nominal design values were used in this analysis with two exceptions: (1) a 50.8 cm region of the fuel assembly lattice was modeled as expanded into the available space to simulate fuel assembly damage observed during HAC drop testing and (2) non-fuel lattice locations (guide and instrument tubes) were modeled as water. The SAR analysis shows that HAC conditions are typically the most reactive. Therefore, this assessment used an HAC model with simulated fuel damage and optimum preferential region flooding. A 17×17 fuel assembly design is used to represent PWR designs.

For the rod pipe model, fuel pin gap and clad are modeled as moderator (polyethylene) and an optimum pitch, and pellet radius search was performed to maximize k_{eff} , which is consistent with the SAR.

For TSUNAMI-3D calculations, a single package with reflective boundary conditions or 30 cm water reflection was used instead of an array of packages to facilitate reasonable execution times and computer resource requirements. This accommodation is justified for two reasons: (1) most Traveller HAC arrays are large (24–150 packages) and (2) with preferential region flooding and Boral absorbers in the Clamshell, neutronic interaction between packages is low. Appendix C describes a limited study of the effect of using package arrays that are different from the bounding criticality array in TSUNAMI-3D calculations. Generally, more accurate similarity results are expected when the TSUNAMI and criticality models are the same.

Table 1 provides fuel assembly and material descriptions. Table 2 shows Clamshell and Outerpack dimensions and material descriptions. In the fuel assembly model, guide tubes and instrument tubes were modeled as moderators, and 2 kg of polyethylene packaging were included as a liner in the Clamshell. Similarly, in the rod pipe model, fuel pins were modeled as a triangular pitch UO_2 lattice with no cladding. The non-fuel region in the pipe was modeled as polyethylene packaging.

Table 1. Traveller model 17×17 fuel assembly data.

Parameter	Value
Assembly lattice	17×17
Assembly pitch	21.5 cm
Fuel rods	264
Guide tubes	24
Instrument tubes	1
Fuel rod pitch	1.26 cm (nominal)
Fuel rod pitch	1.355 cm (damaged)
UO ₂ pellet diameter	0.7831 cm
UO ₂ effective density	10.96 g/cm ³
Clad inner diameter	0.7937 cm
Clad outer diameter	0.9004 cm
Fuel stack height	365 cm
Temperature	293 K
Full water density	0.9986 g/cm ³

Table 2. Traveller design data.

Parameter	Value
Clamshell	
Outside length	439.4 cm
Boral length	426.7 cm
Boral width	15.2 cm
Clamshell material	Al
Clamshell wall thickness	0.714 cm
Clamshell inner height/width	23.17 cm
Outerpack	
Outside length	500.4 cm
Outside diameter	63.5 cm
Outer shell material	304 SS
Outer shell thickness	0.266 cm
Inner shell thickness	0.266 cm
Inner shell inside width*	43.2 cm
Cavity length	455.8 cm
Polyethylene block length	457.2 cm
Upper poly block width	24.1 cm
Upper poly block thickness	3.18 cm
Large lower poly block width	23.7 cm
Large lower poly block thickness	2.54 cm
Small lower poly block width	19.94 cm
Small lower poly block thickness	1.91 cm
Rod pipe	
Rod pipe outside diameter	16.84 cm
Rod pipe inside diameter	15.41 cm

*Measured along horizontal centerline

Figure 2 shows cutaway views of the Traveller standard model with a 17×17 fuel assembly centered in the Clamshell and with no fuel. Figure 3 shows the same model with individual moderator regions indicated by color. Separate moderator regions inside the Clamshell (red), inside the Outerpack (yellow), in the foam region (purple), and outside the Outerpack (blue) are used to determine the flooding configuration that maximizes k_{eff} . The foam region is modeled as an annulus that is a simple approximation sufficient to confirm whether void, foam, or water results in the highest reactivity.

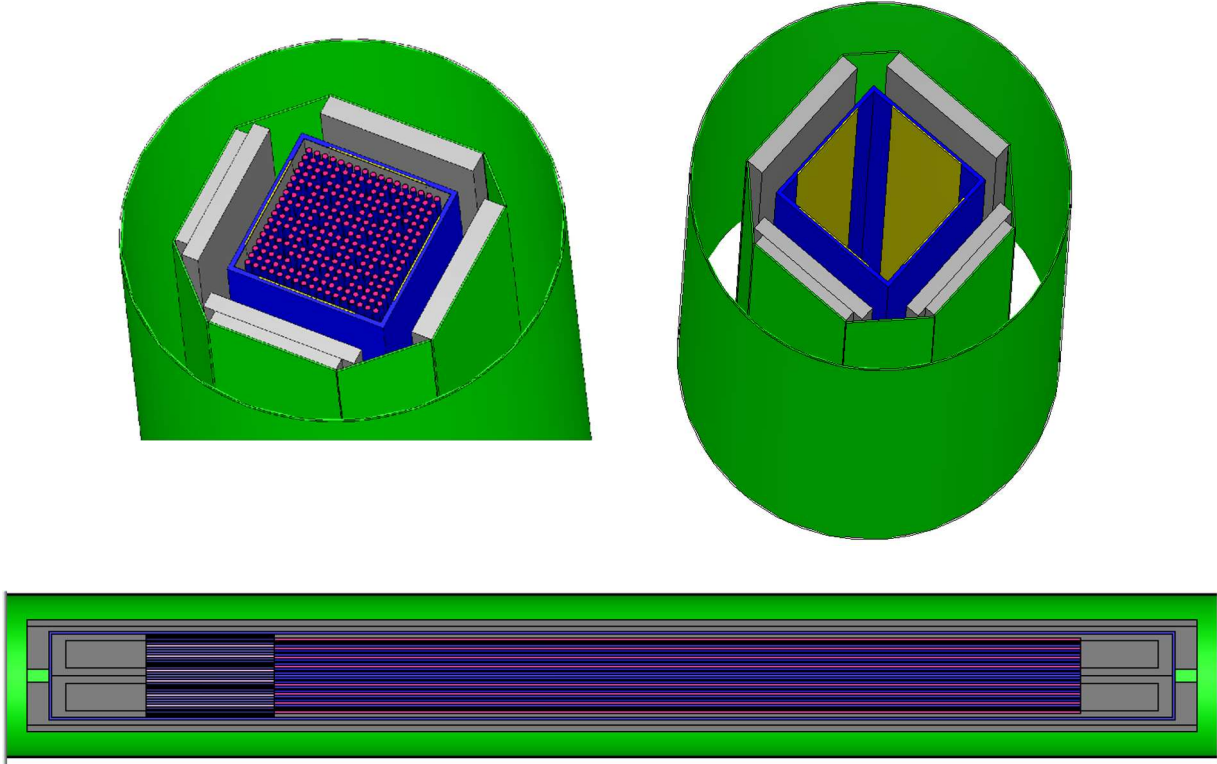


Figure 2. Traveller STD fuel assembly model.

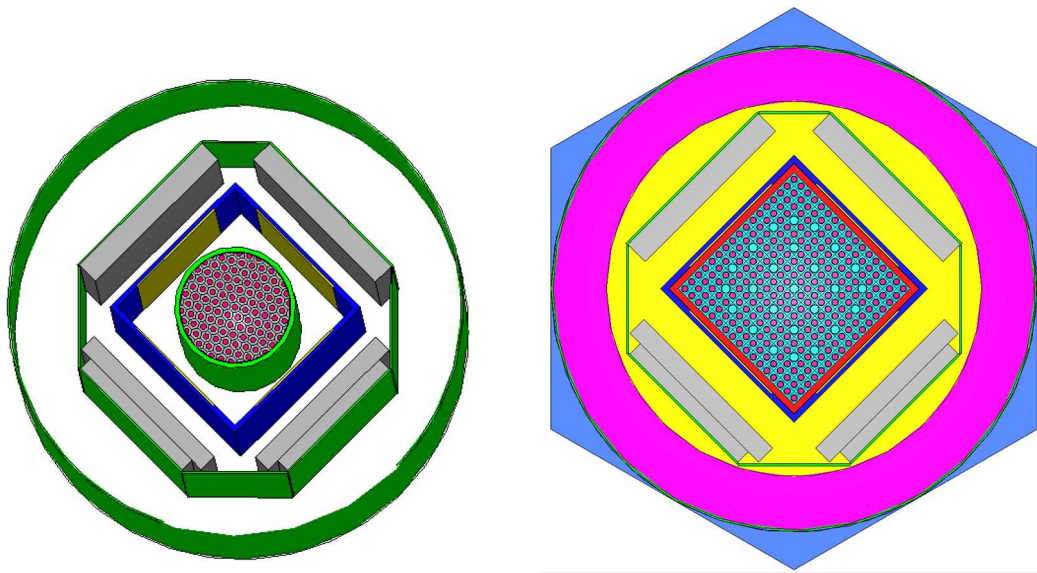


Figure 3. Traveller STD fuel assembly model moderator regions.

Figure 4 shows the rod pipe model. The rod pitch and rod diameter are variable and were used to identify the combination that maximizes k_{eff} . Partial fuel rods bisected by the rod pipe are retained in the model for convenience.

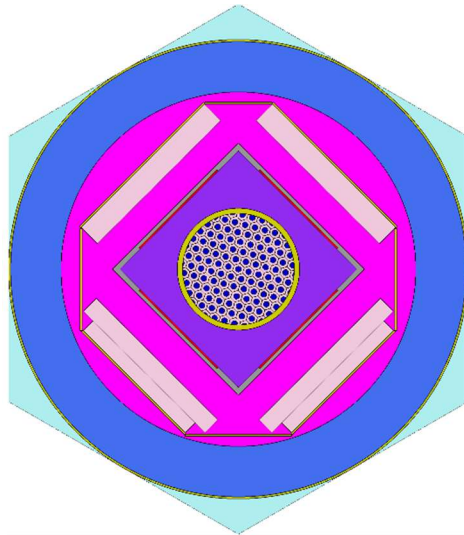


Figure 4. Traveller STD rod pipe model.

2.3 Traveller Fuel Assembly Model Criticality Calculations

KENO-VI cases were run with various combinations of flooding to establish maximum k_{eff} conditions. Preferential full-density water flooding inside the Clamshell, inside the Outerpack, in the foam region, and outside the Outerpack were considered separately and in combination. Outside the Outerpack, optimum-density water was also considered.

The Traveller SAR indicates that the maximum analyzed k_{eff} with 5 wt.% fuel assemblies is close to the upper safety limit (~ 0.94). The analysis bounds all versions of the Traveller package, all allowable fuel assembly types, maximum HAC array size, and all penalties. The Traveller STD model with 17×17 fuel used in this analysis is representative but is not bounding. Therefore, for this evaluation, the maximum k_{eff} of the 5 wt.% base case was used as a target k_{eff} for cases with higher enrichment fuel. The base case comprises an infinite array of packages with each package containing a 5 wt.% 17×17 fuel assembly. Increased enrichment will increase k_{eff} well above the target with no other changes to the package. Two options were considered for reducing maximum k_{eff} with up to 8 wt.% fuel: (1) reduced transportation array size and (2) integral fuel burnable absorber (IFBA) rods.

Table 3 shows the results of preferential flooding calculations for the base case KENO-VI infinite array model, which is a hexagonal array with the sides of the packages touching and reflective boundary conditions. Neutron spectrum hardness is indicated by the energy of the average lethargy of fission (EALF). Two different fuel enrichments were used: 5 and 8 wt.% ^{235}U . The highest k_{eff} occurred with the Clamshell, fuel lattice, and pellet-clad gap region flooded for both enrichments. The 8 wt.% maximum k_{eff} exceeded the target by about 0.06.

Table 3. Traveller fuel assembly k_{eff} cases.

Enrichment (wt. % ^{235}U)	Water flooding					k_{eff}	EALF
	Clamshell ¹	Outerpack	Foam	External	Array		
5.0	No	No	No	No	Infinite	0.2822	83.4
5.0	Yes	No	No	No	Infinite	0.8916	0.248
5.0	No	Yes	No	No	Infinite	0.2329	74.6
5.0	No	No	Yes	No	Infinite	0.2007	174.8
5.0	No	No	No	Yes	Infinite	0.2417	105.0
5.0	Yes	Yes	No	No	Infinite	0.8560	0.237
5.0	Yes	No	Yes	No	Infinite	0.8353	0.255
5.0	Yes	No	No	Yes	Infinite	0.8623	0.253
5.0	Yes	Yes	Yes	Yes	Infinite	0.8525	0.239
5.0	Yes	No	No	Yes (0.05)	Infinite	0.8884	0.248
5.0	Yes	No	No	Yes (0.1)	Infinite	0.8857	0.248
8.0	No	No	No	No	Infinite	0.3310	88.1
8.0	Yes	No	No	No	Infinite	0.9548	0.375
8.0	No	Yes	No	No	Infinite	0.2674	81.0
8.0	No	No	Yes	No	Infinite	0.2310	175.2
8.0	No	No	No	Yes	Infinite	0.2805	108.3
8.0	Yes	Yes	No	No	Infinite	0.9187	0.351
8.0	Yes	No	Yes	No	Infinite	0.8960	0.378
8.0	Yes	No	No	Yes	Infinite	0.9250	0.380
8.0	Yes	Yes	Yes	Yes	Infinite	0.9152	0.352
8.0	Yes	No	No	Yes (0.05)	Infinite	0.9523	0.377
8.0	Yes	No	No	Yes (0.1)	Infinite	0.9492	0.376
8.0 ²	Yes	No	No	Yes	Single	0.8876	0.386
8.0²	Yes	Yes	No	Yes	Single	0.9147	0.354
8.0 ²	Yes	Yes	Yes	Yes	Single	0.9141	0.351
8.0³	Yes	No	No	No	Infinite	0.8983	0.432

¹Includes fuel pellet-clad gap

²Single package (N = 0.5, criticality safety index = 100)

³Fuel includes 52 IFBA rods

Replacing 52 fuel rods with the IFBA rods included in the 8 wt.% fuel assembly lattice produced a maximum k_{eff} similar to the 5 wt.% base case. Reducing the array size of the 8 wt.% case to a single package (20 cm water reflector with vacuum boundary conditions) reduced k_{eff} by 0.03, which was insufficient to reach the target. Nevertheless, the 8 wt.% single package case was used to evaluate cross section S/U and similarity to benchmark critical experiments. The single package case k_{eff} was maximized with Clamshell, Outerpack, and external flooding.

The single package case k_{eff} was maximized with Clamshell, fuel lattice, pellet-clad gap region, Outerpack, and external flooding. The 5 wt.% base case, 8 wt.% 52 IFBA case, and 8 wt.% single package case highlighted in Table 3 were used in the TSUNAMI calculations.

Table 4 contains additional cases to provide enrichment and array size k_{eff} sensitivity. Enrichment sensitivity is approximately 0.02 $\Delta k/\text{wt. \% } ^{235}\text{U}$. Sensitivity to HAC array size is highly nonlinear. The total reduction in k_{eff} for a single package relative to an infinite array is approximately 0.04 Δk .

Determining a trade-off between array size and enrichment for the Traveller is complex because as currently licensed, Traveller criticality safety index (CSI) values range from 0.7 to 4.2 (equivalent to analyzed HAC array sizes of 12 to 72) [6]. With the Table 4 results, a maximum k_{eff} margin of roughly

0.03 Δk could be gained by increasing the CSI to 50 (equivalent to 1.5% enrichment increase). The Traveller safety analysis also shows that the Traveller STD is less reactive than the XL version by 0.01–0.02 Δk , which could allow a higher enrichment limit for the STD version. Explicitly modeling the set of limiting conditions for each fuel design and package version could also provide some margin relative to the bounding design and bounding penalty method.

Table 4. Traveller fuel assembly enrichment and array size sensitivity cases.

Water flooding							
Enrichment (wt% ^{235}U)	Clamshell ¹	Outerpak	Foam	External	Array	CSI	k_{eff}
5	Yes	No	No	No	Infinite	0	0.8916
6	Yes	No	No	No	Infinite	0	0.9157
7	Yes	No	No	No	Infinite	0	0.9345
8	Yes	No	No	No	Infinite	0	0.9548
Array size sensitivity cases							
5	Yes	No	No	No	Infinite	0	0.8916
5	Yes	No	No	Yes	53	1.9	0.8804
5	Yes	No	No	Yes	33	3.1	0.8768
5	Yes	No	No	Yes	18	5.6	0.8705
5	Yes	No	No	Yes	14	7.2	0.8661
5	Yes	No	No	Yes	11	9.1	0.8620
5	Yes	No	No	Yes	7	14.3	0.8560
5	Yes	Yes	No	Yes	4	25.0	0.8515
5	Yes	Yes	No	Yes	2	50.0	0.8518
5	Yes	Yes	No	Yes	1	100.0	0.8522

CSI = 50/N rounded up to the nearest 0.1, where N = analyzed HAC array size/2

2.4 Traveller Fuel Assembly Model TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for the three highlighted cases from Table 3. Table 5 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 5. Traveller fuel assembly model TSUNAMI-3D case data.

Parameter	5 wt.% infinite array	8 wt.% single package	8 wt.% 52 IFBA infinite array
Grid mesh	$40 \times 42 \times 44$	$44 \times 44 \times 58$	$40 \times 42 \times 44$
Particles/gen.	10,000 fwd. / 30,000 adj.	10,000 fwd. / 30,000 adj.	10,000 fwd. / 30,000 adj.
SDF file name	T3D_Trav_FA_wet1_mm2	T3D_Trav_FA8_wet2a_single_axial2	T3D_Trav_FA8I_wet1_mm
Forward k_{eff}	0.89139 ± 0.00034	0.91447 ± 0.00028	0.89772 ± 0.00034
Adjoint k_{eff}	0.89098 ± 0.00099	0.91425 ± 0.00089	0.89868 ± 0.00099
EALF	0.247 eV	0.350 eV	0.433 eV
Cross section uncertainty	0.671% $\Delta k/k$	0.877% $\Delta k/k$	0.633% $\Delta k/k$

TSUNAMI input adequacy was confirmed by comparing TSUNAMI-calculated nuclide sensitivity with KENO direct perturbation (DP) sensitivity. Figures 5, 6, and 7 summarize the sensitivity results calculated by each method for the highest sensitivity nuclide/region combinations. There is good agreement between the DP (% $\Delta k/\rho$) and TSUNAMI (% $\Delta k/\Sigma$) sensitivities, which confirms that the TSUNAMI SDFs properly represent the models.

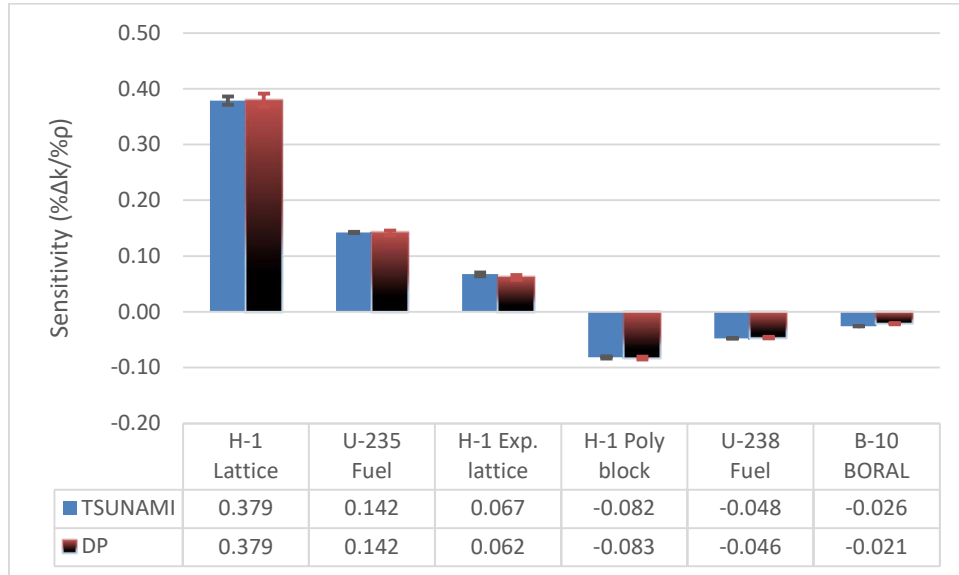


Figure 5. Sensitivity of the infinite array of 5 wt.% fuel assembly packages.

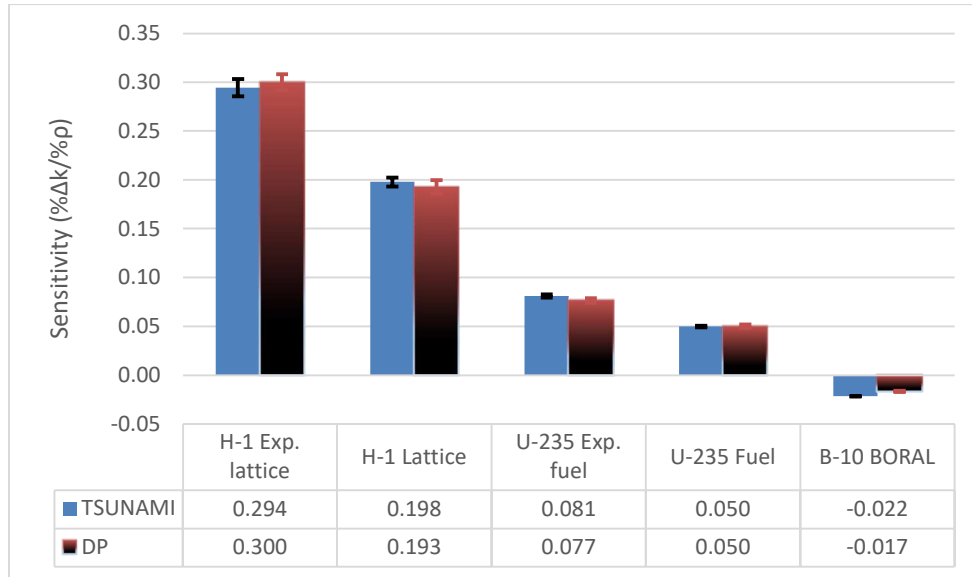


Figure 6. Sensitivity of the single package model with an 8 wt.% fuel assembly.

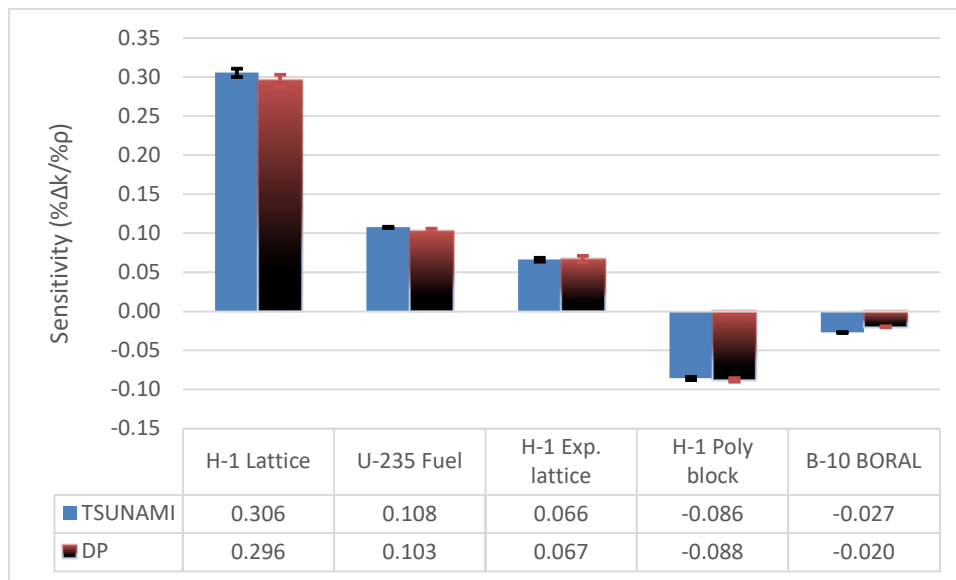


Figure 7. Sensitivity of the infinite array of 8 wt.% 52 IFBA rod fuel assembly packages.

Sensitivity results provided insight into which materials and regions are most important for criticality control. For example, in the infinite array models (Figures 4 and 6), k_{eff} is most sensitive to H in the regular fuel lattice water (increasing ^1H increases k_{eff}). In the single package model (Figure 5), k_{eff} is most sensitive to H in the expanded pitch fuel lattice water (increasing ^1H increases k_{eff}).

Table 6 lists the sensitivity for each mixture in each model. Values greater than 0.01 $\% \Delta k / \% \Sigma$ are highlighted. The two infinite array models (5 wt.% and 8 wt.% with 52 IFBA rods) have similar sensitivities. Materials with the highest positive sensitivity (k_{eff} increases with density) are water in the fuel lattice and UO_2 . Polyethylene blocks and Boral have the most significant negative sensitivities. The biggest difference between the infinite package array models is that sensitivity is split between IFBA and non-IFBA fuel lattice materials. In contrast to the infinite package array models, the 8 wt.% single package model has: (1) higher sensitivity in the expanded lattice region than in the physically larger

regular lattice region, (2) small positive sensitivity to water in the overpack, and (3) almost no sensitivity to the polyethylene blocks. The latter two observations are explained by recognizing that water in the overpack in package arrays increases moderation but tends to reduce interaction between packages, whereas water in the overpack in a single package only increases moderation.

Table 6. Traveller fuel assembly model sensitivity by mixture.

Mixture	Description	5 wt% 17x17 Inf. Array		8 wt% 17x17 Single		8 wt% 17x17 IFBA Inf. Array	
		Sensitivity	Std. Dev.	Sensitivity	Std. Dev.	Sensitivity	Std. Dev.
1	UO ₂ (NL)	0.114	0.6%	0.051	0.9%	0.101	0.6%
2	Fuel clad (NL)	0.007	1.1%	0.005	0.9%	0.006	1.0%
3	Fuel lattice water (NL)	0.413	0.9%	0.218	1.1%	0.333	0.8%
4	SS structure	-0.006	1.0%	0.000	7.2%	-0.006	1.0%
5	BORAL	-0.023	0.3%	-0.018	0.4%	-0.024	0.3%
6	Clamshell water	0.030	2.0%	0.018	2.7%	0.028	2.1%
7	Clamshell aluminum	0.004	1.2%	0.009	0.6%	0.004	1.2%
8	Polyethylene blocks	-0.078	1.2%	0.001	79.6%	-0.083	1.3%
10	Polyethylene packaging	0.004	3.6%	0.005	5.3%	0.003	4.1%
13	Fuel-clad gap water (NL)	0.005	7.1%	0.002	9.5%	0.004	6.2%
14	Water in outerpack	0.000	0.7%	0.010	11.4%	0.000	0.7%
15	Water in outerpack foam	0.000	0.4%	0.000	0.4%	0.000	0.4%
16	Water reflector	0.000	0.8%	0.000	17.4%	0.000	0.8%
21	UO ₂ (EL)	0.023	1.2%	0.085	1.0%	0.018	1.3%
22	Fuel clad (EL)	0.001	2.3%	0.008	1.2%	0.001	2.4%
23	Fuel lattice water (EL)	0.075	2.2%	0.329	1.3%	0.054	2.1%
33	Fuel-clad gap water (EL)	0.001	19.3%	0.001	11.4%	0.000	17.1%
101	UO ₂ (INL)					0.035	0.9%
102	Fuel clad (INL)					0.001	3.4%
103	Fuel lattice water (INL)					0.071	1.7%
113	Fuel-clad gap water (INL)					0.001	16.4%
114	IFBA (INL)					-0.005	1.4%
121	UO ₂ (IEL)					0.006	2.1%
122	Fuel clad (IEL)					0.000	8.2%
123	Fuel lattice water (IEL)					0.012	4.5%
124	Fuel-clad gap water (IEL)					-0.001	4.4%
133	IFBA (IEL)					0.000	50.2%

Region codes: NL (normal fuel lattice), EL (expanded fuel lattice), INL (IFBA pin in normal fuel lattice), IEL (IFBA pin in expanded fuel lattice)

2.5 Traveller Fuel Assembly Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for each of the three SDF files in Table 4 and the library of 1,584 critical experiment SDF files. Figures 8, 9, and 10 show the results with different symbols representing different types of experiments. IEU includes all intermediate enrichment experiments, LEU includes low enrichment experiments not captured by the other categories, LCT includes LEU-COMP-THERM experiments, LMP includes LEU-MET-THERM experiments, and LST includes LEU-SOL-THERM experiments. Table 7 shows the number of experiments in each category with $c_k \geq 0.9$ and the median c_k of the 1,584 experiments for each of the three Traveller models. A full list of experiments with c_k values is provided in Appendix A. The TSUNAMI results show that many experiments are likely to be applicable for code validation for the Traveller PWR fuel assembly models with UO_2 fuel enrichment up to 8 wt.% ^{235}U .

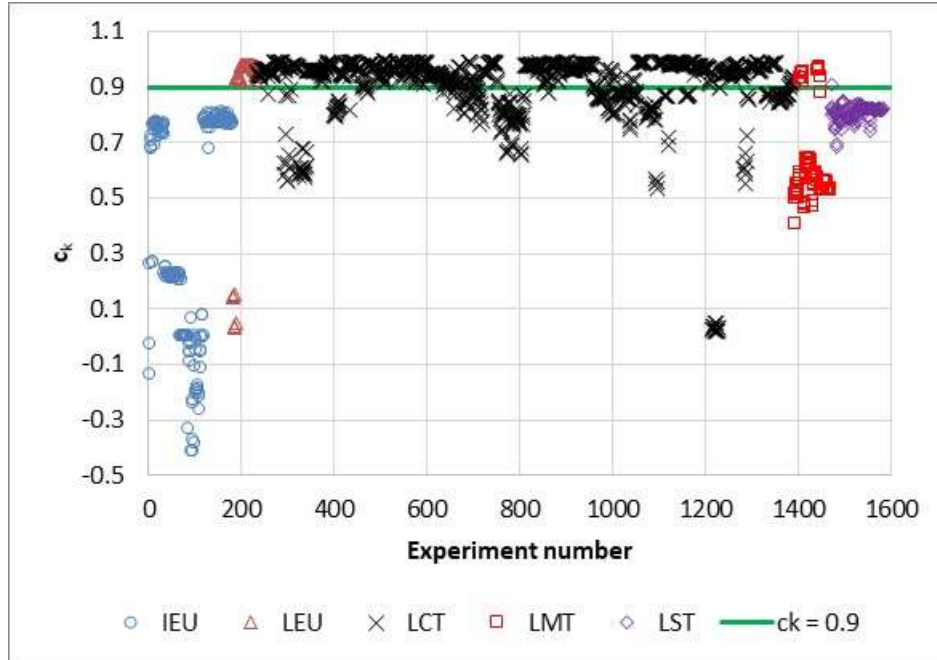


Figure 8. Traveller c_k for the infinite array of packages with 5 wt.% fuel assemblies.

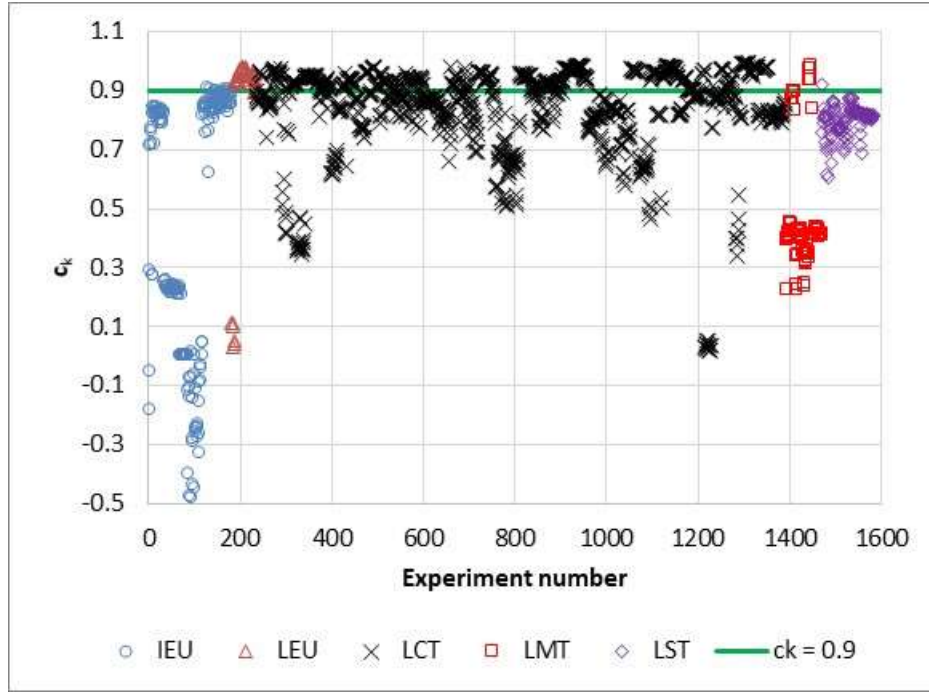


Figure 9. Traveller c_k for a single package with an 8 wt.% fuel assembly.

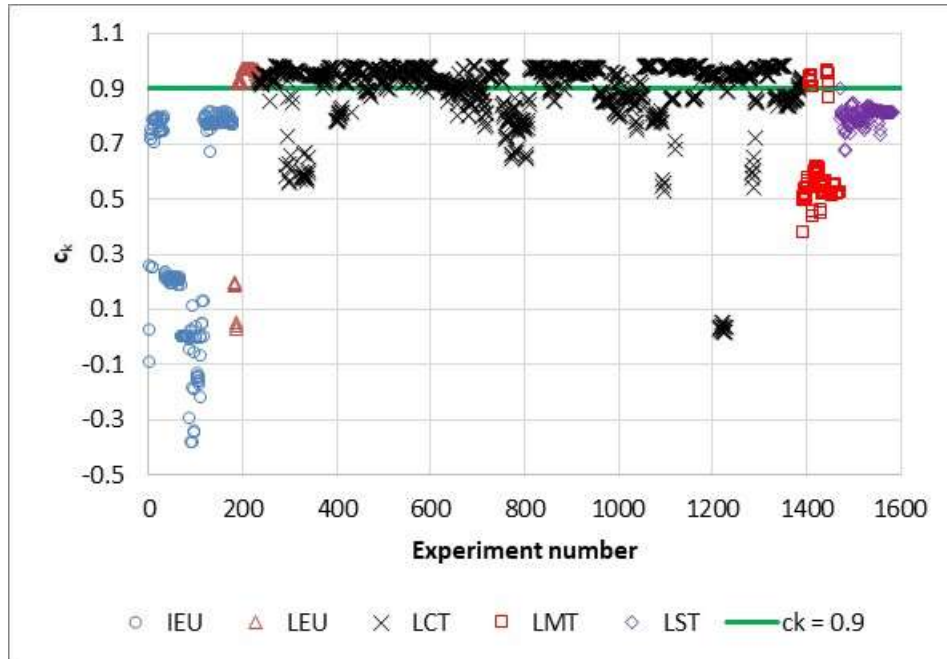


Figure 10. Traveller c_k for the infinite array of packages with 8 wt.% 52 IFBA rod fuel assemblies.

Table 7. Traveller fuel assembly model TSUNAMI-IP similarity summary.

Category	Experiments with $c_k \geq 0.9$		
	5 wt.% array	8 wt.% single	8 wt.% 52 IFBA array
IEU $c_k \geq 0.9$	0	5	0
LEU $c_k \geq 0.9$	48	47	48
LCT $c_k \geq 0.9$	830	528	801
LMT $c_k \geq 0.9$	13	7	13
LST $c_k \geq 0.9$	1	1	1
Median c_k	0.931	0.864	0.921

2.6 Traveller Rod Pipe Model Criticality Calculations

The Traveller package was also used to transport fuel rods in a rod pipe. To cover potential combinations of fuel pellet outer diameters (OD) and the number of rods in the pipe, Sampler was used to direct KENO infinite array calculations for 11 pellet OD and 11 fuel rod pitch values (121 cases). Pellet OD ranged from 0.78 to 1.3 cm. Rod pitch varied from 0.1 to 1.0 cm larger than the pellet OD. No fuel clad is modeled, polyethylene moderator fills the non-fuel space in the rod pipe, and water flooding is assumed in the Clamshell. Other regions are dry.

Sampler/KENO k_{eff} results for 5 wt.% UO_2 fuel rods are shown in Figure 11. Maximum reactivity occurs with pellet OD 0.78 cm and 1.42 cm rod pitch. Results for 10 wt.% UO_2 fuel rods are shown in Figure 12. Maximum reactivity occurs with pellet OD 0.884 cm and 1.70 cm rod pitch.

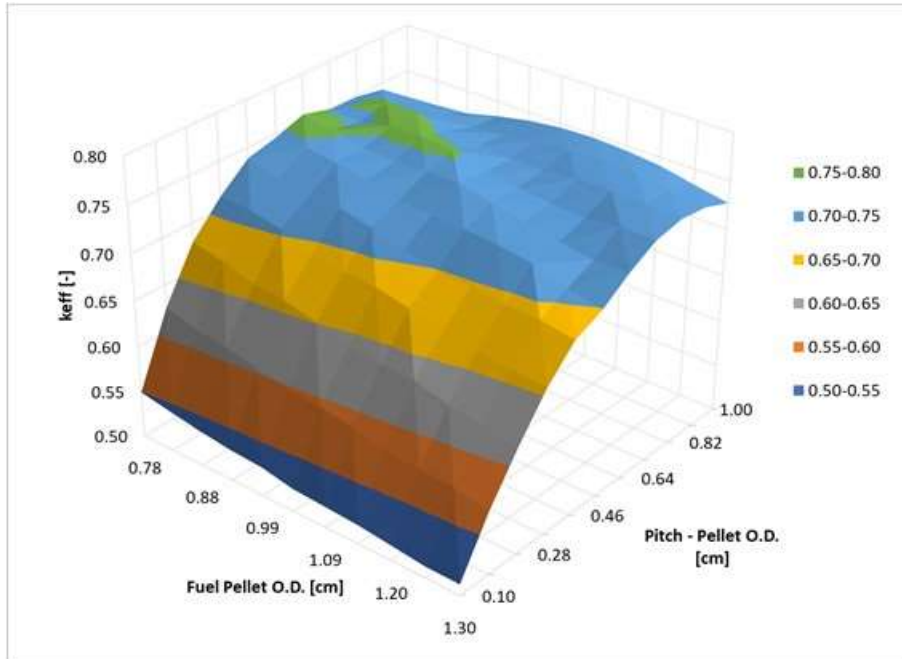


Figure 11. Rod pipe model k_{eff} for fuel pellet OD and rod pitch combinations for 5 wt.% UO_2 .

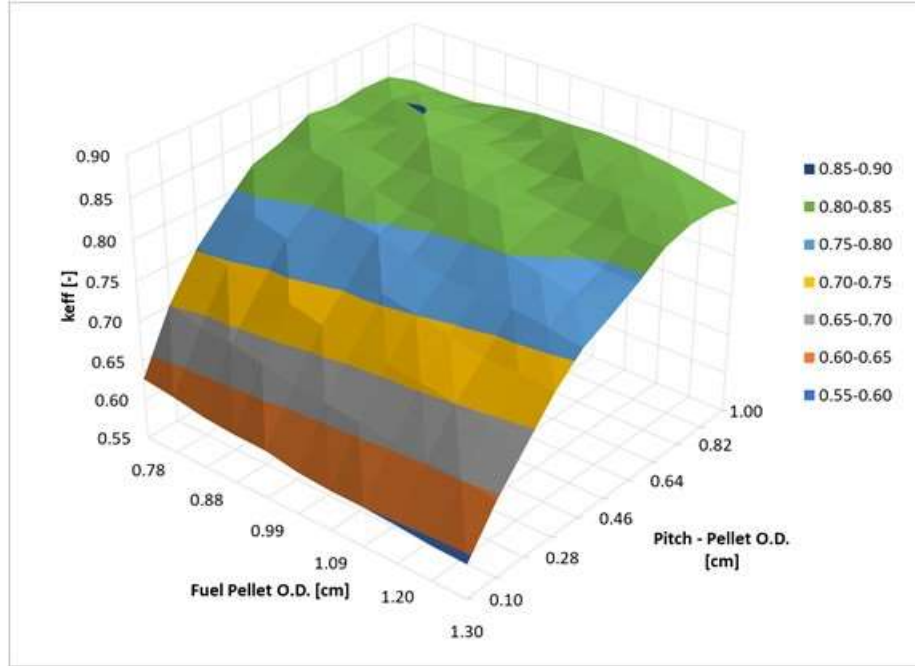


Figure 12. Rod pipe model k_{eff} for fuel pellet OD and rod pitch combinations for 10 wt.% UO_2 .

Additional preferential flooding cases (i.e., overpack, foam, and external) were run by using the Sampler maximum reactivity cases. The flooding cases confirmed that the assumed Clamshell-only flooding produces the highest k_{eff} . With 10 wt.% UO_2 fuel rods, the Traveller rod pipe k_{eff} (0.851) is substantially less than the base case target (0.892). This means that the Traveller package in its current form can likely support the transportation of UO_2 fuel rods up to 10 wt.% ^{235}U .

2.7 Traveller Rod Pipe Model TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for the 5 and 10 wt.% most reactive rod pipe cases. Table 8 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 8. Traveller rod pipe model TSUNAMI-3D case data.

Parameter	5 wt.% infinite array	10 wt.% infinite array
Grid mesh	$40 \times 42 \times 44$	$40 \times 42 \times 44$
Particles/gen.	10,000 fwd. / 30,000 adj.	10,000 fwd. / 30,000 adj.
SDF file	T3D Trav RP5	T3D Trav RP10
Forward k_{eff}	0.75819 ± 0.00049	0.84951 ± 0.00049
Adjoint k_{eff}	0.75800 ± 0.0014	0.8491 ± 0.0014
EALF	0.181 eV	0.255 eV
Cross section uncertainty	0.904 % $\Delta k/k$	0.880 % $\Delta k/k$

Figures 13 and 14 summarize the sensitivity results calculated by TSUNAMI and DP KENO cases for the highest sensitivity nuclide/region combinations. There is good agreement between the DP and TSUNAMI sensitivities, which confirms that the TSUNAMI SDFs properly represent the models. The results also provide insight into what materials and regions are most important for criticality control. For example, in each model, k_{eff} is most sensitive to H in the fuel lattice region polyethylene (increasing 1H increases k_{eff}).

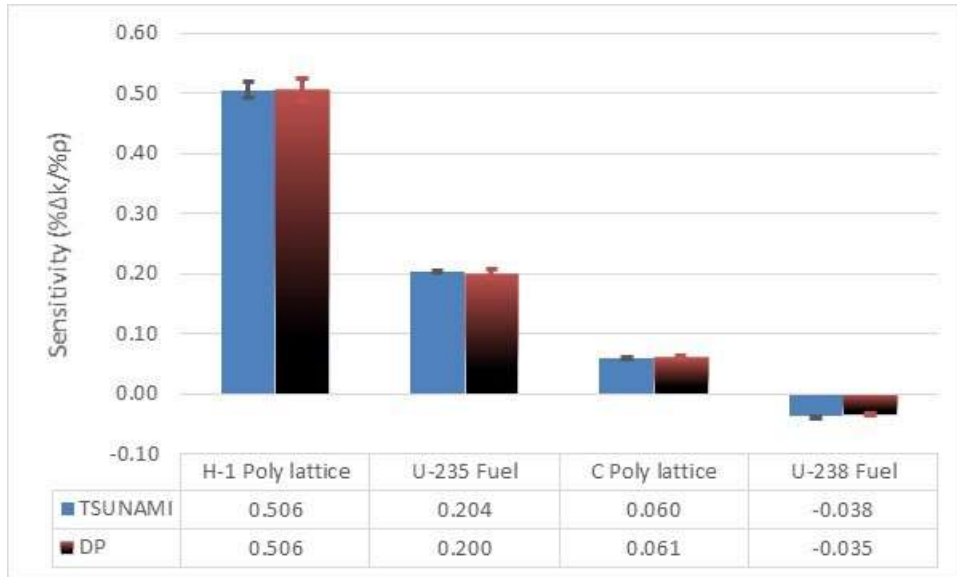


Figure 13. Sensitivity of the infinite array of packages with 5 wt.% UO₂ fuel rods.

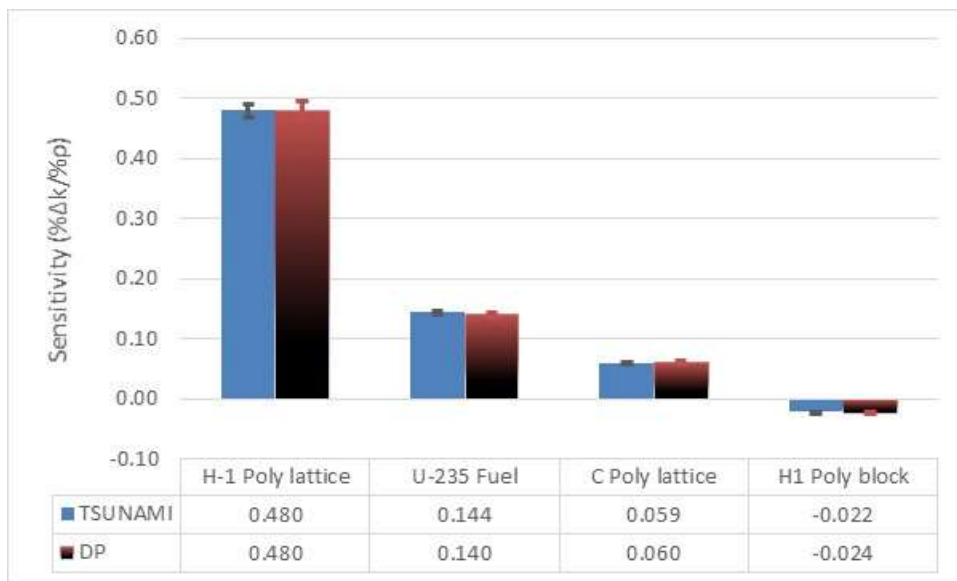


Figure 14. Sensitivity of the infinite array of packages with 10 wt.% UO₂ fuel rods.

Table 9 lists the sensitivity for each mixture in each model. Values greater than 0.01 % Δk /% Σ are highlighted. The two rod pipe models have very similar mixture sensitivities. One interesting feature is that Boral is unimportant for criticality control as compared with SS shells or polyethylene blocks. This is probably due to the SS shells and polyethylene blocks reducing package-to-package neutron interaction in the package array.

Table 9. Traveller rod pipe model sensitivity by mixture.

Mixture	Description	5 wt.% rod pipe		10 wt.% rod pipe	
		Sensitivity	% std. dev.	Sensitivity	% std. dev.
1	UO ₂	0.190	0.6%	0.150	0.7%
3	Fuel lattice polyethylene	0.567	1.3%	0.539	1.1%
4	SS structure	-0.018	2.2%	-0.014	2.4%
5	Boral	-0.002	1.9%	-0.002	1.7%
6	Clamshell water	0.053	6.1%	0.051	5.9%
7	Clamshell Al	0.001	2.6%	0.001	2.4%
8	Polyethylene blocks	-0.021	1.2%	-0.021	1.1%
14	Water in Outerpack	0.000	1.0%	0.000	0.9%
15	Water in Outerpack foam	0.000	0.5%	0.000	0.4%
16	Water reflector	0.000	0.9%	0.000	0.8%

2.8 Traveller Rod Pipe Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for the two SDF files in Table 7 and the library of 1,584 critical experiment SDF files. Figures 15 and 16 show the results with different symbols representing different types of experiments. Table 10 shows the number of experiments in each category with $c_k \geq 0.9$ for the two Traveller rod pipe models. A full list of experiments with c_k values is provided in Appendix A. The TSUNAMI results show that many experiments are applicable for code validation for Traveller rod pipe models with UO₂ fuel enrichment up to 10 wt.% ²³⁵U.

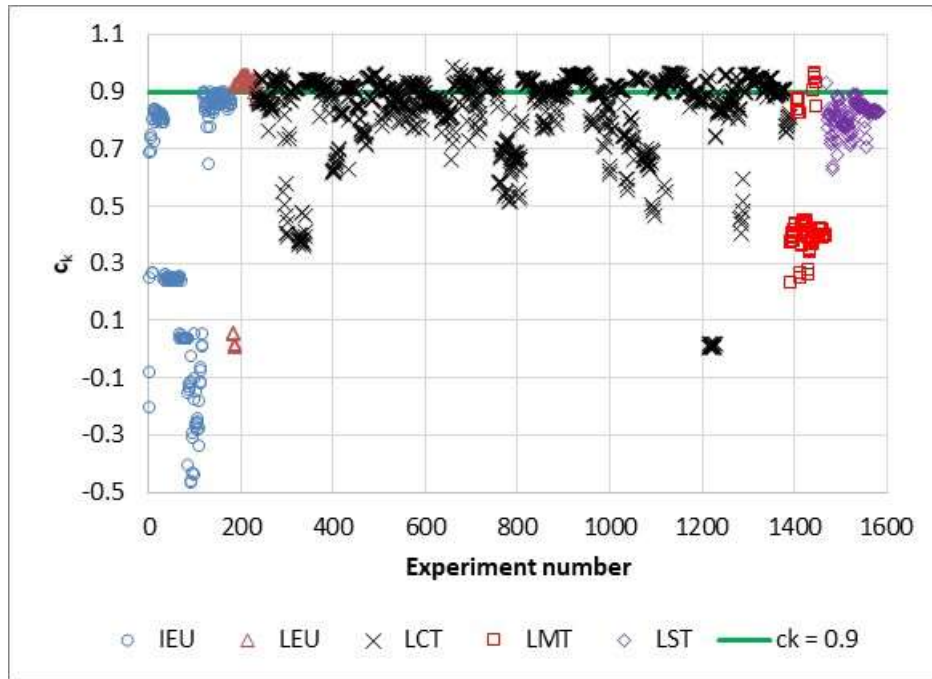


Figure 15. Traveller c_k for the infinite array of packages with 5 wt.% UO₂ fuel rods.

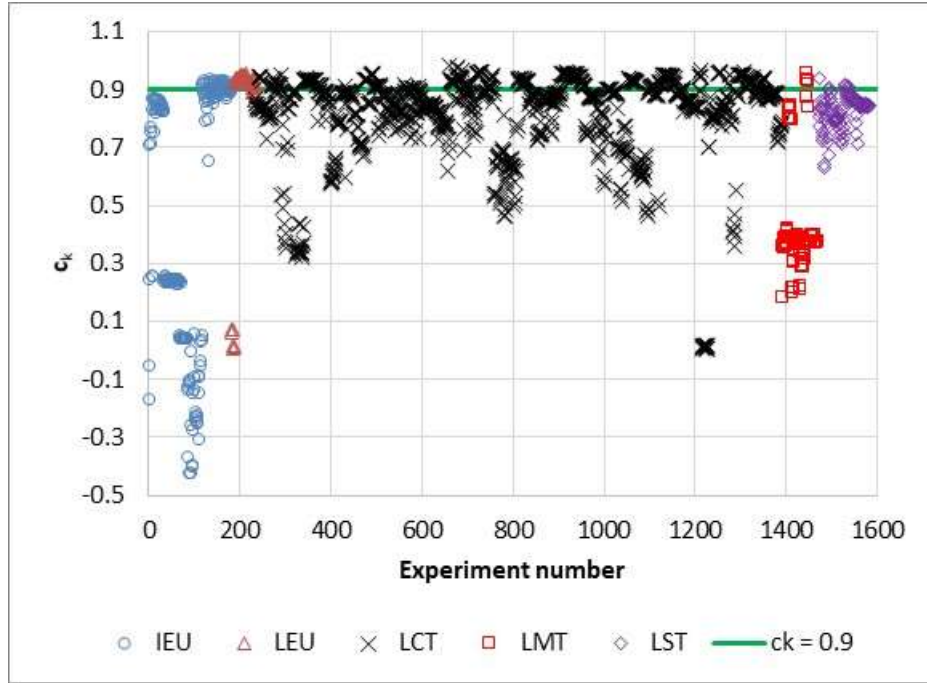


Figure 16. Traveller c_k for the infinite array of packages with 10 wt.% UO_2 fuel rods.

Table 10. Traveller rod pipe model TSUNAMI-IP similarity summary.

Category	Experiments with $c_k \geq 0.9$	
	5 wt.% UO_2 rods	10 wt.% UO_2 rods
IEU $c_k \geq 0.9$	1	32
LEU $c_k \geq 0.9$	45	44
LCT $c_k \geq 0.9$	560	363
LMT $c_k \geq 0.9$	5	4
LST $c_k \geq 0.9$	1	6
Median c_k	0.873	0.860

3. UO₂ POWDER AND PELLETS

3.1 CHT-OP-TU Package Description

The CHT-OP-TU is a cube-shaped package designed to transport uranium oxide in powder or pellet form [7, 8]. UO₂ enrichment is currently limited to ≤ 5 wt.% ²³⁵U. Overall dimensions are 45 × 45 × 62 in. tall. Package construction is of 11 ga carbon or SS with foam and ceramic fiber insulation. UO₂ is contained in four steel oxide vessels (OVs) placed within steel sleeves. Three different sizes of OVs may be used, which have nominal inside diameters of 8, 7.5, and 6 in. The OV minimum wall thickness is 0.22 in., and the maximum internal cavity height is 41 in. The vessels are arranged in a square lattice with a 22.5 in. pitch. Table 11 summarizes the modeled package dimensions, which are based on the HAC models in the SAR.

Table 11. CHT-OP-TU model data.

Parameter	Value (cm)
Outside width	113.51
Outside length	113.51
Outside height	140.14
Outer steel wall thickness	0.305
OV #1 inner diameter	20.824
OV #2 inner diameter	19.558
OV #3 inner diameter	15.748
OV maximum internal height	105.18
OV minimum wall thickness	0.5588
OV pitch	56.992
Sleeve outer diameter	27.305
Sleeve thickness	0.366

Since package design drawings are redacted from the public version of the SAR, a SCALE 6.3.b11 KENO-VI HAC model was constructed by converting the SCALE 4.3 input provided in the SAR. HAC dimensions and conditions were chosen because they produced the highest SAR k_{eff} . HAC model package dimensions are slightly different than the nominal design [8]. A cutaway representation of a 4 × 4 × 3 array of 48 CHT-OP-TU packages is shown in Figure 17. The outermost region is water reflector.

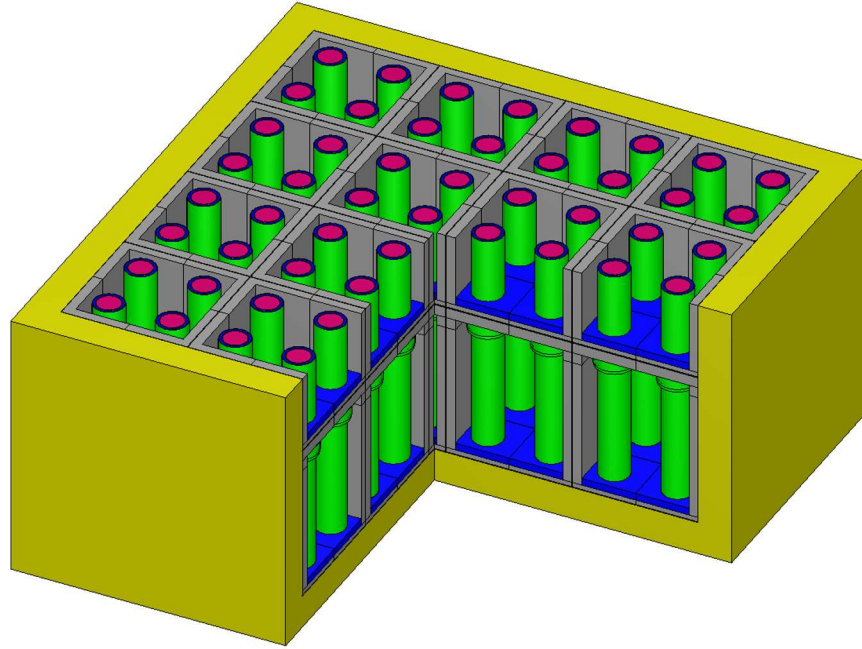


Figure 17. CHT-OP-TU model UO₂ powder model (4 × 4 × 3 package array).

Two versions of the 48 package HAC array model were used to compare optimum moderation conditions and k_{eff} with the CHT-OP-TU SAR results. Table 12 lists the CHT-OP-TU SAR HAC limiting conditions and k_{eff} with 5 wt.% ²³⁵U UO₂ powder and 5 wt.% ²³⁵U UO₂ pellets. Polyethylene packaging increases k_{eff} by 0.001–0.002, but it is ignored in this study for simplicity. The SAR HAC array is 4 × 4 × 3 + 2 (50 packages).

Table 12. CHT-OP-TU safety analysis bounding HAC results.

Number of packages	Array size	Moderator	k_{eff}
50	4 × 4 × 3 + 2	Water reflector, homogenous water/UO ₂ mix in 8 in. OV, other regions dry. H/X ratio 150–200.	0.9381 ± 0.0007
50	4 × 4 × 3 + 2	Water reflector, heterogenous water/UO ₂ mix in 7.5 in. OV, other regions dry. OV water/fuel ratio ~3.0.	0.9255 ± 0.0007

The KENO-VI 4 × 4 × 3 array model was used to confirm HAC optimum moderation package configuration with a homogenous mixture of water and UO₂. The array model has 30 cm of water reflection. KENO-VI and Sampler were used to calculate k_{eff} with varying water volume fractions in the OV sleeve gap, in the internal package void space, and inside the OV (UO₂ vf = 1 – water VF). Five-hundred combinations of moderator VF were run with k_{eff} statistical uncertainty (one sigma) ≤ 0.001. Figure 18 shows the maximum k_{eff} vs. water volume fraction for each of the three variables. The maximum k_{eff} (0.941), which matches the SAR value within the uncertainty of the calculations, occurs with no water in the OV sleeve gap or in the package void spaces and 78% water VF in the 8 in. diameter OV (H/X = 196).

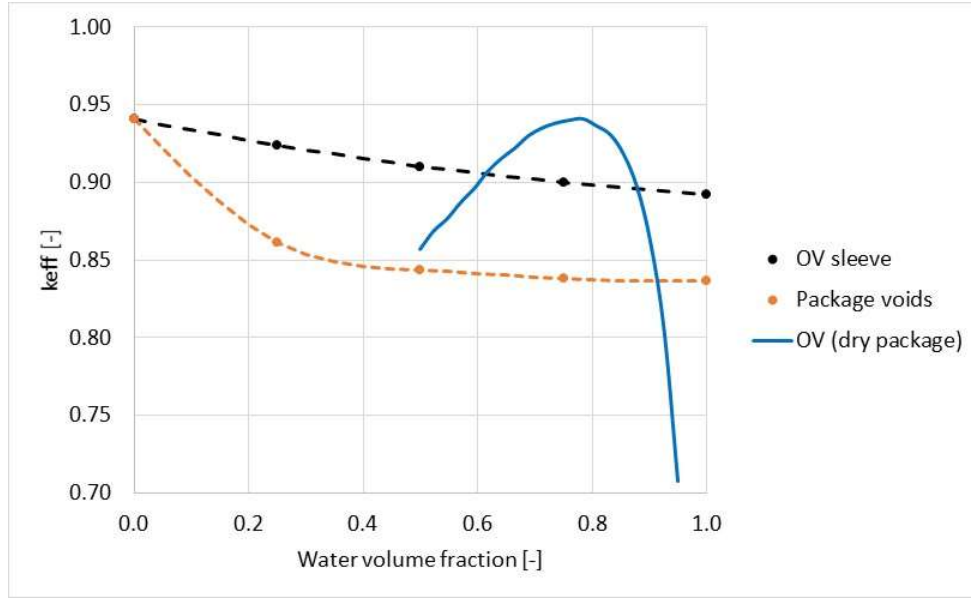


Figure 18. CHT-OP-TU UO₂ powder model optimum moderation results.

The KENO-VI $4 \times 4 \times 3$ package array pellet model was used to confirm HAC optimum package configuration with a heterogenous mixture of water and UO₂ pellets. UO₂ pellets were arranged in triangular pitch stacks. Partial pellets are included in the model where pellet stacks intersect the OV wall.

Sampler/KENO-VI was used to determine optimum pellet OD and pellet stack pitch combinations with water filling the non-pellet space in the OV. Except for 30 cm of external water reflector, all other non-OV regions of the package were dry. A total of 256 combinations of pellet OD and pitch were run with k_{eff} statistical uncertainty (one sigma) ≤ 0.0005 . Tighter convergence was used in this Sampler set to better resolve maximum reactivity conditions. Figure 19 shows k_{eff} as a function of OD and pitch. There are several combinations of pellet OD and pitch at which statistically equivalent maximum k_{eff} occurs. The largest best estimate value (0.930) occurs with 0.6 cm pellet OD and 1.1 cm pitch, which corresponds to a water/fuel ratio of 2.7.

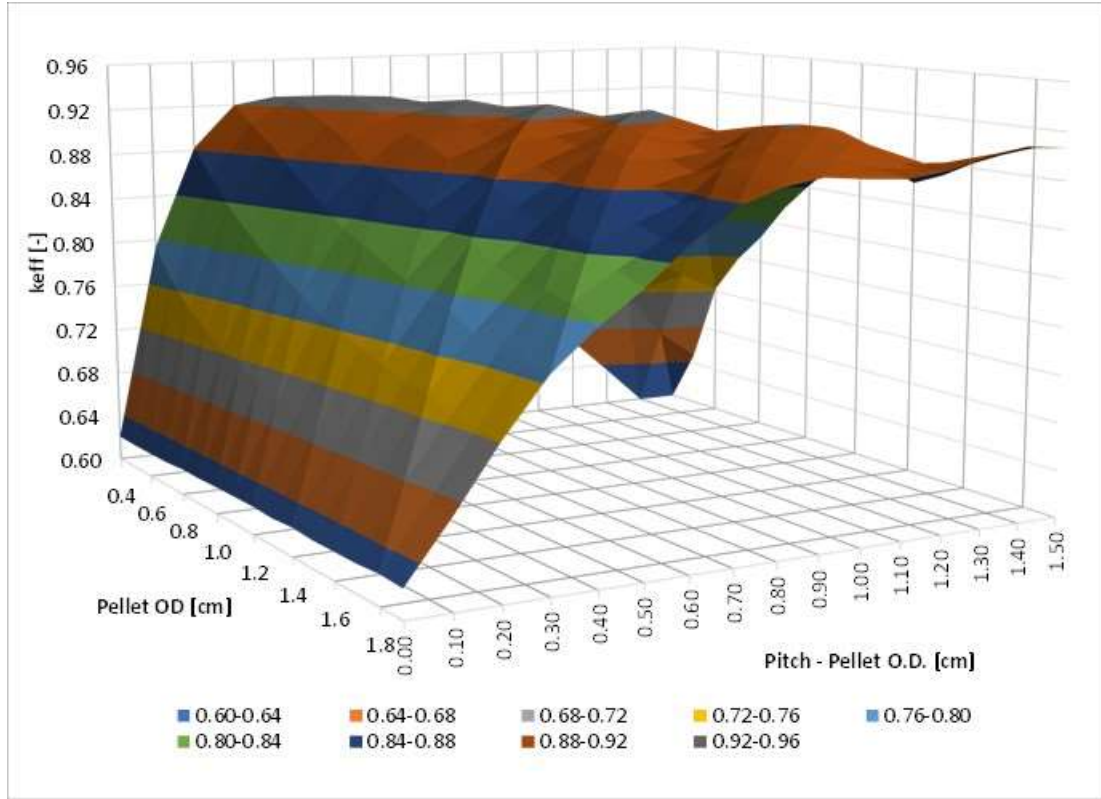


Figure 19. CHT-OP-TU UO₂ pellet model optimum moderation results.

The two $4 \times 4 \times 3$ HAC array KENO models produced bounding condition results very similar to the SAR results. There is little, if any, k_{eff} margin available to accommodate increased enrichment without changing some aspect of the allowable configurations. Compensating for increased enrichment by reducing the HAC array size and reducing the OV diameter will be evaluated with the bounding models.

3.2 CHT-OP-TU Powder Model Criticality Calculations

Table 13 shows the variation of the UO₂ powder model k_{eff} with enrichment, HAC array size, and OV size. Combinations of these characteristics were varied to establish k_{eff} close to 0.94, which is the approximate upper bound from the SAR. Each case maintains the optimum moderator conditions determined in Section 3.1. Cube-shaped array configurations were selected to minimize neutron leakage. Although not comprehensive, the results in Table 13 suggest that by reducing the size of the HAC array and/or reducing the OV diameter, the CHT-OP-TU could be adapted to the transport of increased enrichment UO₂.

Table 13. CHT-OP-TU UO₂ powder model criticality summary.

Enrichment (wt.%)	Array size	CSI	OV diameter (in.)	k_{eff}	EALF (eV)
5	4 × 4 × 3	2.1	8.0	0.9424 ± 0.00049	0.127
6.25	4 × 4 × 3	2.1	7.5	0.9420 ± 0.00049	0.150
7.25	3 × 3 × 3	3.8	7.5	0.9404 ± 0.00049	0.171
8	3 × 3 × 2	5.6	7.5	0.9416 ± 0.00049	0.189
10	4 × 4 × 3	2.1	6	0.8592 ± 0.00049	0.240
18	4 × 4 × 3	2.1	6	0.9331 ± 0.00049	0.507
18*	4 × 4 × 3	2.1	6	0.9390 ± 0.00049	0.314

*After Sampler search for optimum moderation

The EALF of all cases indicates a thermal spectrum, which suggests that ample low-enriched, compound form, thermal energy spectrum (LCT) critical benchmark experiments are likely to be neutronically similar and useful for code validation. A review of 1,236 ICSBEP LCT experiment EALF values shows a range of 0.011 to 6.56 eV with a median value of 0.24 eV [14].

Given the large increase in enrichment considered, the optimum moderator conditions determined in Section 3.1 for 5 wt.% UO₂ might not be bounding for 18 wt.% UO₂. A Sampler/KENO optimum moderation search was performed for the 18 wt.% case. The maximum k_{eff} (0.9390) occurs with no water in the OV sleeve gap or in the package void spaces and 82.5% water VF in the 6 in. diameter OV.

The Table 13 results confirm that there are multiple combinations of package array and OV diameter that would support the transporation of UO₂ powder enriched to >5 wt.% ²³⁵U.

3.3 CHT-OP-TU Pellet Model Criticality Calculations

Table 14 shows the variation of the UO₂ pellet model k_{eff} with enrichment, HAC array size, and OV size. Combinations of these characteristics were varied to establish a k_{eff} close to 0.94, which is the approximate upper bound from the SAR. Each case maintains the optimum moderator conditions determined in Section 3.1. Cube-shaped array configurations were selected to minimize neutron leakage. Although not comprehensive, the Table 13 results suggest that by reducing the size of the HAC array and/or reducing the OV diameter, the CHT-OP-TU could be adapted to transport increased enrichment UO₂.

Table 14. CHT-OP-TU UO₂ pellet model criticality summary.

Enrichment (wt.%)	Array size	CSI	OV diameter (in.)	k_{eff}	EALF (eV)
5	4 × 4 × 3	2.1	7.5	0.9297 ± 0.00049	0.203
5.5	4 × 4 × 3	2.1	7.5	0.9397 ± 0.00049	0.212
6.25	3 × 3 × 3	3.8	7.5	0.9411 ± 0.00049	0.245
6.9	3 × 3 × 2	5.6	7.5	0.9408 ± 0.00049	0.271
17	4 × 4 × 3	2.1	6	0.9390 ± 0.00049	0.807
17*	4 × 4 × 3	2.1	6	0.9454 ± 0.00049	0.346
16.5	4 × 4 × 3	2.1	6	0.9423 ± 0.00049	0.334

*After Sampler search for optimum moderation

The EALF of all cases indicates a thermal spectrum, which suggests that ample low-enriched, compound form, thermal energy spectrum (LCT) critical benchmark experiments are likely to be neutronically similar and useful for code validation.

A Sampler/KENO optimum moderation search was performed for the 17 wt.% case. The maximum k_{eff} (0.9454) occurs with no water in the OV sleeve gap or in the package void spaces, 0.6 cm pellet OD and 1.1 cm pitch (water/fuel ratio of 3.3).

The Table 14 results confirm that there are multiple combinations of package array and OV diameter that would support the transporation of UO₂ pellets enriched to >5 wt.% ²³⁵U.

3.4 CHT-OP-TU Powder Model TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for two cases from Table 13. Table 15 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 15. CHT-OP-TU UO₂ powder model TSUNAMI-3D case data.

Parameter	5 wt.%, 8 in. diameter OV, 48 packages	8 wt.%, 7.5 in. diameter OV, 18 packages
Grid mesh	50 × 50 × 30	38 × 38 × 24
Particles/gen.	30,000 fwd. / 90,000 adj.	30,000 fwd. / 90,000 adj.
SDF file name	T3D_HAC_48_5wt_8in_rev3	T3D_HAC_48_8wt_7-5in_rev3*
Forward k_{eff}	0.94038 ± 0.00049	0.94136 ± 0.00036
Adjoint k_{eff}	0.9409 ± 0.0014	0.9427 ± 0.0014
EALF	0.127 eV	0.189 eV
Cross section uncertainty	0.658% Δk/k	0.727% Δk/k

*Name indicates 48 package array. Actual array size is 18.

The adequacy of the TSUNAMI input is confirmed by comparing TSUNAMI-calculated nuclide sensitivity with KENO DP sensitivity. Figures 20 and 21 summarize the sensitivity results calculated by each method for the highest sensitivity nuclide/region combinations. There is good agreement between the DP and TSUNAMI sensitivities, which confirms that the TSUNAMI SDFs properly represent the models. The two models have the same sensitivity ranking and similar sensitivity values.

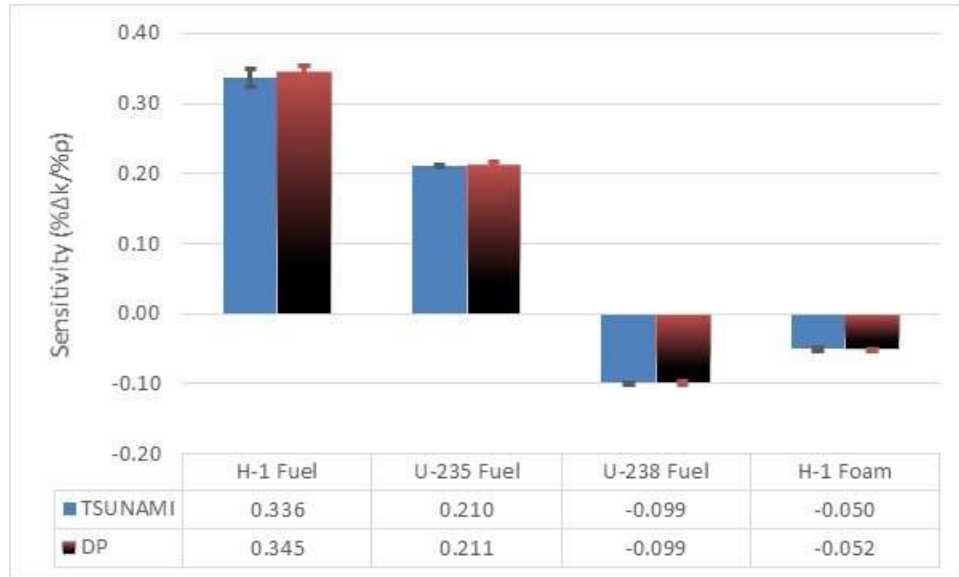


Figure 20. CHT-OP-TU UO₂ powder model sensitivity (48 packages, 5 wt.%, 8 in. OV).

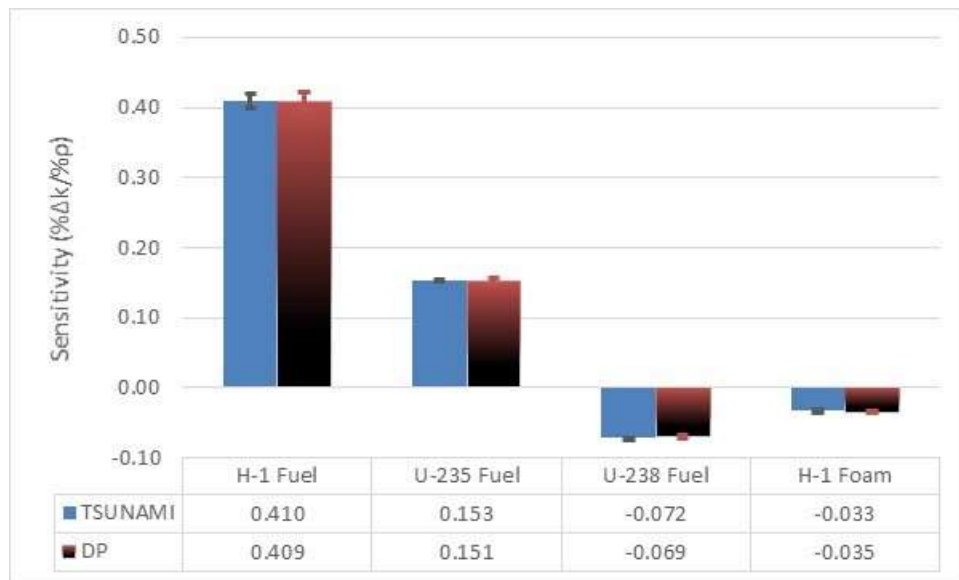


Figure 21. CHT-OP-TU UO₂ powder model sensitivity (18 packages, 8 wt.%, 7.5 in. OV).

Table 16 lists the sensitivity for each mixture in each model. Values greater than 0.01 %Δk/%Σ are highlighted. The CHT-OP-TU models have few regions and materials. The UO₂/water mixture in the OV, the OV and sleeve walls, and the low-density foam have the highest mixture sensitivities.

Table 16. CHT-OP-TU UO₂ powder model sensitivity by mixture.

Mixture	Description	5 wt.%, 8 in. diameter OV, 48 packages		8 wt.%, 7.5 in. diameter OV, 18 packages	
		Sensitivity	% std. dev.	Sensitivity	% std. dev.
1	UO ₂ and water in OV	0.482	1.4%	0.534	1.0%
2	Water outside OV	0.000	3.4%	0.000	3.9%
3	Steel package wall	-0.007	6.9%	-0.005	7.8%
4	OV and sleeve 304 SS	-0.034	2.8%	-0.021	3.2%
5	Water reflector	0.000	N/A	0.000	N/A
6	Low-density foam	-0.045	2.6%	-0.026	4.0%
7	High-density foam	-0.008	6.5%	-0.004	10.2%
8	Water in void spaces	0.000	2.3%	0.000	3.3%

3.5 CHT-OP-TU UO₂ Powder Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for the two SDF files in Table 15 and the library of 1,584 critical experiment SDF files. The 5 wt.% case serves as a reference point for comparison with higher enrichment results. Figures 22 and 23 show the similarity coefficients with different symbols representing different types of experiments. Table 17 shows the number of experiments in each category with $c_k \geq 0.9$ and the median c_k for each CHT-OP-TU powder model. A full list of experiments with c_k values is provided in Appendix A. The TSUNAMI results show that many experiments are likely to be applicable for code validation for the CHT-OP-TU powder models with UO₂ fuel enrichment up to 8 wt.% ²³⁵U. Enrichment higher than 8 wt.% is included in the pellet model evaluation.

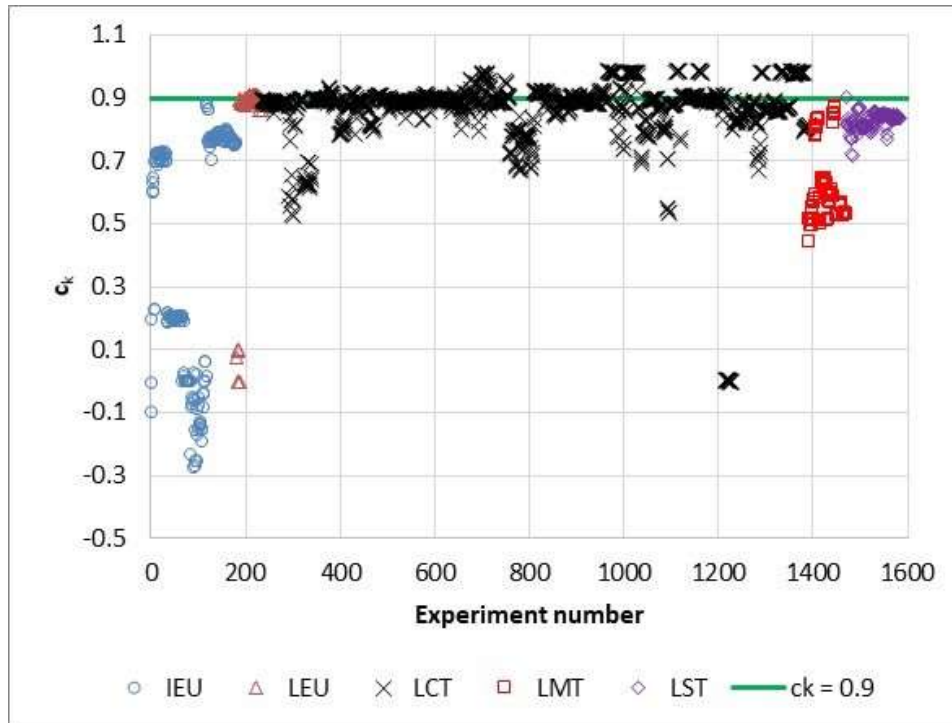


Figure 22. CHT-OP-TU c_k for 5 wt.% UO₂ powder (48 packages, 8 in. diameter OV).

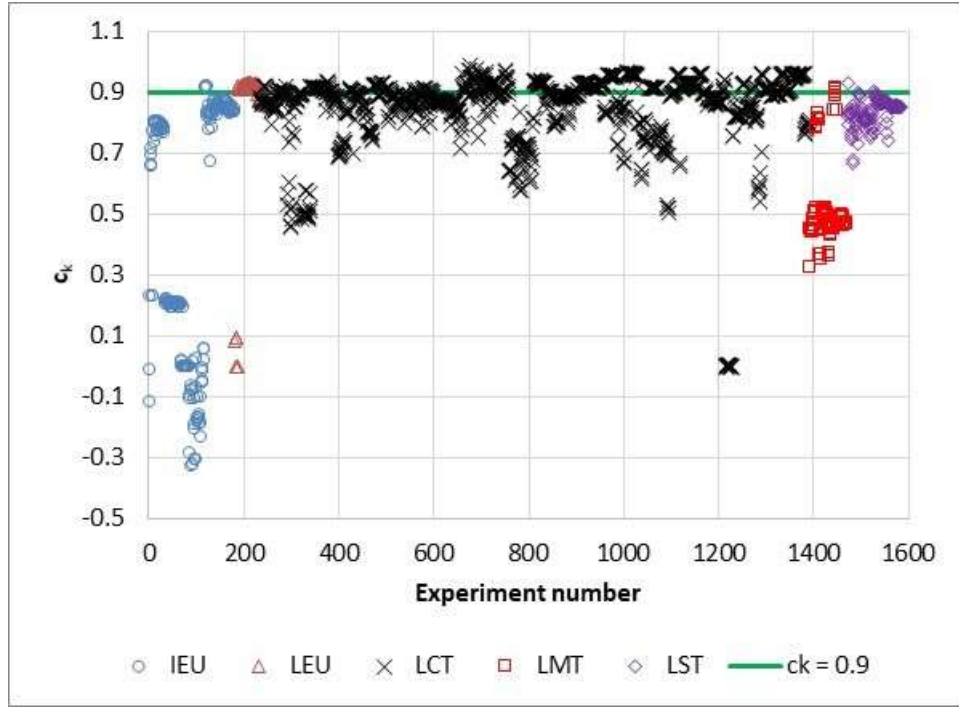


Figure 23. CHT-OP-TU c_k for 8 wt.% UO_2 powder (18 packages, 7.5 in. diameter OV).

Table 17. CHT-OP-TU UO_2 powder model TSUNAMI-IP similarity summary.

Category	5 wt. %	8 wt. %
IEU $c_k \geq 0.9$	0	4
LEU $c_k \geq 0.9$	18	44
LCT $c_k \geq 0.9$	301	476
LMT $c_k \geq 0.9$	0	3
LST $c_k \geq 0.9$	1	2
Median c_k	0.882	0.871

3.6 CHT-OP-TU Pellet Model TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for two cases from Table 14. Table 18 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 18. CHT-OP-TU UO₂ pellet model TSUNAMI-3D case data.

Parameter	6.9 wt.%, 7.5 in. diameter OV 18 packages	16.5 wt.%, 6 in. diameter OV 48 packages
Grid mesh	51 × 51 × 30	50 × 50 × 30
Particles/gen.	100,000 fwd. / 500,000 adj.	30,000 fwd. / 90,000 adj.
SDF file name	T3D_HAC_18_6-9wt_7- 5pel_rev3a	T3D_HAC_48_16-5wt_6pel_rev3
Forward k_{eff}	0.94076 ± 0.00039	0.94247 ± 0.00046
Adjoint k_{eff}	0.9408 ± 0.0011	0.9427 ± 0.0014
EALF	0.271 eV	0.334 eV
Cross section uncertainty	0.720% Δk/k	0.750% Δk/k

The adequacy of the TSUNAMI input is confirmed by comparing TSUNAMI-calculated nuclide sensitivity with KENO DP sensitivity. Figures 24 and 25 summarize the sensitivity results calculated by each method for the highest sensitivity nuclide/region combinations. There is good agreement between the DP and TSUNAMI sensitivities, which confirms that the TSUNAMI SDFs properly represent the models. The two models have the same sensitivity ranking and similar sensitivity values.

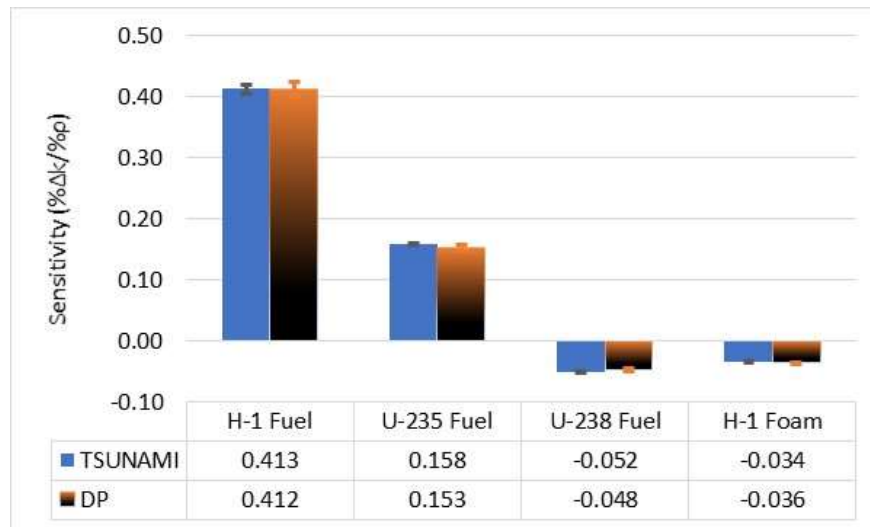


Figure 24. CHT-OP-TU UO₂ pellet model sensitivity (18 packages, 6.9 wt.%, 7.5 in. OV).

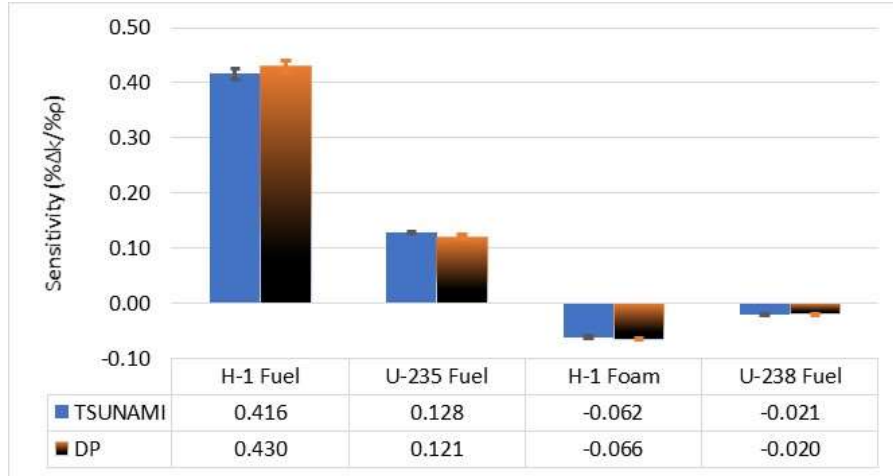


Figure 25. CHT-OP-TU UO₂ pellet model sensitivity (48 packages, 16.5 wt.%, 6 in. OV).

Table 19 lists the sensitivity for each mixture in each model. Values greater than 0.01 %Δk/%Σ are highlighted. The CHT-OP-TU models have few regions and materials. The UO₂ and water mixtures in the OV, OV and sleeve walls, and low-density foam have the highest mixture sensitivities.

Table 19. CHT-OP-TU UO₂ pellet model sensitivity by mixture.

Mixture	Description	6.9 wt.%, 7.5 in. diameter OV, 18 packages		16.5 wt.%, 6 in. diameter OV, 48 packages	
		Sensitivity	% std. dev.	Sensitivity	% std. dev.
1	UO ₂ in OV	0.121	0.5%	0.116	0.9%
2	Water outside OV	0.000	2.2%	0.000	2.1%
3	Steel package wall	-0.005	4.8%	-0.009	5.3%
4	OV and sleeve 304 SS	-0.022	1.7%	-0.035	2.4%
5	Water reflector	0.000	N/A	0.000	N/A
6	Low-density foam	-0.027	2.1%	-0.054	2.1%
7	High-density foam	-0.005	5.6%	-0.011	4.8%
8	Water in void spaces	0.000	1.7%	0.000	1.8%
9	Water in OV	0.446	0.8%	0.448	1.1%

3.7 CHT-OP-TU UO₂ Pellet Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for the two SDF files in Table 18 and the library of 1,584 critical experiment SDF files. The 5 wt.% case serves as a reference point for comparison with higher enrichment results. Figures 26 and 27 show the similarity coefficients with different symbols representing different types of experiments. Table 20 shows the number of experiments in each category with $c_k \geq 0.9$ and the median c_k for each of the CHT-OP-TU powder models. A full list of experiments with c_k values is provided in Appendix A. The TSUNAMI results show that many experiments are likely to be applicable for code validation for the CHT-OP-TU pellet models with UO₂ fuel enrichment up to 16.5 wt.% ²³⁵U, although the 16.5 wt.% package median c_k is substantially lower than for lower enrichment CHT-OP-TU models.

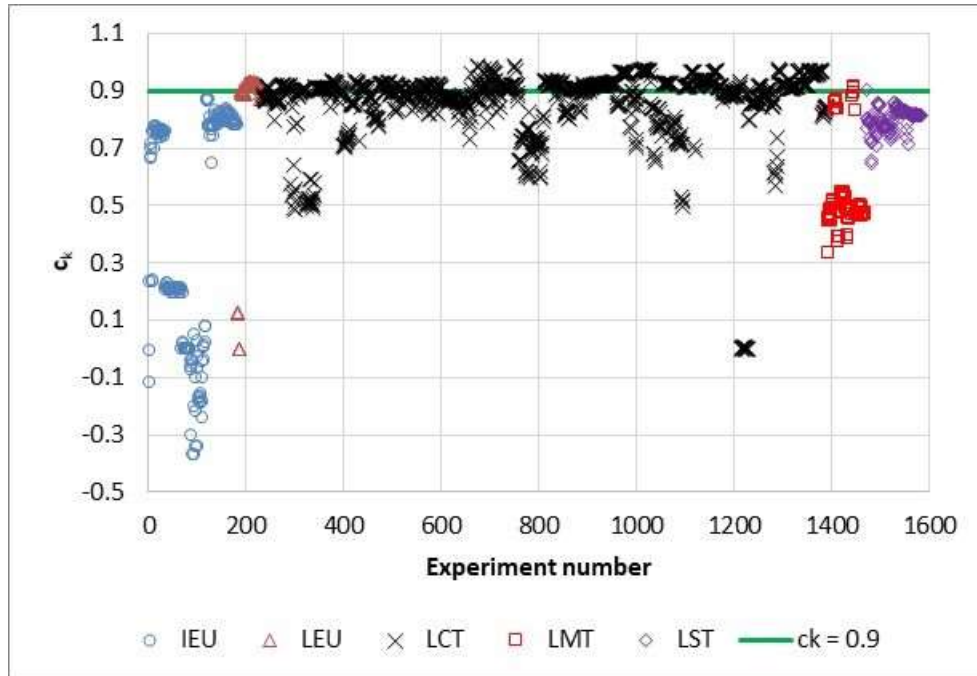


Figure 26. CHT-OP-TU c_k for 6.9 wt.% UO_2 pellets (18 packages, 7.5 in. diameter OV).

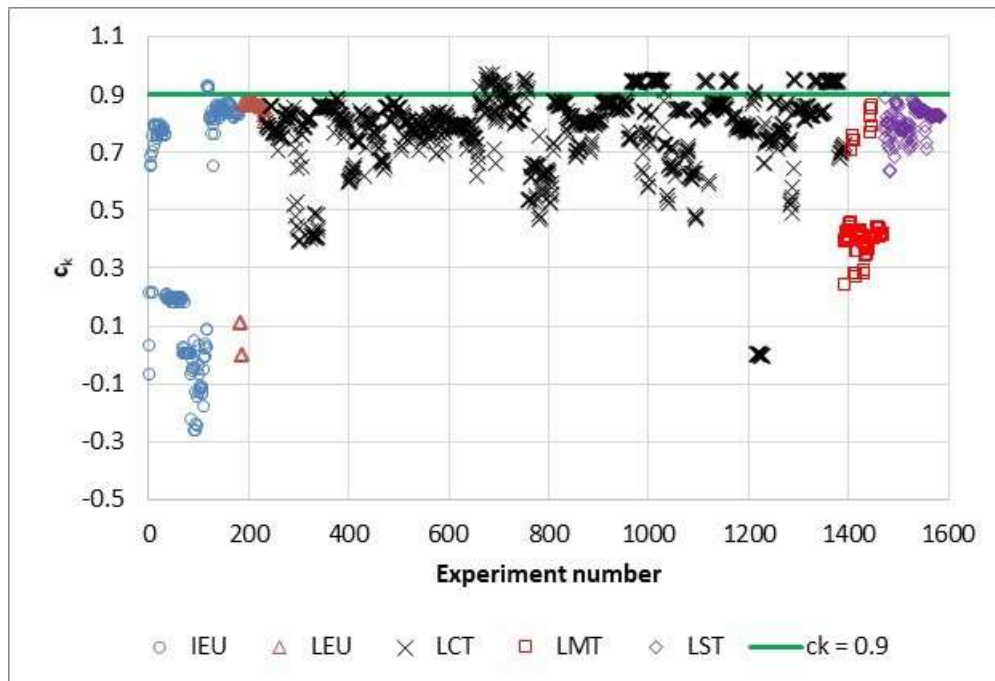


Figure 27. CHT-OP-TU c_k for 16.5 wt.% UO_2 pellets (48 packages, 6 in. diameter OV).

Table 20. CHT-OP-TU UO₂ pellet model TSUNAMI-IP similarity summary.

Category	6.9 wt. %	16.5 wt. %
IEU $c_k \geq 0.9$	0	4
LEU $c_k \geq 0.9$	37	0
LCT $c_k \geq 0.9$	617	137
LMT $c_k \geq 0.9$	3	0
LST $c_k \geq 0.9$	1	0
Median c_k	0.881	0.807

4. U METAL AND ALLOYS

4.1 VERSA-PAC PACKAGE DESCRIPTION

The Versa-Pac is a 55 or 110 gal drum-type package for shipping uranium oxides, uranium metal, uranyl nitrate crystals, uranium carbides, uranyl fluorides, uranyl carbonates, and uranium hexafluoride in 1S or 2S cylinders [9, 10]. Figure 28 shows the major Versa-Pac components. A 5 in. carbon steel pipe container held in place by a “birdcage” device (not pictured) may optionally be used inside the containment body.

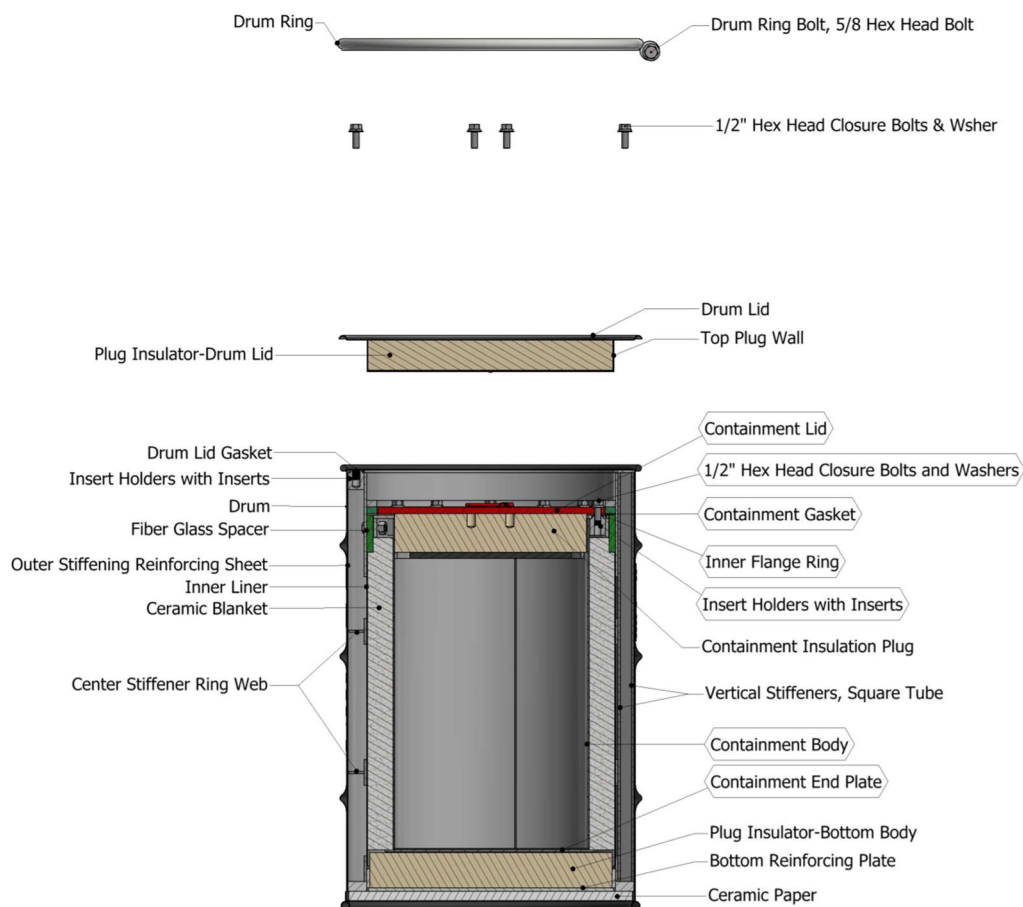


Figure 28. Versa-Pac component illustration [9].

The Versa-Pac package is currently licensed to carry U materials enriched up to 100% ^{235}U with a ^{235}U content maximum allowed mass determined by enrichment bin, as shown in Table 21. Because the Versa-Pac is already licensed to transport HALEU and has mass limits that are a function of enrichment, no additional evaluation is required.

Table 21. Versa-Pac maximum ^{235}U per package (ground/vessel transportation) [15].

^{235}U wt. %	Maximum grams ^{235}U	Packaging type
≤ 100	350	55 or 110 gal drum
≤ 20	410	55 or 110 gal drum
≤ 10	470	55 or 110 gal drum
≤ 5	580	55 or 110 gal drum
≤ 20	605	55 or 110 gal drum, limited hydrogenous packing, CSI = 0.7
≤ 20	635	55 or 110 gal drum, limited hydrogenous packing, CSI = 1.0
≤ 100	695	55 gal drum, 5 in. pipe
≤ 20	1,215	55 gal drum, 5 in. pipe
≤ 10	1,605	55 gal drum, 5 in. pipe
≤ 5	1,065	55 gal drum, 5 in. pipe

5. BWR FUEL RODS AND FUEL ASSEMBLIES

5.1 Framatome TN-B1 Package Description

The TN-B1 is currently licensed to transport two commercial BWR fuel assemblies with lattice average ^{235}U enrichment ≤ 5.0 wt.% or various types of unirradiated fuel rods with ^{235}U enrichment ≤ 5.0 wt.% in a 5 in. SS rod pipe [11, 12]. Multiple fuel assembly design requirements (i.e., Gd rods) and restrictions (i.e., fuel rod OD) are included in the licensing basis that are primarily a function of lattice size.

The TN-B1 package is a rectangular box 29.21 in. tall, 28.35 in. wide, and 199.53 in. long that comprises one inner and one outer SS container. The inner container has a double-wall SS sheet structure with an alumina silicate thermal insulator and foam polyethylene cushioning material. The outer container comprises an angular framework covered with SS plates. A representation of the TN-B1 package from the safety analysis is shown in Figure 29.

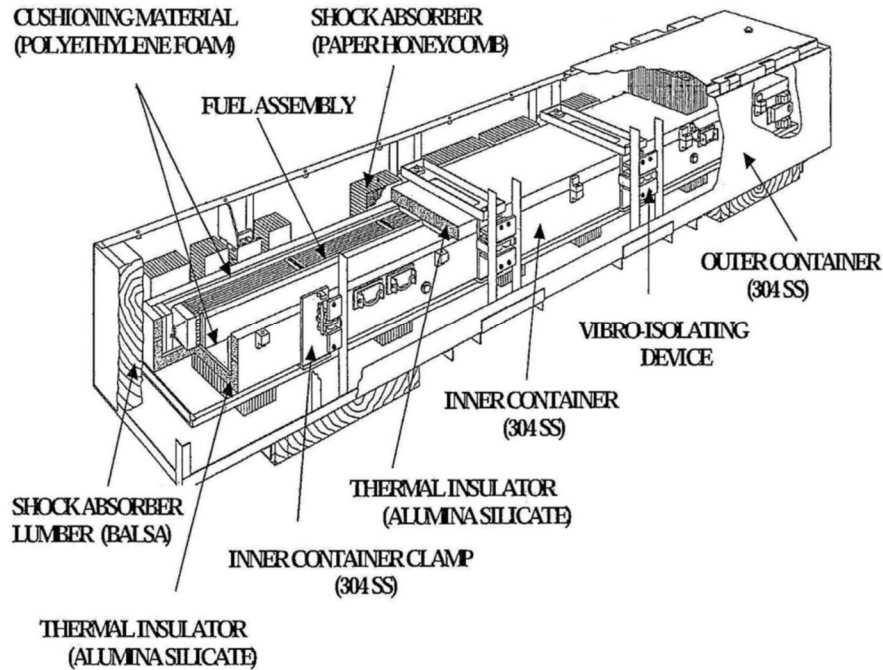


Figure 29. TN-B1 package assembly [11].

The most limiting configuration of the TN-B1 package identified in the criticality safety analysis is the HAC $10 \times 1 \times 10$ array of packages; no space between packages; full flooding in the inner container, including the fuel pellet-clad gap; no water in the outer container or between packages; and 30 cm of water reflector. HAC model dimensions from the criticality safety analysis are shown in Figure 30. Package reactivity is partly controlled by requiring a minimum number of UO_2 rods that contain 2.0 wt.% Gd_2O_3 rods (Gd rods) in the fuel assembly lattice. The 5.0 wt.% ^{235}U 11×11 assembly design requires 13 Gd rods and is the reference design used in this study.

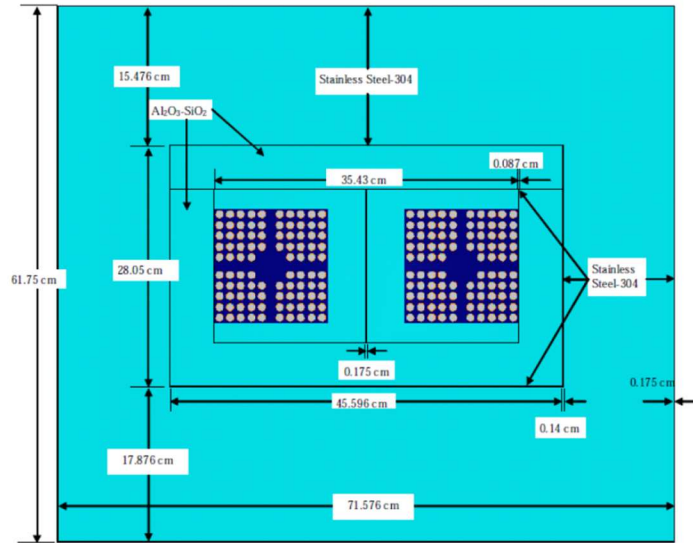


Figure 30. TN-B1 HAC package dimensions [11].

5.2 TN-B1 SCALE KENO-VI Models

A SCALE 6.3.b11 KENO-VI TN-B1 HAC model was constructed by converting a KENO-V.a model provided in the SAR. This base case model consists of a $10 \times 1 \times 10$ array of packages with each package containing two 11×11 5 wt.% fuel assemblies. Each assembly has 13 Gd rods and three axial regions, which differ in the number and configuration of empty lattice locations. Fuel enrichment is 5 wt.% in all fuel rods and axial regions. The base case is used as a representative of TN-B1 characteristics with other fuel designs. The k_{eff} of this HAC case is used as a target for the increased enrichment study. NCT conditions are generally less limiting than HAC conditions and are not modeled for this evaluation.

The effect of increased fuel enrichment fuel in the TN-B1 can be offset by requiring more Gd rods or by reducing the size of the package array. Both approaches are considered in the evaluation. Two cutaway views of a $6 \times 1 \times 6$ package array (top section and front half removed) surrounded by 30 cm of water are shown in Figure 31.

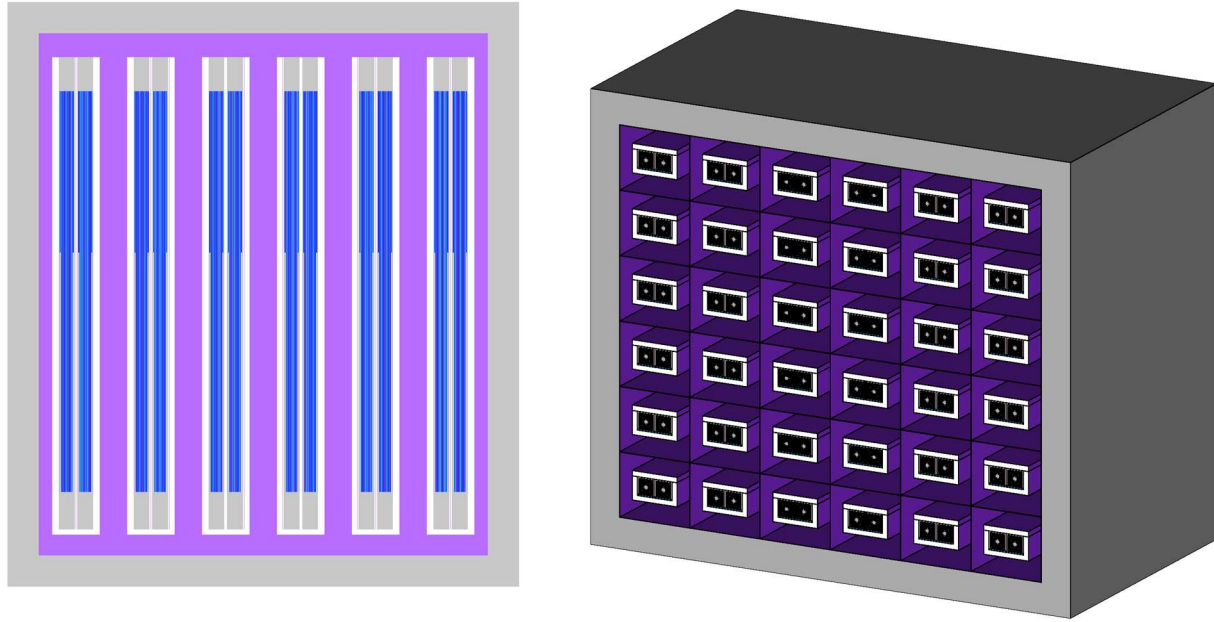


Figure 31. TN-B1 $6 \times 1 \times 6$ package array top and front cutaway views.

5.3 TN-B1 Criticality Calculations

Only one fuel design is used because the objective of this calculation is to assess the effect of increased enrichment. This objective can be met with a representative fuel assembly. Bounding moderator conditions are the same as those determined in the TN-B1 SAR and are not separately verified herein.

Table 22 shows the results of TN-B1 criticality calculations. In the first series of cases, HAC array size is varied from $10 \times 1 \times 10$ to $2 \times 1 \times 2$ incrementally with UO_2 enrichment fixed at 5 wt.%. In the second set, enrichment is increased until k_{eff} is approximately the same as the base case. The last case represents a $10 \times 1 \times 10$ HAC array of packages that contain 8 wt.% fuel assemblies with 24 Gd rods.

Table 22. TN-B1 HAC array criticality calculations.

Enrichment (wt.% ^{235}U)	Gd* rods	Array size	CSI	Fuel assemblies	k_{eff}	EALF (eV)
5	13	$2 \times 1 \times 2$	25	8	0.7108 ± 0.00031	0.293
5	13	$3 \times 1 \times 3$	12.5	18	0.7724 ± 0.00036	0.275
5	13	$4 \times 1 \times 4$	6.3	32	0.8184 ± 0.00033	0.267
5	13	$5 \times 1 \times 5$	4.2	50	0.8528 ± 0.00031	0.260
5	13	$6 \times 1 \times 6$	2.8	72	0.8783 ± 0.00035	0.256
5	13	$7 \times 1 \times 7$	2.1	98	0.8991 ± 0.00030	0.253
5	13	$8 \times 1 \times 8$	1.6	128	0.9148 ± 0.00030	0.251
5	13	$9 \times 1 \times 9$	1.3	162	0.9271 ± 0.00031	0.249
5	13	$10 \times 1 \times 10$	1	200	0.9374 ± 0.00036	0.249
5.55	13	$8 \times 1 \times 8$	1.6	128	0.9371 ± 0.00031	0.269
6	13	$7 \times 1 \times 7$	2.1	98	0.9371 ± 0.00031	0.288

6.7	13	$6 \times 1 \times 6$	2.8	72	0.9377 ± 0.00033	0.316
7.8	13	$5 \times 1 \times 5$	4.2	50	0.9371 ± 0.00036	0.366
9.8	13	$4 \times 1 \times 4$	6.3	32	0.9374 ± 0.00041	0.465
8	24	$10 \times 1 \times 10$	1	200	0.9380 ± 0.00034	0.454

*2.0 wt.% Gd₂O₃

Figure 32 illustrates the trade-off of increased enrichment and reduced array size. Figure 33 compares the $10 \times 1 \times 10$ array 24 Gd rod requirement to extrapolated Gd rod vs. 11×11 fuel enrichment data from the TN-B1 CoC [17]. A log-linear fit line extrapolation provides a good estimate of the number of Gd rods required.

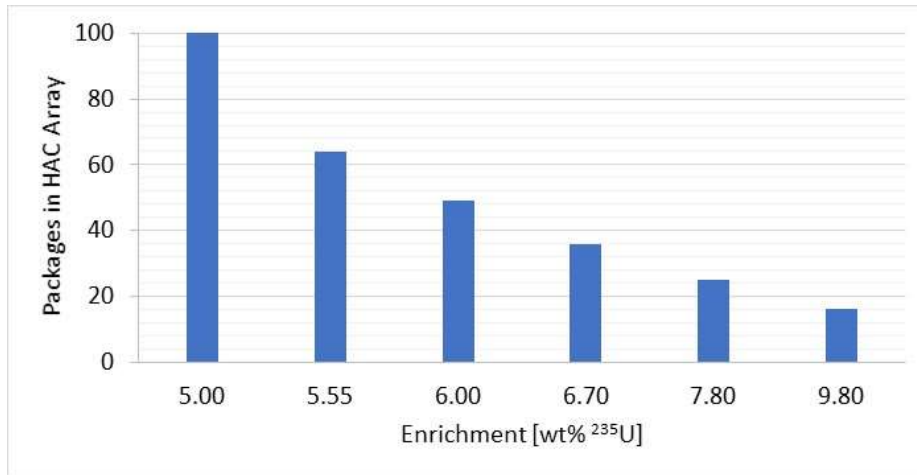


Figure 32. TN-B1 package array size vs. fuel assembly enrichment.

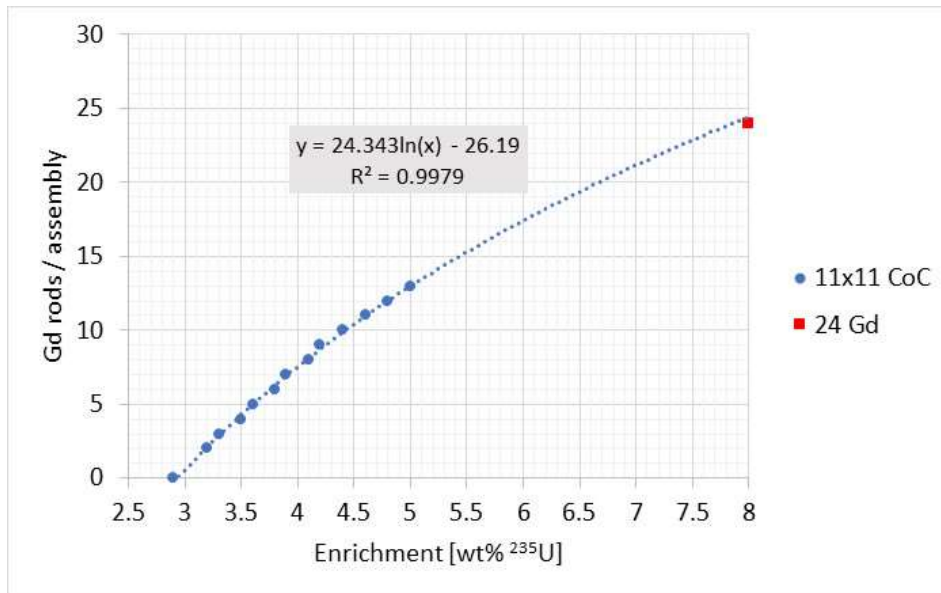


Figure 33. TN-B1 $10 \times 1 \times 10$ package Gd rods required vs. fuel assembly enrichment.

These results show that the TN-B1 could be used for the transportation of increased enrichment fuel by reducing the size of transportation arrays, increasing the number of Gd rods, or a combination of the two. From this set of cases, three were selected for TSUNAMI similarity calculations that cover a range of enrichment with reasonable transportation array size:

- 1) 5.0 wt.% ^{235}U , $10 \times 1 \times 10$ array, 13 Gd rods/fuel assembly;
- 2) 6.7 wt.% ^{235}U , $6 \times 1 \times 6$ array, 13 Gd rods/fuel assembly; and
- 3) 8.0 wt.% ^{235}U , $10 \times 1 \times 10$ array, 24 Gd rods/fuel assembly.

5.4 TN-B1 TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for three cases from Table 22. Table 23 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 23. TN-B1 HAC model TSUNAMI-3D case data.

Parameter	5.0 wt.%, $10 \times 1 \times 10$ package array, 13 Gd rods	6.7 wt.%, $6 \times 1 \times 6$ package array, 13 Gd rods	8.0 wt.%, $10 \times 1 \times 10$ package array, 24 Gd rods
Grid mesh	$52 \times 52 \times 40$	$38 \times 38 \times 40$	$52 \times 52 \times 40$
Particles/gen.	100,000 fwd. / 300,000 adj.	50,000 fwd. / 150,000 adj.	100,000 fwd. / 300,000 adj.
SDF file name	T3D_HAC_5wt_13Gd_10x10a	T3D_HAC_6-7wt_13Gd_6x6	T3D_HAC_8wt_24Gd_10x10a
Forward k_{eff}	0.93688 ± 0.00037	0.93679 ± 0.00031	0.93763 ± 0.00027
Adjoint k_{eff}	0.9364 ± 0.0011	0.9373 ± 0.0014	0.9370 ± 0.0011
EALF	0.248 eV	0.317 eV	0.454 eV
Cross section uncertainty	0.536% $\Delta k/k$	0.568% $\Delta k/k$	0.522% $\Delta k/k$

The adequacy of the TSUNAMI input was confirmed by comparing TSUNAMI-calculated nuclide sensitivity with KENO DP sensitivity. Figures 34, 35, and 36 summarize the sensitivity results calculated by each method for the highest sensitivity nuclide/region combinations. There is good agreement between the DP and TSUNAMI sensitivities, which confirms that the TSUNAMI SDFs properly represent the models. The two models have the same sensitivity ranking and similar sensitivity values.

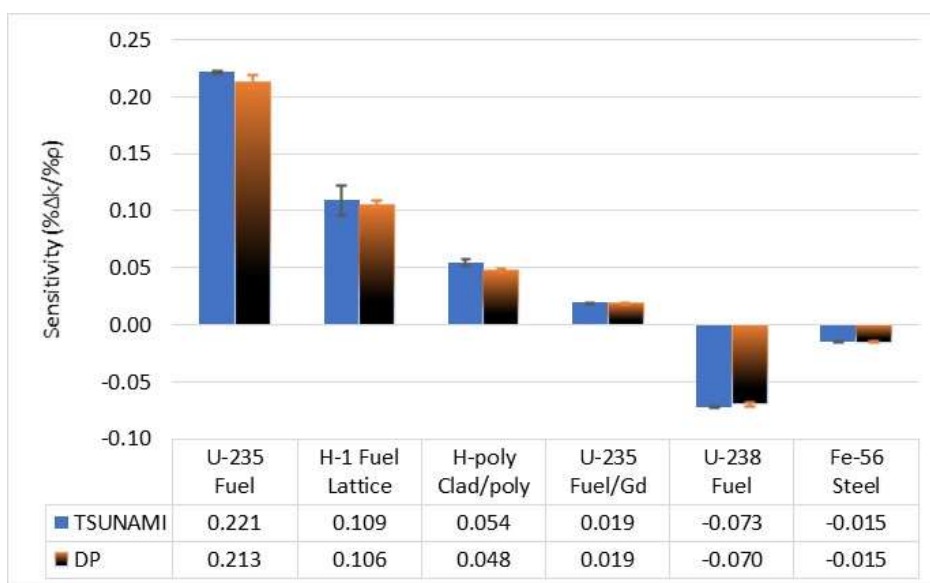


Figure 34. TN-B1 model sensitivity (100 packages, 5 wt.%, 13 Gd rods/fuel assembly).

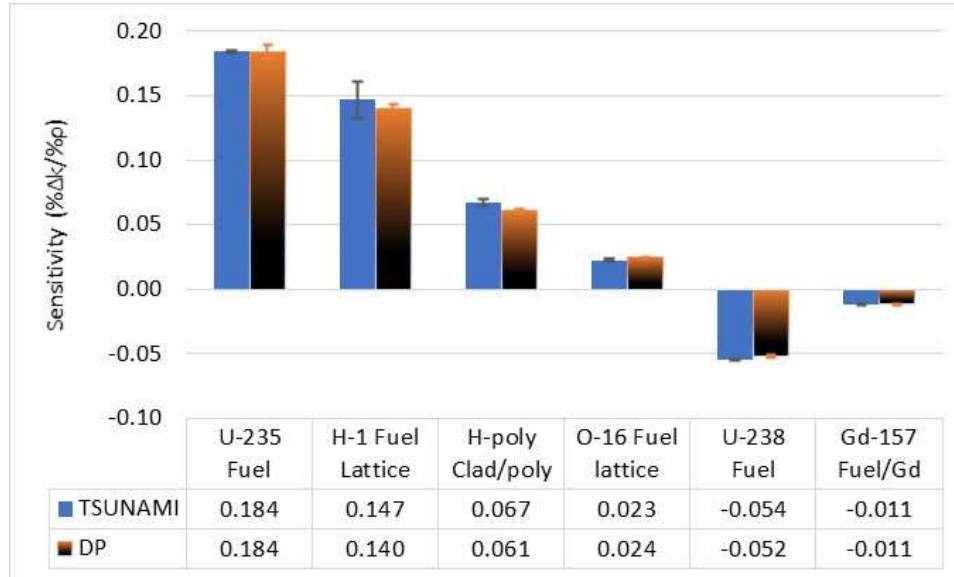


Figure 35. TN-B1 model sensitivity (36 packages, 6.7 wt.%, 13 Gd rods/fuel assembly).

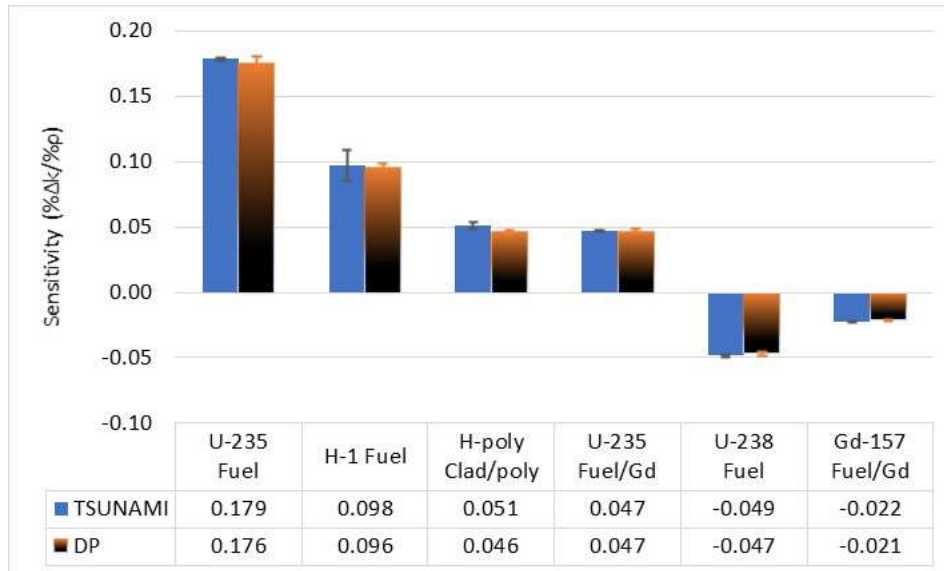


Figure 36. TN-B1 model sensitivity (100 packages, 8 wt.%, 24 Gd rods/fuel assembly).

Table 24 lists the sensitivity for each mixture in each model. Values greater than 0.01 % Δk /% Σ are highlighted. Sensitivities are similar with UO₂ in the non-Gd fuel rods that have the highest sensitivity. The largest difference occurs for lattice/reflector water in the 6 × 1 × 6 array, possibly because the reflector has more importance in a system with more neutron leakage.

Table 24. TN-B1 model sensitivity by mixture.

	5 wt.%, 13 Gd rods/assembly, 100 packages	6.7 wt.%, 13 Gd rods/assembly, 36 packages	8 wt.%, 24 Gd rods/assembly, 100 packages
--	---	--	---

Mixture	Description	Sensitivity	% std. dev.	Sensitivity	% std. dev.	Sensitivity	% std. dev.
1	UO ₂	0.152	0.4%	0.135	0.5%	0.133	0.5%
2	Clad with polyethylene	0.056	2.3%	0.072	1.8%	0.053	2.3%
4	UO ₂ with Gd	0.000	N/A	0.003	5.8%	0.012	2.3%
6	304 SS structure	-0.029	1.4%	-0.021	1.6%	-0.026	1.7%
7	Water (lattice and reflector)	0.124	5.2%	0.170	4.2%	0.112	5.3%
8	Low-density foam	0.001	33.4%	0.003	12.1%	0.003	17.6%
9	High-density foam	0.002	18.0%	0.003	11.1%	0.003	13.8%
10	Insulation	0.009	1.5%	0.011	1.1%	0.009	1.6%
15	Zr fuel channel	0.000	28.8%	0.002	5.9%	0.000	27.4%

5.5 TN-B1 Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for the three SDF files in Table 23 and the library of 1,584 critical experiment SDF files. The 5 wt.% case serves as a reference point for comparison with higher enrichment results. Figures 37, 38, and 39 show the similarity coefficients with different symbols representing different types of experiments.

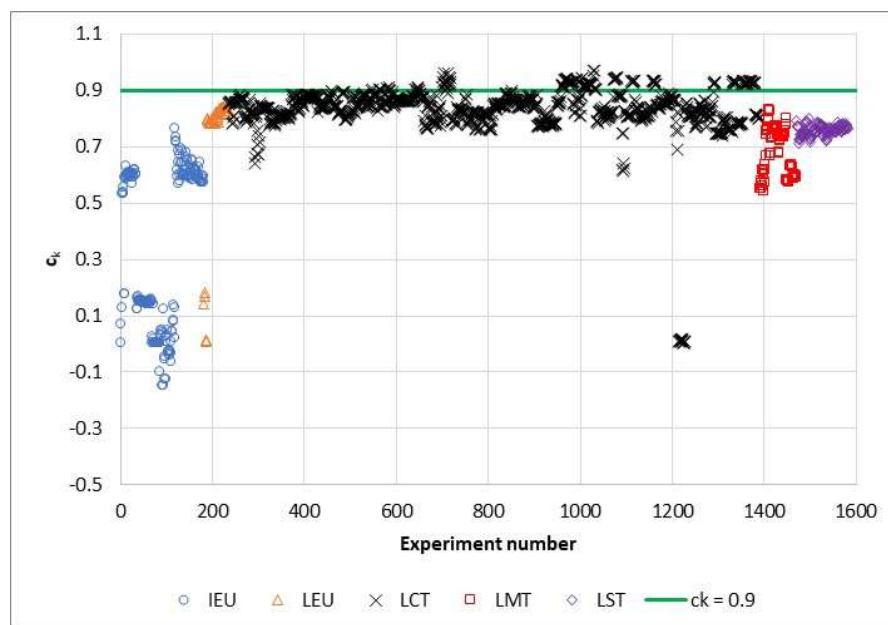


Figure 37. TN-B1 c_k for 5 wt.% UO₂ (100 packages, 13 Gd rods/fuel assembly).

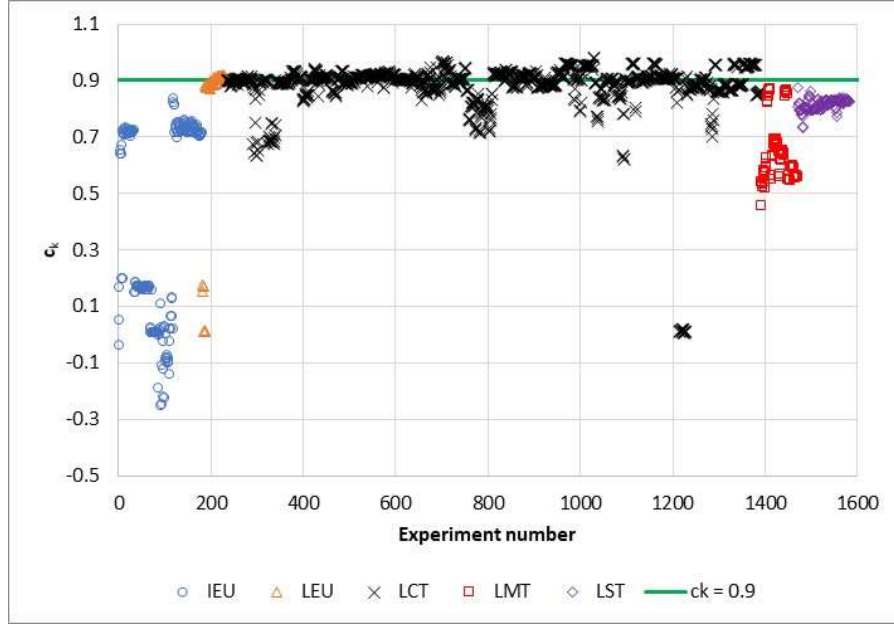


Figure 38. TN-B1 c_k for 6.7 wt.% UO_2 (36 packages, 13 Gd rods/fuel assembly).

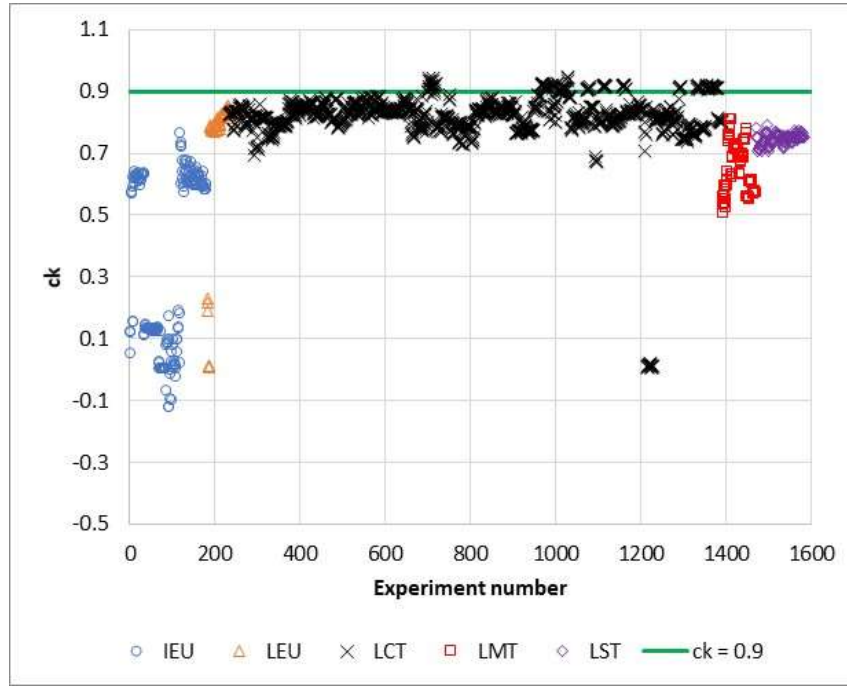


Figure 39. TN-B1 c_k for 8 wt.% UO_2 (100 packages, 24 Gd rods/fuel assembly).

Table 25 shows the number of experiments in each category with $c_k \geq 0.9$ and the median c_k for each TN-B1 model. A full list of experiments with c_k values is provided in Appendix A. There are significantly more experiments with $c_k \geq 0.9$ for the smaller array (36 packages) with the intermediate enrichment (6.7 wt.%). This increase in similarity is coincident with the increased importance of lattice and reflector water. There is only a modest difference in similarity results for the 5 and 8 wt.% 100 package models. Overall, numerous experiments are applicable for code validation (marginally similar with $c_k \geq 0.8$ or similar with $c_k \geq 0.9$) for the TN-B1 models with UO_2 fuel enrichment up to 8 wt.% ^{235}U .

Table 25. TN-B1 model TSUNAMI-IP similarity summary.

Category	5 wt.%, 13 Gd rods/assembly, 100 packages	6.7 wt.%, 13 Gd rods/assembly, 36 packages	8 wt.%, 24 Gd rods/assembly, 100 packages
IEU $c_k \geq 0.9$	0	0	0
LEU $c_k \geq 0.9$	0	25	0
LCT $c_k \geq 0.9$	162	633	132
LMT $c_k \geq 0.9$	0	0	0
LST $c_k \geq 0.9$	0	0	0
Median c_k	0.822	0.890	0.811

6. UF₆

6.1 Daher Nuclear Technologies DN-30 Description

The DN-30 is a nominally 30 in. diameter 30B cylindrical steel container used for the transportation of up to 2,277 kg of ≤ 5 wt.% enriched UF₆ per cylinder. Outside the 30B is protective structural packaging (PSP) comprised largely of inner and outer steel shells with polyisocyanurate rigid foam between [13, 14]. Nominal package dimensions are provided in Table 26. Figure 40 shows the major DN-30 components.

Table 26. DN-30 model data.

Parameter	Value (cm)
30B nominal length	206.0
30B nominal diameter	76.0
30B wall thickness	1.3
PSP nominal length	243.7
PSP nominal diameter	121.6 c
PSP inner shell side thickness	0.2
PSP outer shell side thickness	0.3

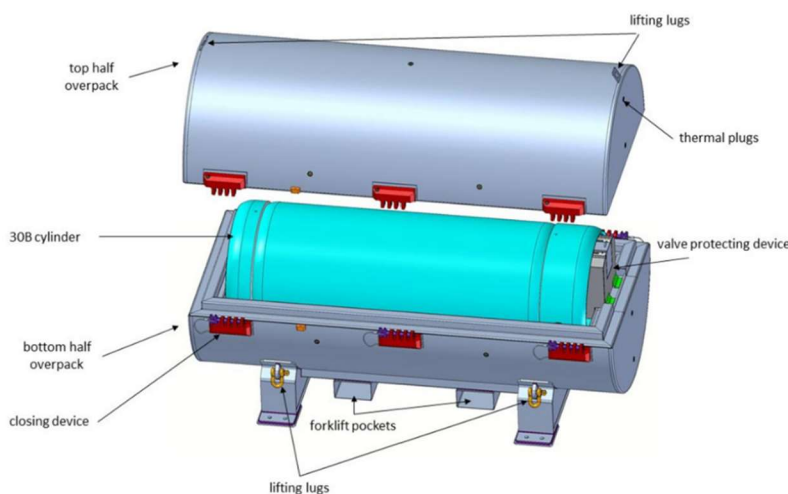


Figure 40. DN-30 package assembly [27].

The most limiting configuration of the DN-30 package identified in the SAR is the HAC infinite package array with a thin cylindrical layer of water between each package in the triangular pitch lattice. Unlike other packages evaluated in this study, UF₆ transportation packages that meet certain requirements are exempt from the 10 CFR 71.55(b) assumption of water leakage into the containment system [20]. This exemption applies to UF₆ enrichment ≤ 5 wt.%. The SAR most reactive 30B contents include 0.5 wt.% HF and 3.9–11.4 kg of hydrogenated uranium residues (HUR). UF₆ occupies the balance of the internal volume of the 30B. The minimum internal volume is 0.736 m³, and the maximum allowed UF₆ loading is 2,277 kg. The CoC lists a maximum allowed H/U ratio of 0.088.

Two 30B models were used in the SAR: one with spherical heads and cylinder skirts on the cylinder ends and one simplified to a right circular cylinder. The maximum OD is 76.8 cm, and the length is 193.5 cm, resulting in a spherical head model internal volume that is almost 10% greater than the minimum. In this work, a simplified model was used for scoping calculations, and a spherical head model was used for documented calculations.

6.2 DN-30 SCALE KENO-VI HAC Models

The DN-30 SAR maximizes the 30B volume by using minimum wall thickness (0.794 cm) and maximal cylinder dimensions. The PSP is assumed to collapse down onto the 30B with only the PSP SS walls (0.5 cm thick radially and 1.4 cm thick axially) and a water layer for optimum moderation between packages.

Four aspects of the SAR HAC model are highly important for criticality calculations:

- 1) the thickness and placement (inside or outside the collapsed PSP shells) of a water layer outside the 30B;
- 2) the presence of the collapsed PSP shells;
- 3) a three-shell spherical model of the HUR with HUR in the center, a shell of UF_6 , and a shell of HF; and
- 4) the position of the HUR sphere.

The nonproprietary SAR does not provide details to allow the SAR HAC model to be replicated. The DN-30 model used in this work includes the important features and produces very similar k_{eff} with 5 wt.% UF_6 . The SAR infinite array HAC k_{eff} is 0.935, including 3 sigma uncertainty. The SAR model has 5.5 g/cc 99.5 wt.% UF_6 and 0.5 wt.% HF filling the volume not occupied by HUR. For the same conditions, k_{eff} that uses the KENO-VI model developed herein is 0.935 (no uncertainty). This model includes 11.4 kg of HUR of the form $\text{UO}_2\text{F}_2 \cdot 3\text{H}_2\text{O}$ with a density of 6.3 g/cc [21].

The SAR bounding material orientation is a complex arrangement of UF_6 and a sphere of UF_6 , HF, and HUR (multiple spherical layers) placed near one end of the cylinder. Scoping calculations confirmed that modeling the HUR as a multilayer sphere produces higher k_{eff} than homogenizing the HUR with UF_6 . The SAR indicated maximum UF_6 density with no void space in the cylinder maximized k_{eff} .

Other work suggests that k_{eff} is maximum at reduced UF_6 density [22]. Scoping calculations with and without the HUR sphere in a 5 wt.% DN-30 model show that the HUR sphere increases k_{eff} significantly and reverses the trend with UF_6 density (Figure 41). The HUR is neutronically important because HUR spheres are positioned to maximize interactions between HUR spheres in adjacent cylinders and because the HUR sphere contains much more moderator than the larger volume of UF_6 . Figure 42 shows the HUR sphere positioning in a KENO-VI 3×2 HAC array model.

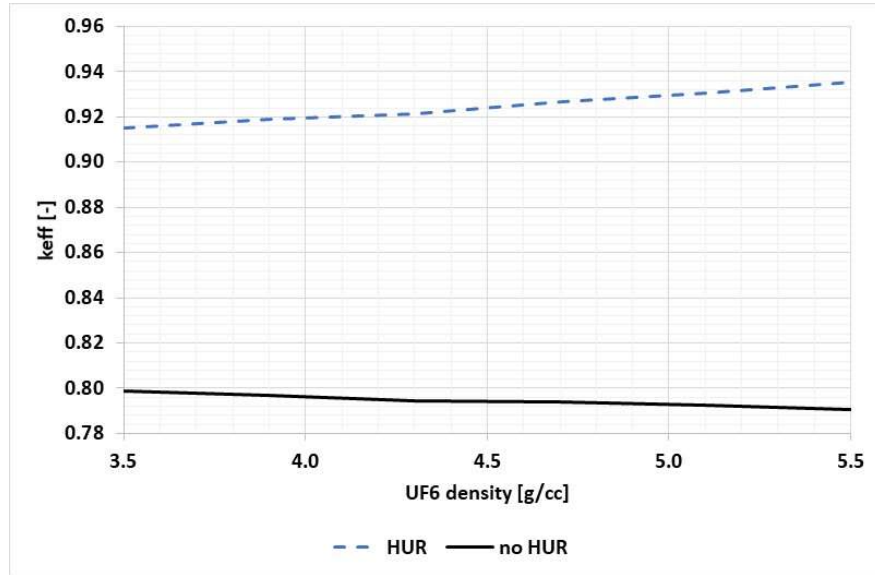


Figure 41. Effect of HUR on k_{eff} .

The enrichment of the U in HUR is important. Increased UF_6 enrichment will lead to increased HUR enrichment. For this work, HUR enrichment is assumed to be the same as UF_6 enrichment. In practice, the HUR enrichment might need to be modeled as the highest enrichment that a cylinder is licensed to transport.

Samplers were used to perform k_{eff} calculations over a range of UF_6 density and water layer thickness. Figure 43 shows k_{eff} results for a 3×2 HAC array with 6.7 wt.% enriched UF_6 . Maximum reactivity occurs with maximum UF_6 density and a 0.4 cm water layer around each 30B cylinder. Several combinations of enrichment and HAC array size were investigated. Unlike the array models, the high-enrichment single cylinder model had maximum reactivity with 1.4 cm of water between the 30B and the PSP steel. For that single package model, increased water layer thickness moves the PSP steel further from the UF_6 but does not increase the distance between packages.

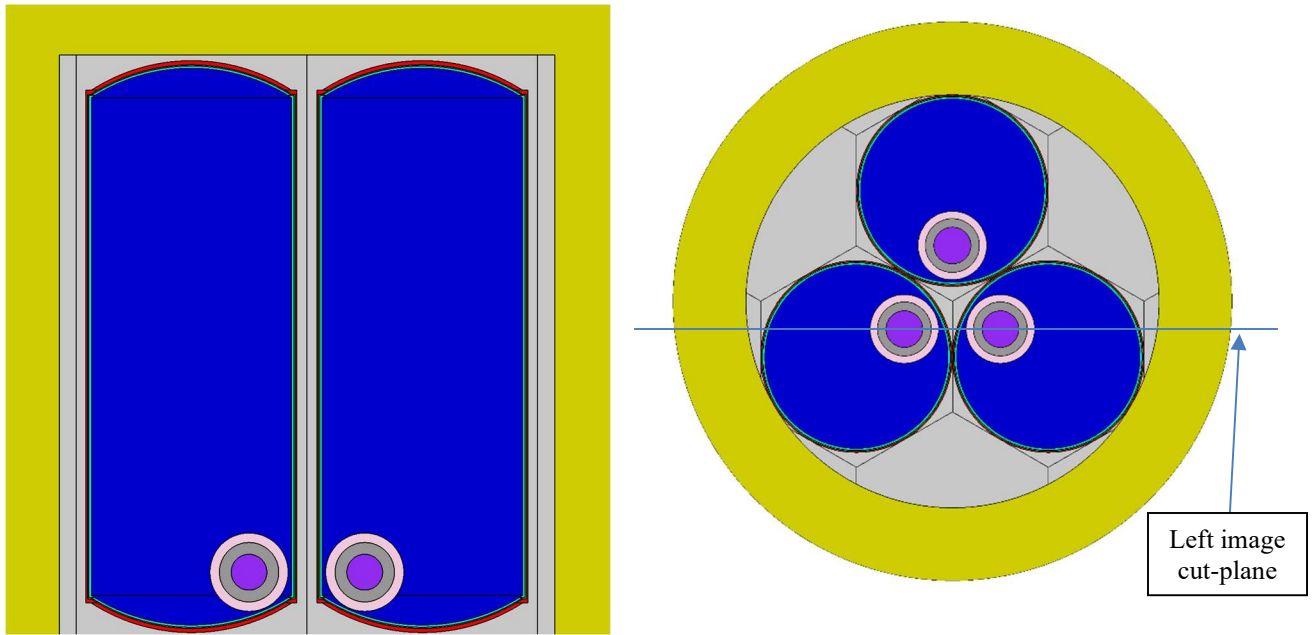


Figure 42. DN-30 3 × 2 HAC array model cutaway views.

6.3 DN-30 Criticality Calculations

Criticality calculations were performed to determine combinations of enrichment and array size with k_{eff} approximately equal to the 5 wt.% infinite array model. Sampler was used to determine the most reactive water layer thickness and UF_6 density. Figures 43 and 44 show the Sampler results for the 3 × 2 and single package models, respectively. Table 27 shows the combinations of enrichment and array size with k_{eff} near 0.935. The trend of enrichment with inverse HAC array size (1/number of packages) is shown in Figure 45. Subcriticality with no water flooding of the 30B interior can be maintained with increased enrichment by reducing the maximum HAC array size (increasing CSI) up to 12.5 wt.%. These results rely partly on the SAR modeling approach, particularly the treatment of HUR. The criticality calculations presented provide useful insights but should not be considered exhaustive.

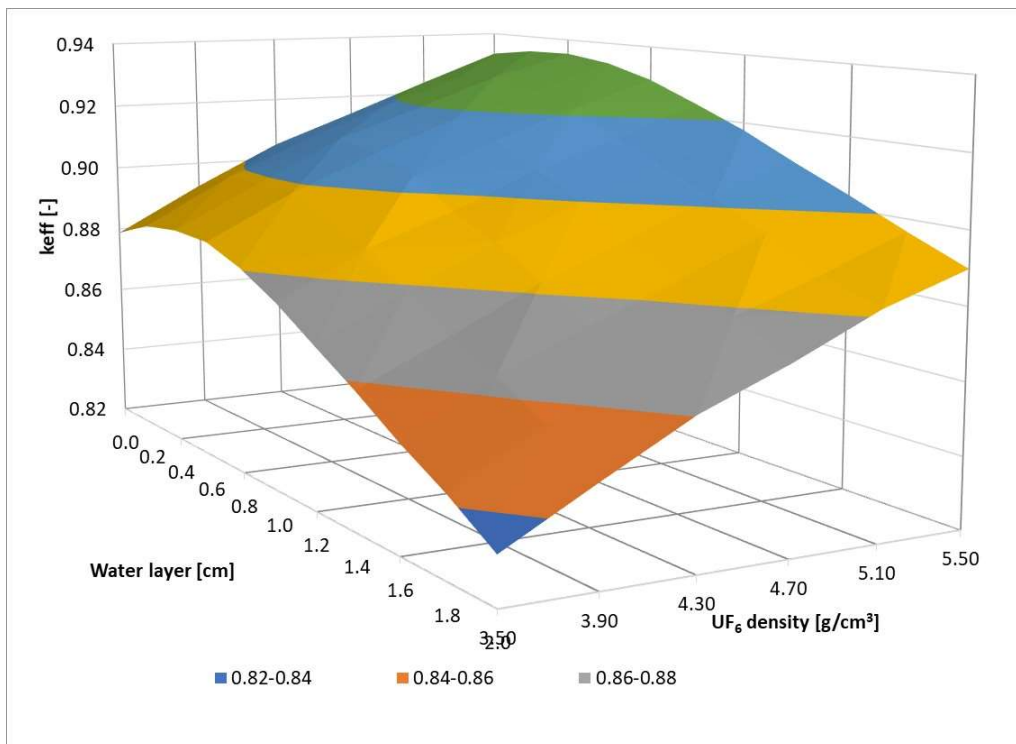


Figure 43. DN-30 3 x 2 HAC array k_{eff} .

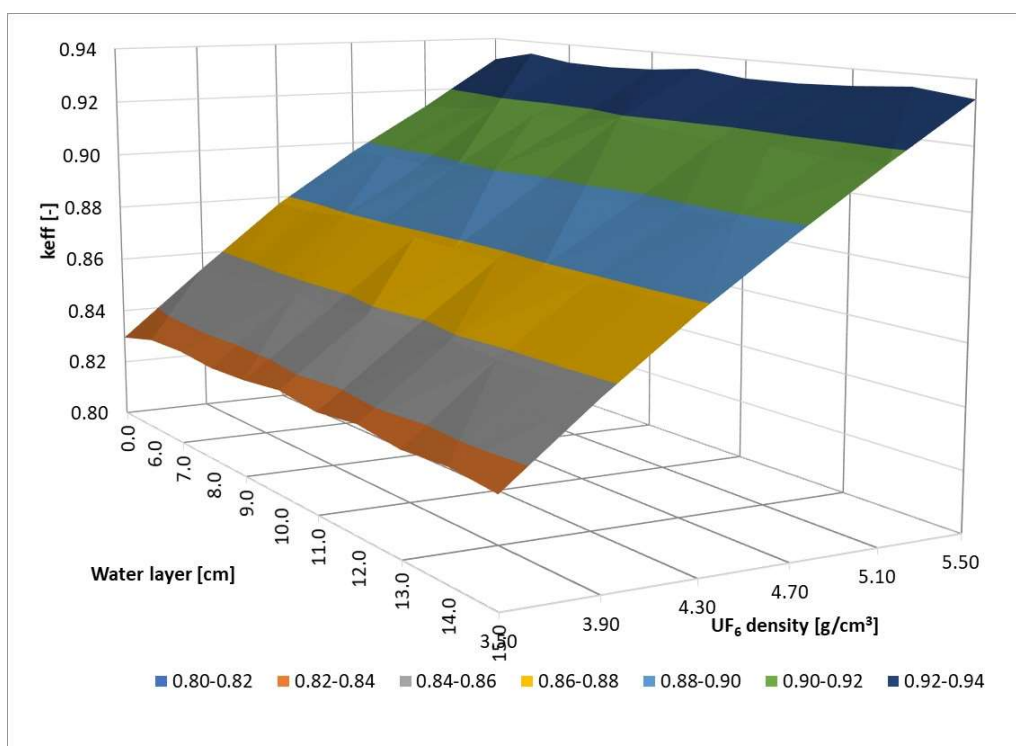


Figure 44. DN-30 HAC single package k_{eff} .

Table 27. DN-30 model enrichment and array size.

Enrichment (wt.% ^{235}U)	HAC array size	1/array size	k_{eff}	EALF (eV)
5	Infinite	0	0.9353 ± 0.00048	45.2
5.8	7×2	0.1	0.9354 ± 0.00049	36.5
6.7	3×2	0.2	0.9350 ± 0.00048	33.2
9.5	1×2	0.5	0.9350 ± 0.00048	69.4
12.5	1×1	1.0	0.9360 ± 0.00048	123.9

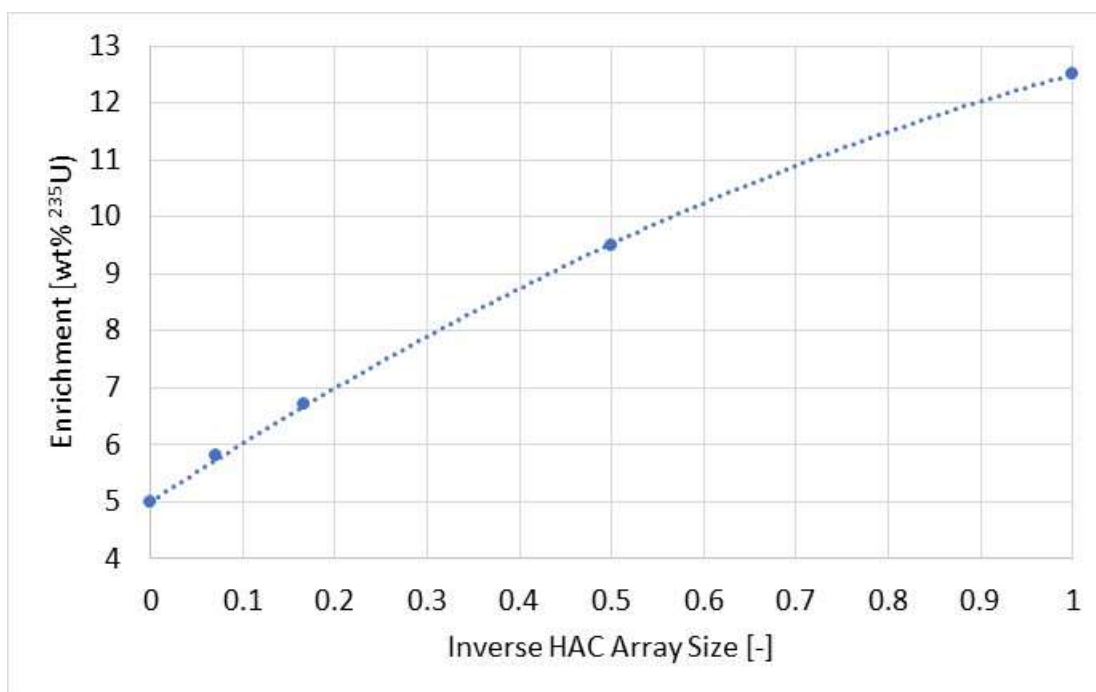


Figure 45. DN-30 model enrichment and array size.

6.4 DN-30 TSUNAMI-3D Calculations

TSUNAMI-3D S/U calculations were performed for three cases from Table 27. Table 28 shows key TSUNAMI input values, forward and adjoint k_{eff} , the energy of the average lethargy of fission, and total cross section uncertainty.

Table 26. DN-30 HAC model TSUNAMI-3D case data.

Parameter	5.0 wt.%, infinite package array	6.7 wt.%, 3 × 2 package array	12.5 wt.%, single package
Grid mesh	40 × 40 × 55	46 × 46 × 36	46 × 46 × 56
Particles/gen.	50,000 fwd. / 300,000 adj.	50,000 fwd. / 250,000 adj.	50,000 fwd. / 300,000 adj.
SDF file name	T3D dn30 hac inf 5wt	T3D dn30 hac 3x2 6-7wt	T3D dn30 hac sgl 12-5wt
Forward k_{eff}	0.93513 ± 0.00031	0.93542 ± 0.00029	0.93229 ± 0.00049
Adjoint k_{eff}	0.9333 ± 0.0014	0.9362 ± 0.0014	0.9346 ± 0.0014
EALF	51.5 eV	34.5 eV	155.1 eV
Cross section uncertainty	0.660% $\Delta k/k$	0.676% $\Delta k/k$	0.915% $\Delta k/k$

The adequacy of the TSUNAMI input is confirmed by comparing TSUNAMI-calculated nuclide sensitivity with KENO DP sensitivity. Figures 46, 47, and 48 summarize the sensitivity results calculated by each method for the highest sensitivity nuclide/region combinations. There is good agreement between the DP and TSUNAMI sensitivities, which confirms that the TSUNAMI SDFs properly represent the models. HUR is a high-sensitivity material in all three models.

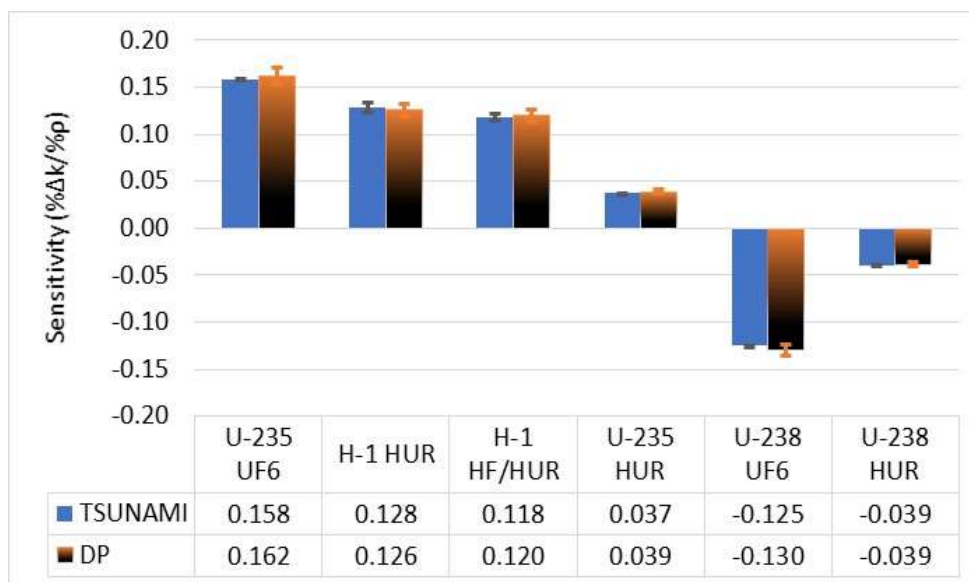


Figure 46. DN-30 model sensitivity (5 wt.%, infinite array).

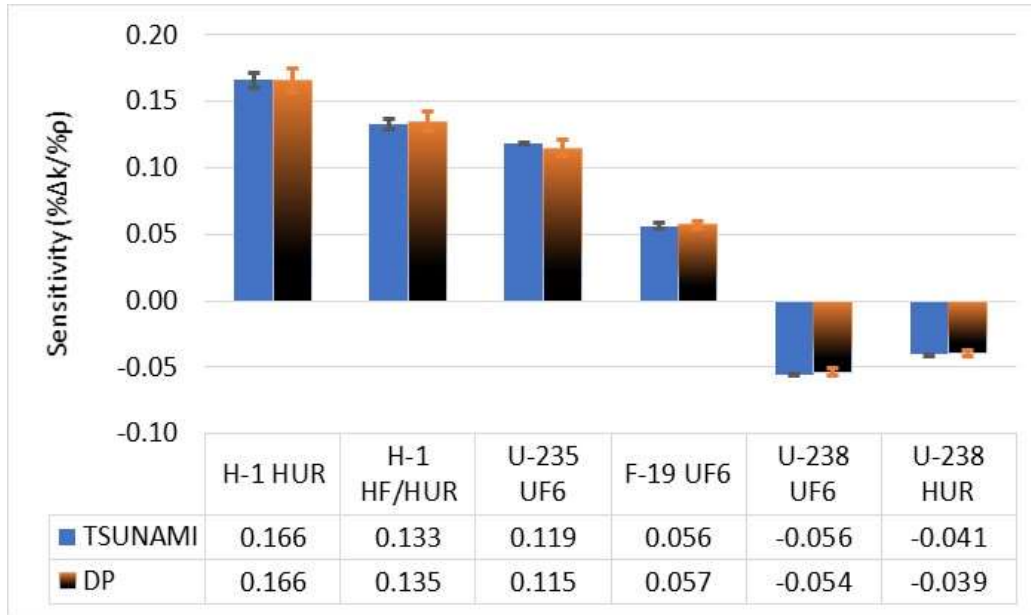


Figure 47. DN-30 model sensitivity (6.7 wt.%, 3×2 array).

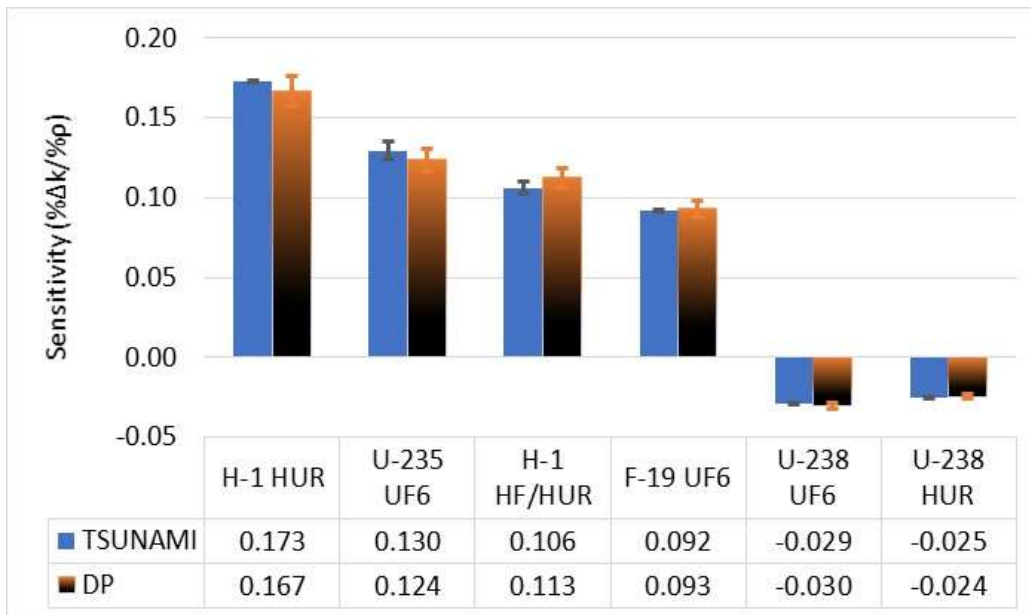


Figure 48. DN-30 model sensitivity (12.5 wt.%, single package).

Table 29 lists the sensitivity for each mixture in each model. Values greater than $0.01 \text{ } \Delta k / \% \Sigma$ are highlighted. The importance of HUR stands out (mixtures 6, 7, and 8). The importance of moderation provided by the 0.5 wt.% HF impurity in the UF_6 increases strongly with increasing enrichment (mixture 1).

Table 27. DN-30 model sensitivity by mixture.

Mixture	Description	5.0 wt.%, infinite package array		6.7 wt.%, 3 × 2 package array		12.5 wt.%, single package	
		Sensitivity	% std. dev.	Sensitivity	% std. dev.	Sensitivity	% std. dev.
1	UF ₆ /HF	0.040	3.0%	0.127	0.8%	0.205	0.5%
2	30B steel	-0.023	1.7%	-0.016	1.7%	-0.018	1.2%
3	H ₂ O layer	0.004	15.6%	0.004	15.4%	0.016	16.0%
4	H ₂ O reflector	N/A	N/A	0.000	N/A	0.000	N/A
5	PSP 304 SS	-0.018	1.7%	-0.005	3.7%	0.000	N/A
6	HUR	0.136	2.0%	0.178	1.7%	0.196	1.5%
7	UF ₆ /HF (HUR)	0.016	4.2%	0.027	2.6%	0.042	1.6%
8	HF (HUR)	0.128	1.6%	0.146	1.3%	0.123	1.3%

6.5 DN-30 Model TSUNAMI-IP Results

TSUNAMI-IP was used to calculate correlation coefficients (c_k) for the three SDF files in Table 28 and the library of 1,584 critical experiment SDF files. The 5 wt.% case serves as a reference point for comparison with higher enrichment results. Figures 49, 50, and 51 show the similarity coefficients with different symbols representing different types of experiments.

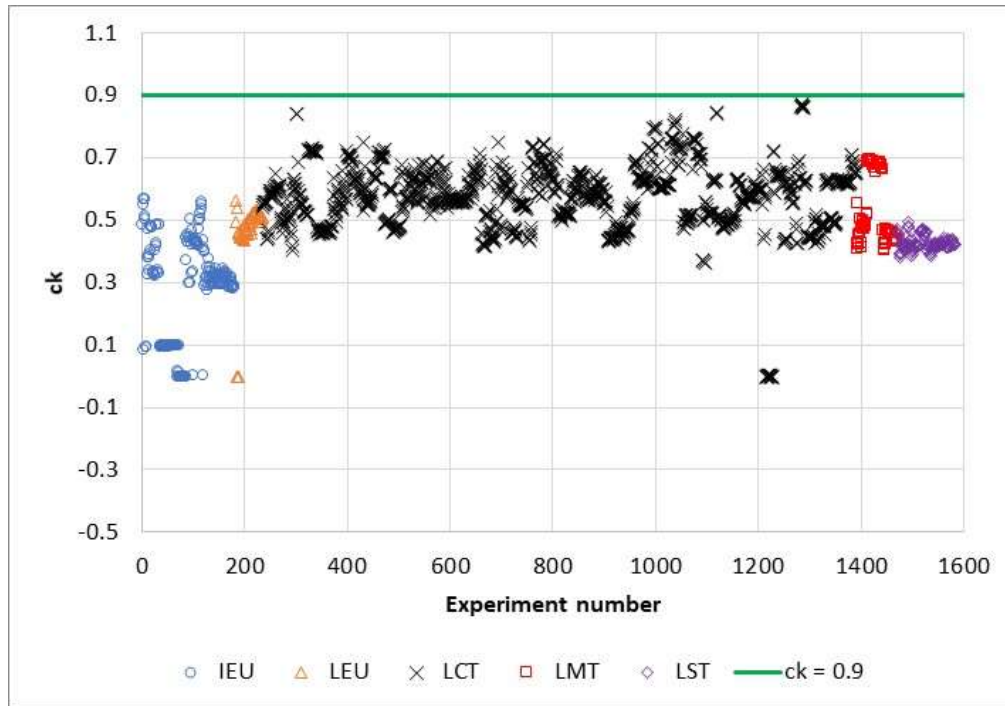


Figure 49. DN-30 c_k for 5 wt.% UF₆ (infinite HAC array).

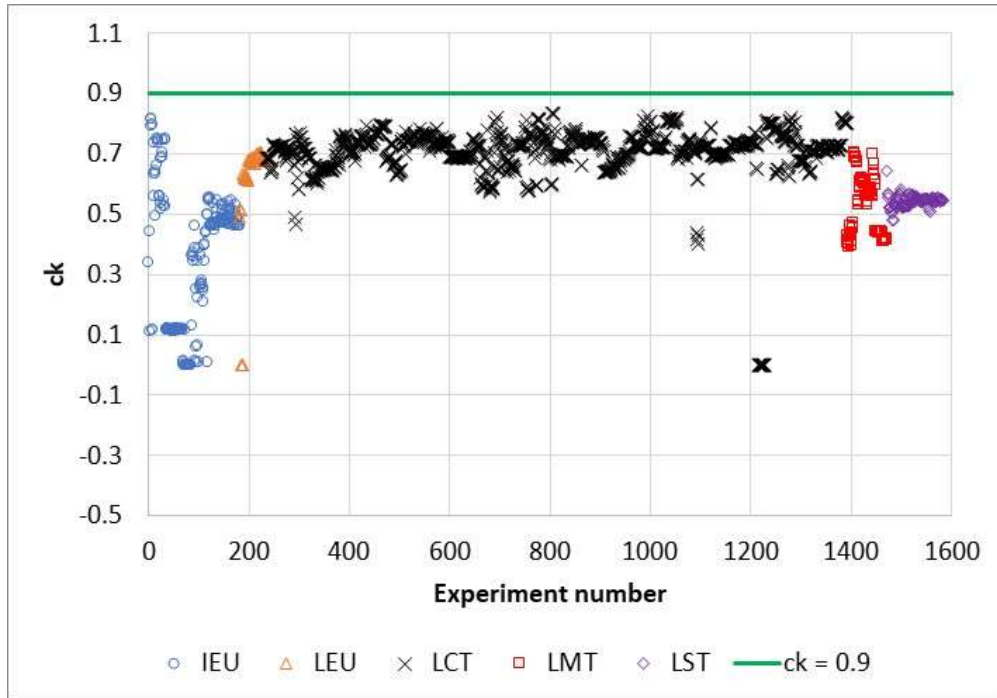


Figure 40. DN-30 ck for 6.7 wt.% UF_6 (3 x 2 HAC array).

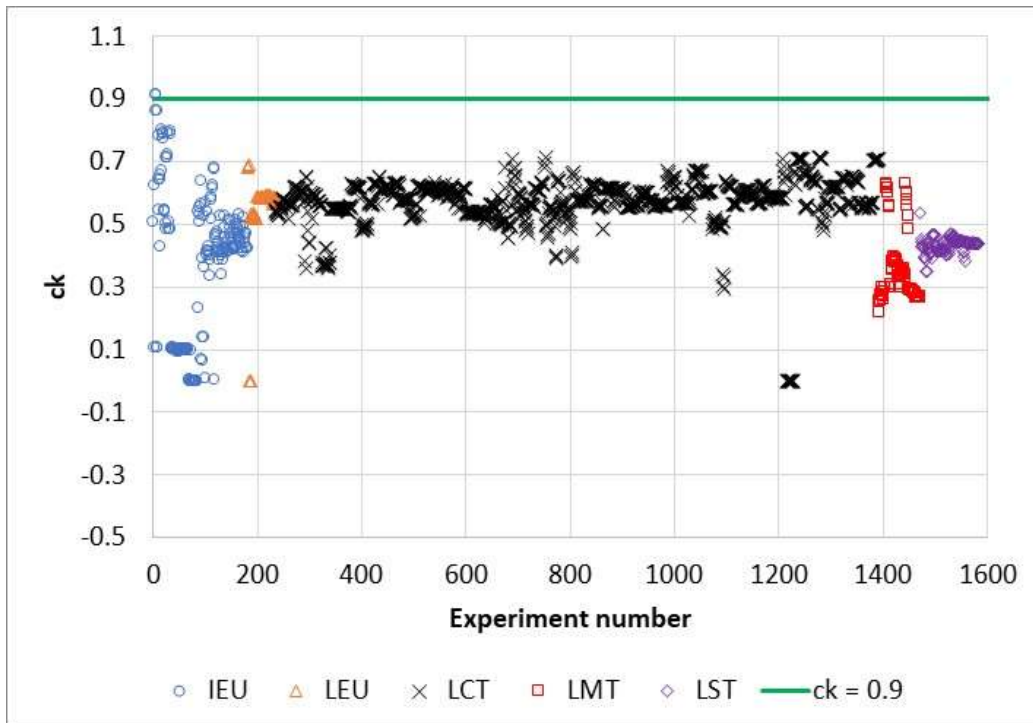


Figure 41. DN-30 ck for 12.5 wt.% UF_6 (single package).

Table 30 shows the number of experiments in each category with $c_k \geq 0.9$ and the median c_k for each of the DN-30 models. A full list of experiments with c_k values is provided in Appendix A. There are only two experiments with $c_k \geq 0.9$ for any of the three DN-30 models. Only the 3×2 6.7 wt.% model has a reasonable number of validation candidates (66) with $c_k \geq 0.8$. The median c_k is also much higher for that enrichment/array size combination. Similarity decreases with increasing enrichment and increases with decreasing array size. Appendix C has an expanded discussion of the trend of similarity with array size.

Table 30. DN-30 model TSUNAMI-IP similarity summary.

Category	5.0 wt.%, infinite package array	6.7 wt.%, 3×2 package array	12.5 wt.%, single package
IEU $c_k \geq 0.9$	0	0	2
LEU $c_k \geq 0.9$	0	0	0
LCT $c_k \geq 0.9$	0	0	0
LMT $c_k \geq 0.9$	0	0	0
LST $c_k \geq 0.9$	0	0	0
IEU $c_k \geq 0.8$	0	2	5
LEU $c_k \geq 0.8$	0	0	0
LCT $c_k \geq 0.8$	15	66	0
LMT $c_k \geq 0.8$	0	0	0
LST $c_k \geq 0.8$	0	0	0
Median c_k	0.548	0.699	0.567

The lack of experiments with a c_k value in excess of 0.8 does not mean that a validation is impossible; a validation must be performed for all computed analysis results. The lack of highly applicable experiments indicates that the bias resulting from these benchmarks might not be highly representative of the bias for the application system. The solution to this is to apply an additional reactivity margin to ensure that the aggregate margin included in the bias, bias uncertainty, and additional margin conservatively represents the bias that is expected for the application. S/U techniques provide tools for generating a quantitative, defensible estimate of what an appropriate margin might be.

Examining the nuclides and reactions that contribute significantly to data-induced uncertainty will indicate the important processes to be validated. Some elements, such as F, might be entirely absent from the validation set or only poorly represented. For these nuclides, the data-induced uncertainty can provide an estimate for the magnitude of the bias that occurs in the application. This approach is essentially the same as that used in several other works [23, 24, 25].

In other cases, important nuclides will be present in the validation suite, but the energy-dependent sensitivity profiles will differ significantly. These profiles can be reviewed to determine whether validation exists for an energy range or perhaps multiple energy ranges. For example, it might be evident that high-energy cross sections are validated because fission neutrons are born at high energies in all systems. Thermal cross sections are generally well-validated due to the many available thermal benchmark experiments. Therefore, an estimate of the unvalidated portion of the profile can be generated and used to estimate the magnitude of the remaining potential bias in the application in the energy ranges with weaker validation. In some cases, an energy range in the application might have significantly less sensitivity than is present in relevant benchmarks. An additional margin for these situations is likely not needed because the low sensitivity directly indicates a low potential for bias. The margin estimates generated for the partially validated nuclides are likely to be less precise than those resulting from an entirely unrepresented nuclide and thus should be developed with some deliberate conservatism.

Overall, this approach is similar to the PENALTY assessment in TSUNAMI-IP [26], but it does not necessarily give credit for single experiments that cover an energy range. This option might still be useful as a reference value. The magnitude of the data-induced uncertainty in the application also provides a bound on the estimated magnitude of the bias given no applicable benchmarks. Using this value might be more efficient than investing effort in developing and defending a lower additional margin.

7. CONCLUSIONS

A criticality assessment of five representative transportation packages was performed to determine whether existing package designs can be used to transport unirradiated increased enrichment (within the HALEU range) LWR fuel materials of different forms. The following representative packages were evaluated:

- 1) Traveller (PWR fuel assemblies, PWR and BWR fuel pins),
- 2) CHT-OP-TU (UO₂ powder and pellets),
- 3) VersaPac (U-metal/TRISO),
- 4) TN-B1 (BWR fuel assemblies), and
- 5) DN-30 (UF₆)

The results provided for each package evaluation include enrichment and packaging limits (e.g., maximum HAC package array size as a function of enrichment) and the identification of benchmark critical experiments that are appropriate candidates for use in computer code validation (determination of k_{eff} bias and bias uncertainty for the application).

Table 31 summarizes the range of enrichment and transportation array size combinations that each design could support based on criticality calculations. In some cases, additional trade-off options to permit increased enrichment are indicated (i.e., increased Gd rod credit in BWR assemblies). These criticality analysis results indicate that there are viable means for increasing enrichments into the HALEU range across the spectrum of fuel forms with differing increase amounts available for different packages.

The Traveller package can support transportation of PWR and BWR UO₂ fuel rods up to 10 wt% in the rod pipe container. Determining an upper fuel assembly enrichment limit for the Traveller is difficult due to the complexity of the safety analysis, which covers numerous fuel designs and three versions of the package. Subcritical margin is relatively insensitive to package array size due to the use of Boral plates and polyethylene moderator blocks, which limit neutronic interaction between packages. The Traveller standard version could support transportation of 5.5 to 6.5 wt% ²³⁵U (assembly average) PWR fuel assemblies for some fuel designs through a combination of transportation array size limits and safety analysis margin harvesting. In addition, maximum enrichment can be increased by crediting minimum integral poisons in the fuel assembly, similar to the TN-B1 BWR assembly package. Numerous critical experiment candidates are available for validation of 5 to 8 wt% ²³⁵U Traveller models.

The CHT-OP-TU package can be configured to transport up to 18 wt% UO₂ powder and up to 16.5 wt% UO₂ pellets through a combination of oxide vessel diameter and package array size. Numerous critical experiment candidates are available for validation of 5 to 16.5 wt% ²³⁵U CHT-OP-TU models.

The Versa-Pac package is currently licensed to transport U materials enriched up to 100% ²³⁵U with a ²³⁵U content maximum allowed mass determined by enrichment bin and packaging type. Because the Versa-Pac is already licensed to transport HALEU and has mass limits that are a function of enrichment, no additional evaluation was performed.

The TN-B1 package can support transportation of BWR fuel assemblies up to 10 wt% (assembly average) using a combination of package array size and gadolinia rod credit. Subcritical margin is highly sensitive to package array size in the un-poisoned TN-B1. Numerous critical experiment candidates were identified for validation of 5 to 8 wt% ²³⁵U TN-B1 models.

The DN-30 package can support transportation of UF₆ up to 9.5 wt% by reducing transportation array size from unlimited (5 wt% ²³⁵U) to 2 packages (9.5 wt% ²³⁵U). These results are based on retaining the 10

CFR 71.55(b) exemption from the assumption of water leakage into the containment system. Because the limiting accident conditions do not include water in-leakage, the neutron energy spectrum of the DN-30 is harder than other evaluated packages and only a few critical experiments were identified with a similarity index (c_k) of 0.8 or higher. Discussion of methods for validation penalty assessment is provided in the DN-30 analysis.

Table 31. Package array criticality summary.

Package	Fuel form	Enrichment (wt.% ^{235}U)	HAC array size	Notes
Traveller	PWR FA ¹	5	Varies	Current limit.
Traveller	PWR FA ¹	~6	Small	Enrichment increases ~0.5% with array size halved. Additional margin is available for some fuel designs and package versions.
Traveller	PWR FA ¹	~7	1	Approximate limit for a single package without additional margin credit.
Traveller	PWR FA ¹	8	Large	Same array size as for the current limit with credit for 52 IFBA per fuel assembly.
Traveller	PWR/BWR fuel pins	>10	Infinite	Additional margin is available to support higher enrichment.
CHT-OP-TU	UO ₂ powder	5	50	Current limit, 8 in. pipe.
CHT-OP-TU	UO ₂ powder	8	18	7.5 in. pipe.
CHT-OP-TU	UO ₂ powder	18	48	6 in. pipe.
CHT-OP-TU	UO ₂ pellets	5	50	Current limit, 7.5 in. pipe.
CHT-OP-TU	UO ₂ pellets	6.9	18	7.5 in. pipe.
CHT-OP-TU	UO ₂ pellets	16.5	48	6 in. pipe.
Versa-Pac	Multiple	10	100	55 gal drum, 5 in. pipe, 1,605 g ^{235}U .
Versa-Pac	Multiple	20	100	55 gal drum, 5 in. pipe, 1,215 g ^{235}U .
TN-B1	BWR FA ²	5	100	Current limit, 13 Gd rods/assembly.
TN-B1	BWR FA ²	6	49	13 Gd rods/assembly.
TN-B1	BWR FA ²	7.8	25	13 Gd rods/assembly.
TN-B1	BWR FA ²	9.8	16	13 Gd rods/assembly.
TN-B1	BWR FA ²	8	100	24 Gd rods/assembly.
DN-30	UF ₆	5	Infinite	Current limit. Few benchmark candidates.
DN-30	UF ₆	6.7	6	HUR sphere governs.
DN-30	UF ₆	12.5	1	HUR sphere governs. Few benchmark candidates.

¹PWR FA = PWR fuel assembly, one per package, assembly average enrichment

²BWR FA = BWR fuel assemblies, two per package, assembly average enrichment

Appendix A summarizes the results of similarity calculations for representative cases from four of the five package designs; the Versa-Pac is already licensed for enrichments up to 100%. Color-coding identifies critical experiments that are similar (green, $c_k \geq 0.9$) and that are marginally similar (yellow, $c_k \geq 0.8$). These experiments are considered valid candidates for criticality code validation for the analyzed packages at limiting conditions, subject to further screening based on the appropriateness of materials and geometry. Numerous experiments are indicted by c_k to be generally applicable across the range of analyzed packages.

Appendix B addresses the effect of using multiple vs. single water compositions on c_k . Appendix C investigates the effect of array size on benchmark experiment similarity.

ACKNOWLEDGMENTS

Support for this work was provided by the NRC Office of Nuclear Regulatory Research and the Office of Nuclear Material Safety and Safeguards. The authors would like to thank many ORNL staff members for their feedback on the contents and presentation in this report.

REFERENCES

- [1] M. Diaz, 2019, DSFM Regulatory Conference, “Advanced Fuels Update on the Front End of the Fuel Cycle,” <https://www.nrc.gov/docs/ML1925/ML19255F598.pdf>.
- [2] F. Pimental et al., “The Economic Benefits and Challenges with Utilizing Increased Enrichment and Fuel Burnup for Light-Water Reactors,” Nuclear Energy Institute (2019).
- [3] B. T. Rearden and M. A. Jessee, *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.3, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2018).
- [4] B. T. Rearden et al., “Sensitivity and Uncertainty Analysis Capabilities and Data in SCALE,” *Nucl. Technol.* 174, 236–288 (2011).
- [5] Westinghouse Electric Company, “Application for Certificate of Compliance for the Traveller PWR Fuel Shipping Package,” NRC ADAMS ML 19098A933 (Safety Analysis Report Revision 14) (2019).
- [6] US NRC, Certificate of Compliance 9297, Revision 11 (2019).
- [7] Columbiana Hi Tech, LLC, *Safety Analysis Report for the Model CHT OP-TU*, Revision 7 (2006).
- [8] US NRC, Certificate of Compliance 9288, Revision 11 (2018).
- [9] Daher-TLI, *Versa-Pac Safety Analysis Report*, Rev. 10, ADAMS Accession number ML18087A454 (2018).
- [10] US NRC, Certificate of Compliance 9342, Revision 15 (2020).
- [11] Framatome, Inc., *Framatome TN-B1 Safety Analysis Report*, Rev. 9, ADAMS Accession number ML19045A485 (2019).
- [12] US NRC, Certificate of Compliance 9372, Revision 2 (2019).
- [13] Daher-TLI, *Safety Analysis Report of the DN30 Package*, Rev. 3, ADAMS Accession number ML19200A133 (2019).
- [14] US NRC, Certificate of Compliance 9362, Revision 2 (2019).
- [15] J. M. Scaglione, D. E. Mueller, J. C. Wagner, and W. J. Marshall, *An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses—Criticality (keff) Predictions*, NUREG/CR-7109 (ORNL/TM-2011/514), Oak Ridge National Laboratory, Oak Ridge, Tennessee (2012).
- [16] B. L. Broadhead et al., “Sensitivity- and Uncertainty-Based Criticality Safety Validation Techniques,” *Nucl. Sci. Eng.* 146, 340–366 (2004).
- [17] *International Criticality Safety Benchmark Evaluation Project ICSBEP Handbook*, NEA/NSC/DOC(95)03, Organisation for Economic Co-Operation and Development /Nuclear Energy Agency (2019).
- [18] W. J. Marshall and B. T. Rearden, “The SCALE Verified, Archived Library of Inputs and Data – VALID,” ANS Nuclear Criticality Safety Division Topical Meetings (NCSD2013), Wilmington, North Carolina (2013).
- [19] J. B. Clarity, W. J. Marshall, and E. M. Saylor, “User Experiences with ICSBEP Distributed Sensitivity Data Profiles with the SCALE Sensitivity and Uncertainty Methods as of Winter 2019,” Data, Analysis and Operations in Nuclear Criticality Safety-III (2019).
- [20] 10 CFR 71, NRC Regulations, *Packaging and Transportation of Radioactive Material*.

- [21] W.C. Jordan J.C. Turner, *Estimated Critical Conditions for UO_2F_2 - H_2O Systems in Fully Water-Reflected Spherical Geometry*, ORNL/TM-12292 (1992)
- [22] L. Begue et al., “Criticality Safety of Enriched UF6 Cylinders.” *Proceedings of the 17th International Symposium on the Packaging and Transportation of Radioactive Materials* (2013).
- [23] J. M. Scaglione, D. E. Mueller, J. C. Wagner, and W. J. Marshall, *An Approach for Validating Actinide and Fission Product Burnup Credit Criticality Safety Analyses-Criticality (k_{eff}) Predictions*, NUREG/CR 7109 (ORNL/TM-2011/514), Oak Ridge, Tennessee (2012).
- [24] W. J. Marshall, B. J. Ade, S. M. Bowman, I. C. Gauld, G. Ilas, U. Mertuyrek, and G. Radulescu, *Technical Basis for Peak Reactivity Burnup Credit for BWR Spent Nuclear Fuel in Storage and Transportation Systems*, NUREG/CR-7194 (ORNL/TM-2014/240), Oak Ridge, Tennessee (2015).
- [25] W. J. Marshall, J. B. Clarity, and S. M. Bowman, *Validation of k_{eff} Calculations for Extended BWR Burnup Credit*, NUREG/CR-7252 (ORNL/TM-2018/797), Oak Ridge, Tennessee (2018).
- [26] B. T. Rearden, M. L. Williams, M. A. Jessee, D. E. Mueller, and D. A. Wiarda, “Sensitivity and Uncertainty Analysis Capabilities and Data in SCALE,” *Nucl. Technol.* 174, 236–288 (2011).
- [27] “DN30 Package,” Daher Nuclear Technologies; <https://daher-nuclear-technologies.com/en/dn30-package> (current as of Nov. 4, 2020).

APPENDIX A. BENCHMARK EXPERIMENT SIMILARITY TABLE

Appendix A summarizes the results of similarity calculations for representative cases from four of the five package designs. Table A-1 contains the column code index descriptions. Cells highlighted yellow have $c_k \geq 0.8$. Cells highlighted green have $c_k \geq 0.9$.

Table A-1. Similarity table package number description.

Package #	Package description	Enrichment (wt% 235U)	# Packages	Type
1	Traveller fuel assembly (17x17)	5	Infinite	PWR FA
2	Traveller fuel assembly	8	1	PWR FA
3	Traveller fuel assembly, 54 IFBA / FA	8	Infinite	PWR FA
4	Traveller rod pipe	5	Infinite	Pins
5	Traveller rod pipe	10	Infinite	Pins
6	CHT-OP-TU UO2 powder	5	48	Powder
7	CHT-OP-TU UO2 powder	8	18	Powder
8	CHT-OP-TU UO2 pellets	6.9	18	Pellets
9	CHT-OP-TU UO2 pellets	16.5	48	Pellets
10	TN-B1 BWR FA (11x11, 13 Gd rods/FA)	5	100	BWR FA
11	TN-B1 BWR FA (11x11, 13 Gd rods/FA)	6.7	36	BWR FA
12	TN-B1 BWR FA (11x11, 24 Gd rods/FA)	8	100	BWR FA
13	DX-30 UF6 in 30B (mod exclusion)	5	Infinite	UF6
14	DX-30 UF6 in 30B (mod exclusion)	6.7	6	UF6
15	DX-30 UF6 in 30B (optimum mod)	12.5	1	UF6

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	IEU-COMP-FAST-004-001_E	-0.14	-0.18	-0.09	-0.20	-0.17	-0.10	-0.12	-0.12	-0.07	0.00	-0.04	0.05	0.49	0.34	0.51
2	IEU-COMP-INTER-005-001_	-0.02	-0.05	0.02	-0.08	-0.05	-0.01	-0.01	0.00	0.03	0.07	0.05	0.12	0.55	0.44	0.62
3	IEU-COMP-INTER-006-001_	0.26	0.29	0.26	0.25	0.24	0.20	0.23	0.23	0.22	0.13	0.17	0.12	0.09	0.11	0.11
4	IEU-COMP-MIXED-001-001_	0.68	0.72	0.71	0.68	0.71	0.60	0.66	0.66	0.65	0.54	0.64	0.58	0.57	0.82	0.91
5	IEU-COMP-MIXED-001-017_	0.71	0.76	0.74	0.73	0.75	0.63	0.70	0.70	0.68	0.54	0.65	0.57	0.50	0.79	0.86
6	IEU-COMP-MIXED-001-021_	0.68	0.72	0.72	0.69	0.71	0.60	0.66	0.67	0.66	0.54	0.64	0.58	0.57	0.81	0.91
7	IEU-COMP-MIXED-001-022_	0.73	0.77	0.75	0.75	0.77	0.65	0.71	0.71	0.70	0.56	0.67	0.59	0.51	0.80	0.86
8	IEU-COMP-MIXED-004-004_	0.27	0.28	0.25	0.27	0.26	0.23	0.23	0.24	0.22	0.18	0.20	0.16	0.10	0.12	0.11
9	IEU-COMP-MIXED-004-005_	0.27	0.27	0.25	0.27	0.26	0.23	0.23	0.24	0.22	0.18	0.20	0.16	0.10	0.12	0.11
10	IEU-COMP-THERM-001-002_	0.76	0.82	0.79	0.80	0.83	0.70	0.77	0.76	0.76	0.59	0.71	0.62	0.47	0.74	0.79
11	IEU-COMP-THERM-001-003_	0.77	0.84	0.79	0.84	0.87	0.72	0.81	0.77	0.79	0.60	0.72	0.62	0.38	0.64	0.64
12	IEU-COMP-THERM-001-004_	0.75	0.83	0.76	0.83	0.86	0.72	0.80	0.76	0.79	0.59	0.71	0.61	0.33	0.56	0.55
13	IEU-COMP-THERM-001-005_	0.69	0.72	0.70	0.72	0.75	0.69	0.74	0.70	0.72	0.63	0.71	0.64	0.34	0.49	0.43
14	IEU-COMP-THERM-001-006_	0.77	0.84	0.79	0.84	0.87	0.72	0.80	0.77	0.79	0.60	0.72	0.62	0.38	0.64	0.65
15	IEU-COMP-THERM-001-007_	0.77	0.84	0.79	0.84	0.87	0.72	0.80	0.77	0.79	0.60	0.73	0.63	0.39	0.65	0.66
16	IEU-COMP-THERM-001-008_	0.78	0.84	0.79	0.83	0.86	0.72	0.80	0.78	0.79	0.61	0.73	0.63	0.40	0.66	0.67
17	IEU-COMP-THERM-001-009_	0.76	0.81	0.78	0.79	0.82	0.69	0.76	0.75	0.75	0.60	0.71	0.63	0.48	0.75	0.80
18	IEU-COMP-THERM-001-010_	0.77	0.82	0.79	0.80	0.83	0.70	0.77	0.76	0.76	0.60	0.72	0.63	0.48	0.75	0.79
19	IEU-COMP-THERM-001-011_	0.77	0.83	0.79	0.81	0.83	0.70	0.78	0.76	0.76	0.60	0.72	0.63	0.48	0.74	0.79
20	IEU-COMP-THERM-001-012_	0.77	0.83	0.80	0.81	0.84	0.71	0.78	0.76	0.77	0.61	0.73	0.64	0.48	0.74	0.78
21	IEU-COMP-THERM-001-013_	0.75	0.83	0.76	0.83	0.86	0.72	0.80	0.76	0.79	0.59	0.71	0.61	0.33	0.56	0.55
22	IEU-COMP-THERM-001-014_	0.75	0.83	0.76	0.83	0.86	0.72	0.80	0.76	0.79	0.59	0.71	0.61	0.33	0.56	0.54
23	IEU-COMP-THERM-001-015_	0.75	0.83	0.77	0.83	0.86	0.73	0.80	0.76	0.79	0.60	0.72	0.62	0.34	0.56	0.54
24	IEU-COMP-THERM-001-016_	0.73	0.79	0.74	0.79	0.83	0.72	0.78	0.74	0.77	0.61	0.71	0.62	0.32	0.52	0.48
25	IEU-COMP-THERM-001-018_	0.76	0.83	0.78	0.82	0.85	0.70	0.78	0.76	0.77	0.57	0.70	0.60	0.40	0.69	0.71
26	IEU-COMP-THERM-001-019_	0.74	0.80	0.75	0.81	0.84	0.72	0.79	0.75	0.78	0.60	0.71	0.62	0.33	0.54	0.51
27	IEU-COMP-THERM-001-020_	0.76	0.82	0.79	0.80	0.83	0.70	0.77	0.76	0.76	0.60	0.72	0.63	0.48	0.75	0.79
28	IEU-COMP-THERM-001-023_	0.77	0.84	0.79	0.83	0.85	0.71	0.79	0.77	0.78	0.59	0.72	0.62	0.42	0.69	0.71
29	IEU-COMP-THERM-001-024_	0.77	0.83	0.78	0.82	0.85	0.71	0.79	0.76	0.77	0.59	0.71	0.62	0.43	0.70	0.72
30	IEU-COMP-THERM-001-025_	0.74	0.80	0.75	0.80	0.84	0.73	0.80	0.75	0.78	0.62	0.73	0.63	0.34	0.54	0.51
31	IEU-COMP-THERM-001-026_	0.73	0.79	0.74	0.79	0.83	0.72	0.79	0.74	0.77	0.62	0.72	0.63	0.33	0.53	0.49
32	IEU-COMP-THERM-001-027_	0.73	0.79	0.74	0.79	0.83	0.72	0.79	0.74	0.77	0.62	0.72	0.63	0.33	0.53	0.49
33	IEU-COMP-THERM-001-028_	0.77	0.82	0.79	0.80	0.83	0.70	0.77	0.76	0.76	0.60	0.72	0.63	0.49	0.75	0.80
34	IEU-COMP-THERM-001-029_	0.77	0.83	0.80	0.81	0.83	0.70	0.78	0.76	0.76	0.61	0.72	0.64	0.48	0.75	0.79
35	IEU-COMP-THERM-015-002_	0.23	0.26	0.22	0.24	0.24	0.19	0.21	0.21	0.20	0.12	0.15	0.11	0.09	0.12	0.11
36	IEU-COMP-THERM-015-003_	0.22	0.24	0.21	0.24	0.23	0.18	0.21	0.21	0.19	0.12	0.15	0.11	0.09	0.12	0.10
37	IEU-COMP-THERM-015-006_	0.25	0.26	0.23	0.26	0.25	0.21	0.22	0.23	0.21	0.16	0.18	0.14	0.10	0.12	0.11
38	IEU-COMP-THERM-015-007_	0.25	0.26	0.23	0.26	0.25	0.22	0.22	0.23	0.21	0.17	0.19	0.15	0.10	0.12	0.11
39	IEU-COMP-THERM-015-008_	0.23	0.24	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.16	0.17	0.13	0.10	0.12	0.10
40	IEU-COMP-THERM-015-009_	0.23	0.24	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
41	IEU-COMP-THERM-015-010_	0.23	0.23	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.16	0.17	0.13	0.10	0.12	0.10
42	IEU-COMP-THERM-015-011_	0.22	0.22	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
43	IEU-COMP-THERM-015-012_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
44	IEU-COMP-THERM-015-013_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
45	IEU-COMP-THERM-015-014_	0.22	0.22	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.16	0.17	0.13	0.10	0.12	0.10
46	IEU-COMP-THERM-015-015_	0.22	0.22	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.16	0.17	0.13	0.10	0.12	0.10
47	IEU-COMP-THERM-015-016_	0.21	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.15	0.16	0.13	0.09	0.11	0.10
48	IEU-COMP-THERM-015-017_	0.21	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.15	0.16	0.13	0.09	0.11	0.10
49	IEU-COMP-THERM-015-018_	0.21	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.15	0.16	0.13	0.09	0.11	0.10
50	IEU-COMP-THERM-016-001_	0.23	0.24	0.22	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
51	IEU-COMP-THERM-016-002_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.21	0.19	0.15	0.16	0.13	0.10	0.12	0.10
52	IEU-COMP-THERM-016-003_	0.22	0.23	0.21	0.25	0.24	0.20	0.20	0.21	0.19	0.15	0.16	0.13	0.10	0.12	0.10
53	IEU-COMP-THERM-016-004_	0.22	0.23	0.21	0.25	0.24	0.20	0.20	0.21	0.19	0.15	0.17	0.13	0.10	0.12	0.10
54	IEU-COMP-THERM-016-005_	0.21	0.22	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.14	0.16	0.12	0.09	0.11	0.10
55	IEU-COMP-THERM-016-011_	0.23	0.24	0.22	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
56	IEU-COMP-THERM-016-012_	0.23	0.24	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
57	IEU-COMP-THERM-016-013_	0.23	0.24	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
58	IEU-COMP-THERM-016-014_	0.23	0.24	0.21	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
59	IEU-COMP-THERM-016-015_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
60	IEU-COMP-THERM-016-016_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
61	IEU-COMP-THERM-016-017_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
62	IEU-COMP-THERM-016-018_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
63	IEU-COMP-THERM-016-019_	0.20	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.15	0.16	0.12	0.10	0.12	0.10
64	IEU-COMP-THERM-016-020_	0.20	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.14	0.16	0.12	0.10	0.12	0.10
65	IEU-COMP-THERM-016-021_	0.23	0.23	0.21	0.25	0.24	0.20	0.21	0.21	0.19	0.15	0.17	0.13	0.10	0.12	0.10
66	IEU-COMP-THERM-016-022_	0.23	0.23	0.21	0.25	0.24	0.20	0.21	0.21	0.19	0.16	0.17	0.14	0.10	0.12	0.10
67	IEU-COMP-THERM-016-024_	0.23	0.24	0.22	0.25	0.24	0.20	0.21	0.21	0.20	0.15	0.17	0.13	0.10	0.12	0.10
68	IEU-COMP-THERM-016-025_	0.22	0.23	0.20	0.25	0.24	0.20	0.20	0.20	0.19	0.15	0.17	0.13	0.10	0.12	0.10
69	IEU-COMP-THERM-016-026_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
70	IEU-COMP-THERM-016-027_	0.00	0.00	0.00	0.05	0.05	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.02	0.01	0.01
71	IEU-COMP-THERM-016-028_	0.00	0.00	0.00	0.05	0.05	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.01	0.01	0.00
72	IEU-COMP-THERM-016-029_	0.21	0.21	0.19	0.24	0.23	0.19	0.19	0.19	0.18	0.14	0.16	0.12	0.10	0.12	0.10
73	IEU-COMP-THERM-016-031_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
74	IEU-COMP-THERM-016-032_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
75	IEU-COMP-THERM-016-033_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
76	IEU-COMP-THERM-016-034_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
77	IEU-COMP-THERM-016-035_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
78	IEU-COMP-THERM-016-036_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
79	IEU-COMP-THERM-016-037_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
80	IEU-COMP-THERM-016-038_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
81	IEU-COMP-THERM-016-039_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
82	IEU-COMP-THERM-016-040_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
83	IEU-COMP-THERM-016-041_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
84	IEU-COMP-THERM-016-042_	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
85	IEU-COMP-THERM-016-043_EN	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
86	IEU-MET-FAST-002-001_EN	-0.33	-0.40	-0.29	-0.41	-0.37	-0.24	-0.28	-0.30	-0.23	-0.10	-0.19	-0.07	0.37	0.13	0.23
87	IEU-MET-FAST-003-001_EN	-0.06	-0.12	-0.01	-0.15	-0.14	-0.08	-0.11	-0.07	-0.07	0.03	0.00	0.08	0.45	0.36	0.54
88	IEU-MET-FAST-004-001_EN	-0.05	-0.11	-0.01	-0.14	-0.13	-0.08	-0.09	-0.06	-0.06	0.03	0.00	0.08	0.45	0.37	0.55
89	IEU-MET-FAST-005-001_EN	-0.09	-0.14	-0.04	-0.13	-0.12	-0.05	-0.07	-0.04	-0.02	0.05	0.01	0.10	0.43	0.35	0.51
90	IEU-MET-FAST-006-001_EN	-0.03	-0.08	0.02	-0.12	-0.11	-0.06	-0.08	-0.05	-0.05	0.04	0.01	0.08	0.43	0.36	0.53
91	IEU-MET-FAST-007-001_EN	-0.41	-0.48	-0.38	-0.47	-0.43	-0.27	-0.33	-0.37	-0.27	-0.15	-0.25	-0.12	0.30	0.01	0.07
92	IEU-MET-FAST-008-001_EN	-0.02	-0.07	0.03	-0.11	-0.10	-0.06	-0.08	-0.04	-0.05	0.05	0.02	0.09	0.45	0.39	0.57
93	IEU-MET-FAST-009-001_EN	0.07	0.02	0.11	-0.02	-0.01	0.03	0.02	0.05	0.05	0.12	0.11	0.17	0.51	0.46	0.64
94	IEU-MET-FAST-010-001_EN	-0.41	-0.48	-0.39	-0.47	-0.42	-0.27	-0.32	-0.37	-0.26	-0.15	-0.25	-0.12	0.30	0.01	0.07
95	IEU-MET-FAST-012-001_EN	-0.23	-0.28	-0.19	-0.30	-0.26	-0.16	-0.19	-0.20	-0.13	-0.04	-0.11	0.00	0.45	0.25	0.39
96	IEU-MET-FAST-013-001_EN	-0.37	-0.44	-0.34	-0.44	-0.40	-0.25	-0.30	-0.34	-0.24	-0.13	-0.22	-0.10	0.33	0.06	0.14
97	IEU-MET-FAST-014-001_EN	-0.24	-0.29	-0.19	-0.31	-0.27	-0.17	-0.21	-0.22	-0.15	-0.05	-0.12	-0.02	0.42	0.23	0.36
98	IEU-MET-FAST-014-002_EN	-0.11	-0.14	-0.06	-0.18	-0.15	-0.09	-0.10	-0.10	-0.05	0.01	-0.03	0.05	0.47	0.34	0.53
99	IEU-MET-FAST-016-001_EN	-0.38	-0.45	-0.35	-0.44	-0.40	-0.26	-0.31	-0.34	-0.24	-0.13	-0.22	-0.10	0.34	0.06	0.14
100	IEU-MET-FAST-018-002_EN	0.00	0.00	0.00	0.05	0.05	0.02	0.03	0.03	0.03	0.03	0.03	0.03	0.00	0.01	0.01
101	IEU-MET-FAST-019-001_EN	-0.01	-0.06	0.04	-0.10	-0.09	-0.05	-0.07	-0.03	-0.04	0.05	0.03	0.10	0.44	0.39	0.57
102	IEU-MET-FAST-019-002_EN	-0.05	-0.11	-0.01	-0.15	-0.13	-0.08	-0.10	-0.07	-0.07	0.03	0.00	0.08	0.44	0.36	0.54
103	IEU-MET-FAST-020-001_EN	-0.20	-0.26	-0.16	-0.28	-0.24	-0.15	-0.18	-0.18	-0.13	-0.03	-0.09	0.01	0.43	0.26	0.40
104	IEU-MET-FAST-020-002_EN	-0.19	-0.24	-0.15	-0.26	-0.23	-0.14	-0.17	-0.17	-0.12	-0.03	-0.08	0.01	0.43	0.27	0.41
105	IEU-MET-FAST-020-003_EN	-0.19	-0.25	-0.15	-0.26	-0.23	-0.14	-0.17	-0.17	-0.12	-0.03	-0.09	0.01	0.43	0.26	0.41
106	IEU-MET-FAST-020-004_EN	-0.18	-0.23	-0.13	-0.25	-0.22	-0.13	-0.16	-0.16	-0.11	-0.02	-0.07	0.02	0.43	0.28	0.43
107	IEU-MET-FAST-020-005_EN	-0.19	-0.24	-0.14	-0.26	-0.23	-0.14	-0.17	-0.17	-0.11	-0.03	-0.08	0.02	0.43	0.27	0.42
108	IEU-MET-FAST-020-006_EN	-0.22	-0.27	-0.17	-0.29	-0.25	-0.16	-0.19	-0.19	-0.14	-0.04	-0.10	0.00	0.42	0.25	0.39
109	IEU-MET-FAST-020-007_EN	-0.20	-0.26	-0.16	-0.28	-0.25	-0.15	-0.18	-0.18	-0.13	-0.03	-0.09	0.01	0.43	0.26	0.40
110	IEU-MET-FAST-021-001_EN	-0.26	-0.33	-0.22	-0.34	-0.31	-0.19	-0.23	-0.24	-0.18	-0.06	-0.14	-0.03	0.42	0.21	0.34
111	IEU-MET-FAST-022-001_EN	-0.11	-0.15	-0.07	-0.18	-0.15	-0.09	-0.10	-0.10	-0.05	0.01	-0.03	0.06	0.47	0.34	0.52
112	IEU-MET-FAST-022-005_EN	-0.05	-0.09	-0.01	-0.12	-0.09	-0.04	-0.05	-0.04	-0.01	0.04	0.02	0.09	0.50	0.40	0.58
113	IEU-MET-FAST-022-006_EN	-0.05	-0.08	0.00	-0.11	-0.09	-0.04	-0.05	-0.04	-0.01	0.04	0.02	0.09	0.50	0.40	0.59
114	IEU-MET-FAST-022-007_EN	0.00	-0.03	0.05	-0.06	-0.04	0.00	0.00	0.01	0.04	0.08	0.06	0.13	0.52	0.44	0.62
115	IEU-MET-INTER-001-002_E	0.00	-0.04	0.05	-0.08	-0.05	0.00	-0.01	0.00	0.02	0.09	0.07	0.13	0.53	0.44	0.62
116	IEU-MET-INTER-001-003_E	0.08	0.04	0.13	0.01	0.03	0.06	0.06	0.08	0.09	0.14	0.13	0.19	0.56	0.50	0.68
117	IEU-MET-INTER-001-004_E	0.08	0.05	0.13	0.01	0.03	0.06	0.06	0.08	0.09	0.13	0.13	0.18	0.55	0.50	0.68
118	IEU-MET-MIXED-001-001_E	0.00	0.00	0.00	0.05	0.05	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.00	0.01	0.01
119	IEU-SOL-THERM-001-001_E	0.78	0.82	0.79	0.88	0.90	0.88	0.92	0.87	0.93	0.77	0.84	0.77	0.43	0.56	0.46
120	IEU-SOL-THERM-001-002_E	0.79	0.84	0.80	0.89	0.92	0.87	0.92	0.87	0.93	0.73	0.82	0.74	0.41	0.55	0.47
121	IEU-SOL-THERM-001-003_E	0.79	0.85	0.79	0.89	0.92	0.86	0.91	0.87	0.92	0.72	0.81	0.73	0.40	0.55	0.46
122	IEU-SOL-THERM-001-004_E	0.80	0.86	0.80	0.90	0.93	0.86	0.92	0.87	0.92	0.72	0.81	0.72	0.40	0.55	0.48
123	IEU-SOL-THERM-002-001_E	0.77	0.86	0.77	0.85	0.89	0.76	0.84	0.78	0.82	0.60	0.71	0.60	0.29	0.46	0.42
124	IEU-SOL-THERM-002-002_E	0.77	0.84	0.77	0.84	0.88	0.77	0.83	0.78	0.82	0.62	0.73	0.62	0.30	0.46	0.41
125	IEU-SOL-THERM-002-003_E	0.77	0.82	0.77	0.83	0.86	0.77	0.82	0.77	0.81	0.65	0.74	0.64	0.32	0.47	0.41
126	IEU-SOL-THERM-002-004_E	0.75	0.76	0.75	0.77	0.79	0.76	0.78	0.74	0.76	0.69	0.75	0.67	0.35	0.47	0.39

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
127	IEU-SOL-THERM-002-005_E	0.77	0.87	0.77	0.86	0.89	0.74	0.84	0.78	0.83	0.57	0.70	0.58	0.28	0.47	0.44
128	IEU-SOL-THERM-002-006_E	0.81	0.91	0.82	0.89	0.92	0.76	0.86	0.81	0.84	0.58	0.72	0.60	0.32	0.54	0.53
129	IEU-SOL-THERM-002-007_E	0.77	0.85	0.77	0.85	0.88	0.76	0.83	0.78	0.82	0.60	0.72	0.61	0.29	0.46	0.42
130	IEU-SOL-THERM-002-008_E	0.77	0.80	0.77	0.81	0.83	0.78	0.81	0.76	0.79	0.67	0.75	0.66	0.34	0.47	0.40
131	IEU-SOL-THERM-002-009_E	0.68	0.62	0.67	0.65	0.65	0.70	0.67	0.65	0.65	0.70	0.71	0.68	0.38	0.45	0.34
132	IEU-SOL-THERM-002-010_E	0.77	0.83	0.77	0.83	0.86	0.77	0.83	0.78	0.81	0.64	0.74	0.64	0.31	0.47	0.41
133	IEU-SOL-THERM-002-011_E	0.75	0.76	0.75	0.78	0.80	0.77	0.78	0.74	0.76	0.69	0.75	0.68	0.35	0.47	0.39
134	IEU-SOL-THERM-002-012_E	0.78	0.83	0.77	0.83	0.86	0.77	0.83	0.78	0.81	0.65	0.74	0.64	0.32	0.47	0.41
135	IEU-SOL-THERM-002-013_E	0.77	0.85	0.77	0.85	0.88	0.76	0.84	0.78	0.83	0.61	0.72	0.61	0.29	0.46	0.42
136	IEU-SOL-THERM-003-001_E	0.81	0.90	0.82	0.90	0.93	0.78	0.87	0.83	0.86	0.61	0.74	0.62	0.34	0.55	0.53
137	IEU-SOL-THERM-003-002_E	0.79	0.89	0.80	0.89	0.92	0.77	0.87	0.82	0.86	0.60	0.73	0.61	0.32	0.52	0.49
138	IEU-SOL-THERM-003-003_E	0.78	0.87	0.78	0.88	0.91	0.77	0.86	0.81	0.85	0.60	0.72	0.61	0.30	0.49	0.46
139	IEU-SOL-THERM-003-004_E	0.77	0.86	0.77	0.87	0.90	0.77	0.85	0.80	0.84	0.60	0.72	0.61	0.29	0.48	0.44
140	IEU-SOL-THERM-003-005_E	0.77	0.85	0.77	0.86	0.89	0.78	0.85	0.80	0.84	0.62	0.73	0.62	0.30	0.47	0.43
141	IEU-SOL-THERM-003-006_E	0.78	0.84	0.78	0.85	0.88	0.78	0.85	0.79	0.84	0.64	0.74	0.64	0.32	0.48	0.42
142	IEU-SOL-THERM-003-007_E	0.78	0.83	0.77	0.84	0.87	0.79	0.84	0.79	0.83	0.66	0.75	0.66	0.33	0.48	0.41
143	IEU-SOL-THERM-003-008_E	0.77	0.81	0.77	0.82	0.85	0.79	0.83	0.78	0.82	0.68	0.76	0.67	0.34	0.48	0.41
144	IEU-SOL-THERM-003-009_E	0.77	0.87	0.78	0.87	0.91	0.77	0.86	0.80	0.85	0.60	0.72	0.61	0.30	0.49	0.45
145	IEU-SOL-THERM-003-010_E	0.78	0.83	0.78	0.84	0.87	0.79	0.84	0.79	0.83	0.66	0.75	0.65	0.32	0.48	0.42
146	IEU-SOL-THERM-003-011_E	0.80	0.90	0.81	0.89	0.93	0.77	0.87	0.82	0.86	0.60	0.73	0.61	0.32	0.53	0.51
147	IEU-SOL-THERM-003-012_E	0.80	0.90	0.81	0.89	0.93	0.78	0.87	0.82	0.86	0.60	0.73	0.62	0.33	0.53	0.52
148	IEU-SOL-THERM-003-013_E	0.79	0.89	0.80	0.89	0.92	0.77	0.86	0.82	0.86	0.60	0.73	0.61	0.31	0.51	0.49
149	IEU-SOL-THERM-003-014_E	0.78	0.88	0.79	0.88	0.91	0.77	0.86	0.81	0.85	0.59	0.72	0.60	0.30	0.50	0.47
150	IEU-SOL-THERM-003-015_E	0.78	0.87	0.78	0.87	0.91	0.76	0.85	0.80	0.85	0.59	0.72	0.60	0.30	0.49	0.46
151	IEU-SOL-THERM-003-016_E	0.77	0.86	0.77	0.87	0.90	0.77	0.85	0.80	0.84	0.60	0.72	0.60	0.29	0.47	0.44
152	IEU-SOL-THERM-003-017_E	0.77	0.86	0.77	0.86	0.90	0.77	0.85	0.80	0.84	0.61	0.73	0.62	0.30	0.47	0.43
153	IEU-SOL-THERM-003-018_E	0.77	0.85	0.77	0.86	0.89	0.78	0.85	0.80	0.84	0.62	0.73	0.62	0.30	0.47	0.43
154	IEU-SOL-THERM-003-019_E	0.77	0.85	0.77	0.86	0.89	0.78	0.85	0.80	0.84	0.63	0.74	0.64	0.31	0.47	0.42
155	IEU-SOL-THERM-003-020_E	0.78	0.84	0.78	0.85	0.88	0.79	0.85	0.80	0.84	0.65	0.75	0.65	0.32	0.48	0.42
156	IEU-SOL-THERM-003-021_E	0.78	0.84	0.78	0.85	0.88	0.79	0.85	0.80	0.84	0.66	0.75	0.65	0.33	0.48	0.42
157	IEU-SOL-THERM-003-022_E	0.78	0.88	0.79	0.88	0.91	0.76	0.85	0.80	0.84	0.59	0.71	0.60	0.30	0.50	0.47
158	IEU-SOL-THERM-003-023_E	0.77	0.86	0.78	0.86	0.89	0.77	0.85	0.79	0.84	0.60	0.72	0.61	0.29	0.47	0.43
159	IEU-SOL-THERM-003-024_E	0.81	0.90	0.82	0.90	0.93	0.80	0.88	0.84	0.88	0.63	0.75	0.64	0.35	0.54	0.51
160	IEU-SOL-THERM-003-025_E	0.80	0.89	0.81	0.89	0.93	0.79	0.88	0.83	0.87	0.62	0.75	0.63	0.34	0.53	0.50
161	IEU-SOL-THERM-003-026_E	0.80	0.89	0.80	0.89	0.92	0.79	0.87	0.83	0.87	0.62	0.74	0.63	0.33	0.52	0.49
162	IEU-SOL-THERM-003-027_E	0.79	0.88	0.80	0.89	0.92	0.79	0.87	0.82	0.87	0.62	0.74	0.63	0.33	0.51	0.48
163	IEU-SOL-THERM-003-028_E	0.79	0.88	0.79	0.88	0.92	0.79	0.87	0.82	0.87	0.62	0.74	0.63	0.32	0.51	0.47
164	IEU-SOL-THERM-003-029_E	0.78	0.87	0.79	0.88	0.91	0.78	0.87	0.82	0.86	0.62	0.73	0.62	0.32	0.50	0.46
165	IEU-SOL-THERM-003-030_E	0.78	0.87	0.78	0.88	0.91	0.79	0.87	0.81	0.86	0.62	0.74	0.63	0.32	0.49	0.45
166	IEU-SOL-THERM-003-031_E	0.81	0.91	0.82	0.90	0.93	0.77	0.87	0.82	0.86	0.60	0.73	0.61	0.33	0.55	0.53
167	IEU-SOL-THERM-003-032_E	0.79	0.89	0.80	0.88	0.92	0.76	0.86	0.81	0.85	0.59	0.72	0.60	0.31	0.51	0.49
168	IEU-SOL-THERM-003-033_E	0.78	0.87	0.78	0.87	0.91	0.76	0.85	0.80	0.84	0.59	0.71	0.60	0.29	0.49	0.46

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
169	IEU-SOL-THERM-003-034_E	0.77	0.86	0.77	0.86	0.90	0.76	0.84	0.79	0.84	0.59	0.71	0.59	0.28	0.47	0.44
170	IEU-SOL-THERM-003-035_E	0.77	0.85	0.77	0.86	0.89	0.76	0.84	0.79	0.83	0.60	0.72	0.61	0.29	0.46	0.42
171	IEU-SOL-THERM-003-036_E	0.77	0.84	0.77	0.85	0.88	0.77	0.84	0.78	0.83	0.63	0.73	0.63	0.30	0.47	0.42
172	IEU-SOL-THERM-003-037_E	0.78	0.83	0.77	0.84	0.87	0.78	0.83	0.78	0.82	0.65	0.74	0.64	0.32	0.47	0.41
173	IEU-SOL-THERM-003-038_E	0.80	0.90	0.81	0.89	0.92	0.76	0.86	0.81	0.85	0.58	0.72	0.60	0.32	0.53	0.52
174	IEU-SOL-THERM-003-039_E	0.79	0.89	0.80	0.88	0.91	0.76	0.85	0.80	0.84	0.58	0.71	0.59	0.30	0.51	0.49
175	IEU-SOL-THERM-003-040_E	0.78	0.88	0.79	0.87	0.91	0.75	0.85	0.80	0.84	0.57	0.70	0.58	0.29	0.49	0.47
176	IEU-SOL-THERM-003-041_E	0.78	0.88	0.78	0.87	0.90	0.75	0.84	0.79	0.83	0.57	0.70	0.58	0.29	0.48	0.46
177	IEU-SOL-THERM-003-042_E	0.77	0.86	0.77	0.86	0.89	0.75	0.84	0.78	0.83	0.58	0.70	0.58	0.28	0.47	0.44
178	IEU-SOL-THERM-003-043_E	0.77	0.86	0.77	0.86	0.89	0.76	0.84	0.78	0.83	0.59	0.71	0.59	0.28	0.46	0.43
179	IEU-SOL-THERM-003-044_E	0.77	0.86	0.77	0.85	0.89	0.76	0.84	0.78	0.83	0.60	0.71	0.60	0.29	0.46	0.42
180	IEU-SOL-THERM-003-045_E	0.78	0.88	0.79	0.87	0.91	0.75	0.85	0.80	0.84	0.57	0.71	0.59	0.29	0.49	0.47
181	IEU-SOL-THERM-003-046_E	0.77	0.85	0.77	0.85	0.89	0.76	0.84	0.78	0.83	0.60	0.71	0.60	0.29	0.46	0.42
182	LEU-COMP-FAST-001-003_E	0.14	0.11	0.19	0.06	0.07	0.08	0.08	0.12	0.11	0.14	0.15	0.19	0.50	0.49	0.68
183	LEU-COMP-MIXED-001-001_E	0.15	0.10	0.20	0.05	0.06	0.10	0.09	0.12	0.11	0.18	0.18	0.23	0.56	0.52	0.69
184	LEU-COMP-MIXED-001-002_E	0.15	0.11	0.20	0.06	0.07	0.10	0.09	0.13	0.12	0.17	0.17	0.22	0.54	0.51	0.69
185	LEU-COMP-MIXED-002-001_E	0.03	0.03	0.03	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
186	LEU-COMP-MIXED-002-002_E	0.04	0.04	0.04	0.02	0.02	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
187	LEU-COMP-MIXED-002-003_E	0.05	0.05	0.05	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
188	LEU-COMP-THERM-001-001_E	0.96	0.90	0.94	0.89	0.87	0.90	0.89	0.89	0.81	0.85	0.90	0.82	0.54	0.68	0.55
189	LEU-COMP-THERM-001-002_E	0.95	0.88	0.93	0.88	0.85	0.89	0.88	0.88	0.80	0.86	0.90	0.83	0.55	0.69	0.54
190	LEU-COMP-THERM-001-003_E	0.94	0.87	0.92	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.68	0.54
191	LEU-COMP-THERM-001-004_E	0.95	0.88	0.93	0.88	0.85	0.89	0.87	0.88	0.80	0.86	0.90	0.83	0.55	0.69	0.54
192	LEU-COMP-THERM-001-005_E	0.94	0.86	0.92	0.86	0.83	0.89	0.86	0.87	0.78	0.86	0.90	0.83	0.56	0.68	0.53
193	LEU-COMP-THERM-001-006_E	0.95	0.87	0.93	0.87	0.85	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.68	0.54
194	LEU-COMP-THERM-001-007_E	0.93	0.86	0.91	0.86	0.83	0.89	0.86	0.86	0.78	0.86	0.90	0.83	0.56	0.68	0.53
195	LEU-COMP-THERM-001-008_E	0.94	0.86	0.92	0.86	0.84	0.89	0.86	0.87	0.78	0.86	0.90	0.83	0.56	0.68	0.53
196	LEU-COMP-THERM-002-001_E	0.96	0.97	0.95	0.95	0.95	0.89	0.92	0.91	0.86	0.78	0.88	0.77	0.44	0.64	0.55
197	LEU-COMP-THERM-002-002_E	0.96	0.96	0.95	0.95	0.95	0.89	0.92	0.91	0.86	0.79	0.88	0.77	0.44	0.64	0.55
198	LEU-COMP-THERM-002-003_E	0.96	0.96	0.95	0.95	0.94	0.89	0.92	0.91	0.86	0.79	0.88	0.78	0.44	0.64	0.55
199	LEU-COMP-THERM-002-004_E	0.96	0.96	0.96	0.94	0.94	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
200	LEU-COMP-THERM-002-005_E	0.96	0.95	0.95	0.94	0.93	0.90	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
201	LEU-COMP-THERM-003-001_E	0.96	0.88	0.95	0.87	0.83	0.88	0.86	0.88	0.77	0.86	0.90	0.83	0.59	0.73	0.58
202	LEU-COMP-THERM-003-002_E	0.97	0.89	0.95	0.88	0.84	0.88	0.86	0.88	0.77	0.85	0.90	0.83	0.58	0.73	0.58
203	LEU-COMP-THERM-003-003_E	0.97	0.89	0.95	0.87	0.84	0.88	0.86	0.88	0.77	0.86	0.90	0.83	0.59	0.73	0.58
204	LEU-COMP-THERM-003-004_E	0.97	0.89	0.95	0.87	0.84	0.88	0.86	0.88	0.77	0.86	0.90	0.83	0.59	0.73	0.58
205	LEU-COMP-THERM-003-005_E	0.96	0.88	0.95	0.87	0.83	0.88	0.86	0.88	0.77	0.86	0.90	0.84	0.59	0.73	0.58
206	LEU-COMP-THERM-003-006_E	0.97	0.89	0.95	0.88	0.85	0.89	0.87	0.89	0.78	0.86	0.91	0.84	0.57	0.72	0.57
207	LEU-COMP-THERM-003-007_E	0.97	0.89	0.95	0.88	0.85	0.89	0.87	0.89	0.78	0.86	0.91	0.83	0.58	0.72	0.58
208	LEU-COMP-THERM-003-008_E	0.97	0.89	0.95	0.88	0.85	0.89	0.87	0.89	0.78	0.86	0.91	0.83	0.57	0.72	0.57
209	LEU-COMP-THERM-003-009_E	0.96	0.87	0.94	0.86	0.83	0.89	0.86	0.87	0.77	0.87	0.91	0.84	0.59	0.72	0.57
210	LEU-COMP-THERM-003-010_E	0.97	0.89	0.95	0.87	0.84	0.89	0.87	0.88	0.78	0.86	0.91	0.84	0.58	0.72	0.57

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
211	LEU-COMP-THERM-003-011_	0.94	0.84	0.92	0.83	0.80	0.88	0.84	0.85	0.75	0.88	0.90	0.85	0.61	0.72	0.55
212	LEU-COMP-THERM-003-012_	0.88	0.74	0.85	0.76	0.73	0.85	0.79	0.80	0.71	0.89	0.88	0.86	0.65	0.71	0.52
213	LEU-COMP-THERM-003-013_	0.96	0.87	0.94	0.86	0.83	0.89	0.86	0.87	0.77	0.87	0.91	0.84	0.59	0.72	0.57
214	LEU-COMP-THERM-003-014_	0.96	0.87	0.94	0.86	0.83	0.89	0.86	0.87	0.77	0.87	0.91	0.84	0.59	0.72	0.57
215	LEU-COMP-THERM-003-015_	0.95	0.87	0.93	0.86	0.82	0.88	0.86	0.87	0.77	0.87	0.90	0.84	0.59	0.72	0.57
216	LEU-COMP-THERM-003-016_	0.95	0.86	0.93	0.85	0.82	0.88	0.85	0.87	0.76	0.87	0.91	0.85	0.60	0.72	0.56
217	LEU-COMP-THERM-003-017_	0.95	0.85	0.93	0.84	0.80	0.88	0.84	0.86	0.75	0.88	0.90	0.85	0.61	0.72	0.56
218	LEU-COMP-THERM-003-018_	0.94	0.84	0.92	0.84	0.80	0.88	0.84	0.86	0.75	0.88	0.90	0.85	0.61	0.72	0.56
219	LEU-COMP-THERM-003-019_	0.95	0.85	0.93	0.84	0.81	0.88	0.84	0.86	0.75	0.87	0.90	0.85	0.60	0.72	0.56
220	LEU-COMP-THERM-003-020_	0.96	0.87	0.94	0.85	0.82	0.88	0.85	0.87	0.76	0.87	0.90	0.84	0.60	0.73	0.57
221	LEU-COMP-THERM-003-021_	0.95	0.86	0.93	0.85	0.81	0.88	0.85	0.87	0.76	0.87	0.90	0.85	0.61	0.73	0.57
222	LEU-COMP-THERM-003-022_	0.95	0.84	0.93	0.84	0.80	0.88	0.84	0.86	0.75	0.87	0.90	0.84	0.61	0.73	0.56
223	LEU-COMP-THERM-004-001_	0.99	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.82	0.80	0.89	0.79	0.49	0.71	0.62
224	LEU-COMP-THERM-004-002_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.80	0.89	0.80	0.51	0.71	0.62
225	LEU-COMP-THERM-004-003_	0.99	0.97	0.98	0.94	0.92	0.88	0.90	0.92	0.82	0.80	0.89	0.79	0.50	0.71	0.62
226	LEU-COMP-THERM-004-004_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.80	0.89	0.80	0.51	0.71	0.62
227	LEU-COMP-THERM-004-005_	0.98	0.98	0.98	0.95	0.94	0.88	0.91	0.92	0.85	0.79	0.89	0.78	0.46	0.68	0.59
228	LEU-COMP-THERM-004-006_	0.99	0.97	0.98	0.95	0.93	0.88	0.91	0.92	0.84	0.80	0.89	0.79	0.48	0.69	0.60
229	LEU-COMP-THERM-004-007_	0.99	0.97	0.98	0.95	0.93	0.89	0.91	0.92	0.84	0.81	0.90	0.80	0.48	0.69	0.60
230	LEU-COMP-THERM-004-008_	0.99	0.96	0.98	0.94	0.92	0.88	0.90	0.92	0.83	0.81	0.90	0.80	0.50	0.70	0.61
231	LEU-COMP-THERM-004-009_	0.99	0.94	0.98	0.92	0.90	0.88	0.89	0.91	0.82	0.83	0.91	0.82	0.53	0.72	0.62
232	LEU-COMP-THERM-004-010_	0.99	0.94	0.98	0.92	0.90	0.89	0.89	0.91	0.82	0.84	0.91	0.82	0.54	0.72	0.61
233	LEU-COMP-THERM-004-011_	0.98	0.92	0.97	0.91	0.88	0.89	0.89	0.90	0.82	0.85	0.92	0.84	0.54	0.71	0.59
234	LEU-COMP-THERM-004-012_	0.96	0.89	0.95	0.88	0.86	0.89	0.87	0.89	0.80	0.87	0.92	0.85	0.57	0.72	0.59
235	LEU-COMP-THERM-004-013_	0.99	0.96	0.98	0.94	0.92	0.89	0.90	0.92	0.83	0.82	0.90	0.81	0.51	0.70	0.61
236	LEU-COMP-THERM-004-014_	0.99	0.96	0.98	0.94	0.92	0.88	0.90	0.92	0.83	0.82	0.90	0.81	0.50	0.70	0.61
237	LEU-COMP-THERM-004-015_	0.99	0.96	0.98	0.94	0.92	0.89	0.90	0.92	0.83	0.82	0.90	0.81	0.50	0.70	0.61
238	LEU-COMP-THERM-004-016_	0.99	0.96	0.98	0.94	0.92	0.89	0.91	0.92	0.84	0.81	0.90	0.81	0.50	0.70	0.61
239	LEU-COMP-THERM-004-017_	0.99	0.95	0.98	0.93	0.91	0.89	0.90	0.92	0.83	0.83	0.91	0.82	0.51	0.71	0.61
240	LEU-COMP-THERM-004-018_	0.99	0.96	0.98	0.94	0.92	0.89	0.90	0.92	0.83	0.82	0.90	0.81	0.51	0.71	0.61
241	LEU-COMP-THERM-004-019_	0.99	0.95	0.98	0.93	0.91	0.89	0.90	0.91	0.82	0.83	0.91	0.82	0.52	0.71	0.61
242	LEU-COMP-THERM-004-020_	0.98	0.93	0.97	0.91	0.89	0.89	0.89	0.91	0.82	0.85	0.91	0.84	0.53	0.71	0.60
243	LEU-COMP-THERM-005-001_	0.98	0.98	0.97	0.96	0.95	0.89	0.92	0.92	0.86	0.79	0.88	0.78	0.45	0.66	0.58
244	LEU-COMP-THERM-005-002_	0.96	0.95	0.95	0.93	0.92	0.87	0.90	0.90	0.84	0.80	0.89	0.81	0.46	0.66	0.57
245	LEU-COMP-THERM-005-003_	0.63	0.56	0.62	0.55	0.53	0.59	0.57	0.58	0.52	0.66	0.68	0.72	0.42	0.49	0.39
246	LEU-COMP-THERM-005-004_	0.59	0.51	0.58	0.51	0.49	0.55	0.53	0.54	0.48	0.64	0.64	0.69	0.41	0.47	0.36
247	LEU-COMP-THERM-005-005_	0.96	0.89	0.96	0.86	0.83	0.84	0.84	0.87	0.75	0.81	0.87	0.80	0.59	0.76	0.65
248	LEU-COMP-THERM-005-006_	0.94	0.85	0.93	0.82	0.78	0.82	0.80	0.84	0.71	0.82	0.87	0.82	0.62	0.77	0.65
249	LEU-COMP-THERM-005-007_	0.87	0.77	0.87	0.74	0.70	0.76	0.74	0.78	0.65	0.81	0.83	0.82	0.63	0.75	0.62
250	LEU-COMP-THERM-005-008_	0.73	0.60	0.73	0.58	0.54	0.66	0.61	0.64	0.53	0.76	0.75	0.79	0.63	0.68	0.54
251	LEU-COMP-THERM-005-009_	0.63	0.49	0.63	0.47	0.44	0.58	0.52	0.55	0.44	0.71	0.68	0.75	0.62	0.62	0.48
252	LEU-COMP-THERM-005-010_	0.56	0.42	0.56	0.40	0.37	0.53	0.46	0.49	0.40	0.68	0.64	0.72	0.61	0.59	0.44

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
253	LEU-COMP-THERM-005-011_	0.56	0.42	0.56	0.40	0.37	0.53	0.46	0.49	0.39	0.67	0.63	0.71	0.60	0.58	0.44
254	LEU-COMP-THERM-005-012_	0.66	0.47	0.66	0.44	0.40	0.62	0.52	0.56	0.44	0.74	0.68	0.72	0.84	0.77	0.60
255	LEU-COMP-THERM-005-013_	0.61	0.42	0.61	0.39	0.35	0.58	0.48	0.52	0.40	0.72	0.65	0.71	0.84	0.76	0.59
256	LEU-COMP-THERM-005-014_	0.97	0.91	0.96	0.90	0.87	0.89	0.88	0.89	0.79	0.85	0.90	0.82	0.56	0.72	0.58
257	LEU-COMP-THERM-005-015_	0.87	0.76	0.85	0.75	0.72	0.81	0.77	0.79	0.68	0.85	0.87	0.86	0.59	0.68	0.52
258	LEU-COMP-THERM-005-016_	0.89	0.75	0.87	0.74	0.69	0.81	0.76	0.79	0.65	0.85	0.85	0.81	0.69	0.76	0.58
259	LEU-COMP-THERM-006-001_	0.97	0.89	0.95	0.87	0.84	0.87	0.86	0.88	0.76	0.84	0.89	0.82	0.58	0.73	0.60
260	LEU-COMP-THERM-006-002_	0.97	0.89	0.95	0.87	0.83	0.87	0.85	0.88	0.76	0.84	0.89	0.81	0.58	0.73	0.60
261	LEU-COMP-THERM-006-003_	0.97	0.89	0.95	0.87	0.83	0.87	0.85	0.88	0.76	0.84	0.89	0.81	0.58	0.73	0.60
262	LEU-COMP-THERM-006-004_	0.98	0.91	0.96	0.90	0.87	0.89	0.88	0.90	0.79	0.84	0.90	0.82	0.56	0.72	0.59
263	LEU-COMP-THERM-006-005_	0.98	0.92	0.96	0.90	0.87	0.88	0.88	0.90	0.79	0.84	0.90	0.81	0.55	0.72	0.59
264	LEU-COMP-THERM-006-006_	0.98	0.92	0.96	0.90	0.87	0.88	0.88	0.90	0.79	0.84	0.90	0.81	0.55	0.72	0.59
265	LEU-COMP-THERM-006-007_	0.98	0.92	0.96	0.90	0.87	0.88	0.88	0.90	0.79	0.83	0.90	0.81	0.55	0.72	0.59
266	LEU-COMP-THERM-006-008_	0.98	0.92	0.96	0.90	0.87	0.88	0.88	0.90	0.79	0.83	0.89	0.81	0.55	0.72	0.59
267	LEU-COMP-THERM-006-009_	0.98	0.93	0.96	0.91	0.89	0.90	0.89	0.90	0.81	0.84	0.90	0.82	0.53	0.70	0.57
268	LEU-COMP-THERM-006-010_	0.98	0.93	0.96	0.92	0.89	0.90	0.89	0.91	0.81	0.84	0.90	0.81	0.53	0.70	0.57
269	LEU-COMP-THERM-006-011_	0.98	0.93	0.96	0.92	0.89	0.90	0.89	0.91	0.81	0.84	0.90	0.81	0.53	0.70	0.57
270	LEU-COMP-THERM-006-012_	0.98	0.93	0.96	0.92	0.89	0.90	0.89	0.91	0.81	0.84	0.90	0.81	0.53	0.70	0.57
271	LEU-COMP-THERM-006-013_	0.98	0.93	0.96	0.91	0.89	0.89	0.89	0.90	0.81	0.84	0.90	0.81	0.53	0.70	0.57
272	LEU-COMP-THERM-006-014_	0.97	0.92	0.95	0.91	0.89	0.90	0.90	0.90	0.82	0.84	0.90	0.82	0.53	0.69	0.56
273	LEU-COMP-THERM-006-015_	0.97	0.93	0.95	0.92	0.89	0.90	0.90	0.90	0.82	0.84	0.90	0.81	0.52	0.69	0.56
274	LEU-COMP-THERM-006-016_	0.97	0.93	0.96	0.92	0.89	0.90	0.90	0.90	0.82	0.84	0.90	0.81	0.52	0.69	0.56
275	LEU-COMP-THERM-006-017_	0.97	0.93	0.96	0.92	0.89	0.90	0.90	0.90	0.82	0.84	0.90	0.81	0.52	0.69	0.56
276	LEU-COMP-THERM-006-018_	0.97	0.93	0.96	0.92	0.89	0.90	0.90	0.90	0.82	0.84	0.90	0.81	0.52	0.69	0.56
277	LEU-COMP-THERM-008-001_	0.58	0.35	0.57	0.37	0.33	0.62	0.49	0.50	0.40	0.78	0.68	0.74	0.73	0.62	0.37
278	LEU-COMP-THERM-008-002_	0.59	0.36	0.58	0.38	0.34	0.63	0.50	0.51	0.41	0.79	0.69	0.75	0.72	0.61	0.37
279	LEU-COMP-THERM-008-003_	0.61	0.39	0.60	0.40	0.36	0.64	0.51	0.53	0.43	0.80	0.70	0.76	0.72	0.62	0.38
280	LEU-COMP-THERM-008-004_	0.59	0.37	0.58	0.38	0.34	0.63	0.50	0.51	0.42	0.79	0.69	0.75	0.72	0.61	0.37
281	LEU-COMP-THERM-008-005_	0.59	0.36	0.58	0.38	0.34	0.62	0.49	0.51	0.41	0.78	0.68	0.75	0.72	0.61	0.37
282	LEU-COMP-THERM-008-006_	0.61	0.38	0.60	0.40	0.36	0.64	0.51	0.52	0.43	0.79	0.70	0.75	0.73	0.62	0.38
283	LEU-COMP-THERM-008-007_	0.60	0.37	0.59	0.38	0.34	0.63	0.50	0.51	0.42	0.79	0.69	0.75	0.72	0.62	0.37
284	LEU-COMP-THERM-008-008_	0.68	0.47	0.67	0.48	0.44	0.69	0.58	0.59	0.49	0.83	0.75	0.79	0.73	0.66	0.42
285	LEU-COMP-THERM-008-009_	0.68	0.47	0.67	0.48	0.44	0.70	0.58	0.59	0.49	0.83	0.75	0.79	0.73	0.66	0.42
286	LEU-COMP-THERM-008-010_	0.59	0.36	0.58	0.38	0.34	0.62	0.49	0.51	0.41	0.78	0.68	0.75	0.72	0.61	0.37
287	LEU-COMP-THERM-008-011_	0.60	0.37	0.59	0.39	0.35	0.63	0.50	0.51	0.42	0.79	0.69	0.75	0.72	0.62	0.37
288	LEU-COMP-THERM-008-012_	0.59	0.36	0.58	0.37	0.33	0.62	0.49	0.50	0.41	0.78	0.68	0.74	0.72	0.61	0.37
289	LEU-COMP-THERM-008-013_	0.58	0.35	0.56	0.36	0.32	0.62	0.48	0.49	0.40	0.78	0.67	0.74	0.72	0.60	0.36
290	LEU-COMP-THERM-008-014_	0.59	0.36	0.58	0.37	0.34	0.62	0.49	0.50	0.41	0.78	0.68	0.74	0.72	0.61	0.37
291	LEU-COMP-THERM-008-015_	0.61	0.38	0.59	0.40	0.36	0.64	0.51	0.52	0.43	0.79	0.70	0.76	0.72	0.62	0.38
292	LEU-COMP-THERM-008-016_	0.62	0.39	0.60	0.41	0.37	0.65	0.52	0.53	0.44	0.80	0.71	0.76	0.72	0.62	0.38
293	LEU-COMP-THERM-008-017_	0.66	0.45	0.65	0.46	0.43	0.69	0.57	0.58	0.48	0.83	0.74	0.79	0.71	0.64	0.40
294	LEU-COMP-THERM-009-001_	0.96	0.94	0.95	0.94	0.93	0.91	0.92	0.92	0.87	0.82	0.90	0.81	0.48	0.66	0.55

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
295	LEU-COMP-THERM-009-002_	0.96	0.95	0.95	0.94	0.93	0.90	0.92	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
296	LEU-COMP-THERM-009-003_	0.96	0.95	0.95	0.94	0.93	0.90	0.92	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
297	LEU-COMP-THERM-009-004_	0.96	0.94	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
298	LEU-COMP-THERM-009-005_	0.96	0.94	0.95	0.93	0.93	0.90	0.92	0.91	0.86	0.82	0.90	0.80	0.48	0.66	0.55
299	LEU-COMP-THERM-009-006_	0.96	0.95	0.95	0.94	0.94	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.45	0.65	0.55
300	LEU-COMP-THERM-009-007_	0.96	0.96	0.95	0.94	0.94	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
301	LEU-COMP-THERM-009-008_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
302	LEU-COMP-THERM-009-009_	0.96	0.94	0.95	0.93	0.93	0.90	0.91	0.91	0.86	0.82	0.90	0.80	0.47	0.65	0.55
303	LEU-COMP-THERM-009-010_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.79	0.47	0.65	0.55
304	LEU-COMP-THERM-009-011_	0.96	0.95	0.95	0.94	0.93	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
305	LEU-COMP-THERM-009-012_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
306	LEU-COMP-THERM-009-013_	0.96	0.94	0.95	0.93	0.93	0.89	0.91	0.91	0.85	0.81	0.89	0.80	0.47	0.65	0.55
307	LEU-COMP-THERM-009-014_	0.96	0.95	0.95	0.94	0.93	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
308	LEU-COMP-THERM-009-015_	0.96	0.94	0.95	0.93	0.93	0.90	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
309	LEU-COMP-THERM-009-016_	0.96	0.95	0.95	0.94	0.93	0.90	0.92	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
310	LEU-COMP-THERM-009-017_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.79	0.46	0.65	0.55
311	LEU-COMP-THERM-009-018_	0.96	0.95	0.95	0.94	0.93	0.90	0.92	0.91	0.86	0.81	0.89	0.79	0.47	0.65	0.55
312	LEU-COMP-THERM-009-019_	0.96	0.95	0.95	0.94	0.93	0.89	0.92	0.91	0.86	0.81	0.89	0.79	0.47	0.65	0.55
313	LEU-COMP-THERM-009-020_	0.96	0.94	0.95	0.93	0.93	0.90	0.91	0.91	0.86	0.82	0.90	0.80	0.47	0.65	0.55
314	LEU-COMP-THERM-009-021_	0.96	0.95	0.95	0.94	0.93	0.89	0.92	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
315	LEU-COMP-THERM-009-022_	0.96	0.94	0.95	0.93	0.93	0.90	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
316	LEU-COMP-THERM-009-023_	0.96	0.95	0.95	0.94	0.94	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
317	LEU-COMP-THERM-009-024_	0.96	0.94	0.95	0.93	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.80	0.47	0.65	0.55
318	LEU-COMP-THERM-009-025_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
319	LEU-COMP-THERM-009-026_	0.96	0.95	0.95	0.94	0.94	0.89	0.92	0.91	0.86	0.80	0.89	0.79	0.46	0.65	0.55
320	LEU-COMP-THERM-009-027_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.79	0.46	0.65	0.55
321	LEU-COMP-THERM-010-001_	0.95	0.93	0.94	0.92	0.91	0.89	0.90	0.90	0.84	0.81	0.89	0.80	0.48	0.66	0.55
322	LEU-COMP-THERM-010-002_	0.96	0.93	0.95	0.93	0.92	0.89	0.91	0.90	0.85	0.82	0.89	0.80	0.48	0.66	0.55
323	LEU-COMP-THERM-010-003_	0.95	0.93	0.95	0.92	0.92	0.89	0.91	0.90	0.85	0.82	0.90	0.80	0.48	0.66	0.55
324	LEU-COMP-THERM-010-004_	0.96	0.93	0.95	0.93	0.92	0.90	0.91	0.90	0.85	0.82	0.90	0.81	0.48	0.65	0.55
325	LEU-COMP-THERM-010-005_	0.92	0.81	0.90	0.81	0.79	0.88	0.84	0.84	0.77	0.89	0.90	0.86	0.64	0.71	0.54
326	LEU-COMP-THERM-010-006_	0.94	0.87	0.93	0.87	0.85	0.90	0.88	0.88	0.81	0.87	0.91	0.85	0.58	0.69	0.54
327	LEU-COMP-THERM-010-007_	0.95	0.90	0.94	0.90	0.89	0.90	0.90	0.89	0.84	0.85	0.90	0.83	0.54	0.67	0.54
328	LEU-COMP-THERM-010-008_	0.95	0.90	0.93	0.90	0.89	0.90	0.90	0.89	0.84	0.84	0.90	0.82	0.52	0.67	0.54
329	LEU-COMP-THERM-010-009_	0.92	0.87	0.91	0.91	0.90	0.93	0.93	0.93	0.88	0.89	0.93	0.87	0.55	0.70	0.56
330	LEU-COMP-THERM-010-010_	0.94	0.89	0.93	0.92	0.91	0.93	0.94	0.94	0.89	0.88	0.94	0.86	0.54	0.69	0.56
331	LEU-COMP-THERM-010-011_	0.95	0.90	0.94	0.93	0.92	0.93	0.93	0.93	0.88	0.87	0.93	0.86	0.53	0.69	0.56
332	LEU-COMP-THERM-010-012_	0.96	0.92	0.95	0.93	0.92	0.92	0.93	0.92	0.87	0.86	0.92	0.84	0.51	0.68	0.56
333	LEU-COMP-THERM-010-013_	0.96	0.92	0.95	0.92	0.91	0.91	0.91	0.91	0.85	0.84	0.91	0.82	0.50	0.66	0.55
334	LEU-COMP-THERM-010-014_	0.97	0.90	0.96	0.91	0.88	0.91	0.90	0.93	0.83	0.88	0.93	0.87	0.60	0.76	0.63
335	LEU-COMP-THERM-010-015_	0.98	0.91	0.97	0.91	0.89	0.91	0.91	0.93	0.84	0.88	0.93	0.86	0.59	0.76	0.63
336	LEU-COMP-THERM-010-016_	0.97	0.90	0.97	0.90	0.88	0.91	0.90	0.92	0.83	0.88	0.93	0.87	0.60	0.76	0.62

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
337	LEU-COMP-THERM-010-017_	0.98	0.92	0.98	0.92	0.89	0.91	0.90	0.93	0.83	0.87	0.93	0.85	0.58	0.75	0.62
338	LEU-COMP-THERM-010-018_	0.99	0.93	0.98	0.92	0.90	0.90	0.90	0.93	0.83	0.86	0.92	0.84	0.57	0.74	0.62
339	LEU-COMP-THERM-010-019_	0.99	0.93	0.98	0.91	0.89	0.89	0.89	0.91	0.82	0.85	0.91	0.83	0.56	0.73	0.62
340	LEU-COMP-THERM-010-020_	0.98	0.92	0.97	0.90	0.88	0.88	0.88	0.90	0.80	0.83	0.90	0.82	0.55	0.73	0.62
341	LEU-COMP-THERM-010-021_	0.99	0.94	0.98	0.92	0.89	0.88	0.89	0.91	0.81	0.83	0.90	0.81	0.54	0.73	0.62
342	LEU-COMP-THERM-010-022_	0.99	0.94	0.98	0.92	0.90	0.88	0.89	0.91	0.81	0.83	0.90	0.81	0.53	0.72	0.62
343	LEU-COMP-THERM-010-023_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.54	0.73	0.62
344	LEU-COMP-THERM-010-024_	0.95	0.84	0.94	0.83	0.79	0.87	0.84	0.86	0.75	0.88	0.91	0.86	0.66	0.77	0.61
345	LEU-COMP-THERM-010-025_	0.97	0.88	0.96	0.86	0.83	0.88	0.86	0.88	0.77	0.87	0.91	0.85	0.63	0.76	0.62
346	LEU-COMP-THERM-010-026_	0.97	0.89	0.96	0.87	0.85	0.89	0.87	0.89	0.79	0.87	0.91	0.85	0.62	0.76	0.62
347	LEU-COMP-THERM-010-027_	0.98	0.90	0.97	0.88	0.86	0.89	0.87	0.90	0.79	0.86	0.91	0.84	0.60	0.75	0.62
348	LEU-COMP-THERM-010-028_	0.98	0.91	0.97	0.89	0.87	0.89	0.88	0.90	0.80	0.86	0.91	0.84	0.59	0.75	0.62
349	LEU-COMP-THERM-010-029_	0.99	0.92	0.98	0.90	0.88	0.89	0.89	0.90	0.81	0.85	0.91	0.83	0.58	0.74	0.62
350	LEU-COMP-THERM-010-030_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
351	LEU-COMP-THERM-011-001_	0.97	0.91	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.90	0.82	0.57	0.72	0.58
352	LEU-COMP-THERM-011-002_	0.80	0.62	0.79	0.62	0.58	0.78	0.69	0.71	0.59	0.87	0.83	0.84	0.72	0.72	0.50
353	LEU-COMP-THERM-011-003_	0.80	0.62	0.78	0.62	0.58	0.79	0.70	0.71	0.60	0.88	0.83	0.84	0.71	0.70	0.48
354	LEU-COMP-THERM-011-004_	0.80	0.61	0.78	0.62	0.58	0.79	0.69	0.71	0.60	0.88	0.83	0.84	0.71	0.70	0.48
355	LEU-COMP-THERM-011-005_	0.80	0.62	0.78	0.62	0.58	0.79	0.69	0.71	0.60	0.88	0.83	0.84	0.71	0.70	0.48
356	LEU-COMP-THERM-011-006_	0.80	0.62	0.79	0.63	0.59	0.79	0.70	0.71	0.61	0.88	0.84	0.84	0.71	0.70	0.48
357	LEU-COMP-THERM-011-007_	0.81	0.64	0.80	0.64	0.60	0.80	0.71	0.72	0.62	0.88	0.84	0.85	0.70	0.71	0.49
358	LEU-COMP-THERM-011-008_	0.82	0.65	0.81	0.65	0.61	0.80	0.72	0.73	0.62	0.88	0.85	0.85	0.70	0.71	0.50
359	LEU-COMP-THERM-011-009_	0.83	0.66	0.81	0.66	0.62	0.81	0.72	0.74	0.63	0.89	0.85	0.85	0.70	0.71	0.50
360	LEU-COMP-THERM-011-010_	0.81	0.64	0.80	0.64	0.60	0.80	0.71	0.72	0.61	0.88	0.84	0.84	0.71	0.71	0.49
361	LEU-COMP-THERM-011-011_	0.83	0.66	0.81	0.66	0.63	0.81	0.72	0.74	0.63	0.88	0.85	0.84	0.69	0.71	0.49
362	LEU-COMP-THERM-011-012_	0.84	0.68	0.83	0.68	0.65	0.82	0.74	0.75	0.65	0.89	0.86	0.85	0.69	0.71	0.50
363	LEU-COMP-THERM-011-013_	0.83	0.67	0.81	0.68	0.64	0.81	0.73	0.74	0.64	0.88	0.85	0.84	0.67	0.69	0.49
364	LEU-COMP-THERM-011-014_	0.85	0.70	0.83	0.70	0.67	0.83	0.75	0.76	0.66	0.88	0.86	0.85	0.67	0.70	0.50
365	LEU-COMP-THERM-011-015_	0.84	0.68	0.81	0.70	0.66	0.81	0.73	0.75	0.65	0.87	0.85	0.83	0.64	0.68	0.49
366	LEU-COMP-THERM-012-001_	0.95	0.85	0.93	0.85	0.81	0.89	0.86	0.88	0.77	0.88	0.91	0.86	0.62	0.74	0.58
367	LEU-COMP-THERM-012-002_	0.94	0.83	0.92	0.82	0.78	0.87	0.83	0.85	0.74	0.88	0.90	0.85	0.63	0.74	0.57
368	LEU-COMP-THERM-012-003_	0.95	0.85	0.93	0.84	0.80	0.88	0.84	0.86	0.75	0.88	0.90	0.85	0.63	0.74	0.57
369	LEU-COMP-THERM-012-004_	0.95	0.84	0.93	0.83	0.79	0.87	0.83	0.85	0.74	0.88	0.90	0.85	0.63	0.74	0.57
370	LEU-COMP-THERM-012-005_	0.94	0.84	0.93	0.82	0.79	0.88	0.84	0.85	0.74	0.88	0.90	0.85	0.63	0.74	0.57
371	LEU-COMP-THERM-012-006_	0.94	0.84	0.93	0.83	0.79	0.88	0.84	0.86	0.74	0.88	0.90	0.85	0.63	0.74	0.57
372	LEU-COMP-THERM-012-007_	0.94	0.83	0.92	0.82	0.78	0.87	0.83	0.85	0.74	0.88	0.90	0.85	0.64	0.74	0.57
373	LEU-COMP-THERM-012-008_	0.94	0.84	0.93	0.83	0.79	0.87	0.83	0.85	0.74	0.88	0.90	0.85	0.63	0.74	0.57
374	LEU-COMP-THERM-012-009_	0.94	0.84	0.92	0.83	0.79	0.87	0.84	0.85	0.74	0.87	0.90	0.85	0.62	0.73	0.56
375	LEU-COMP-THERM-012-010_	0.94	0.83	0.92	0.83	0.79	0.88	0.84	0.85	0.74	0.88	0.90	0.85	0.63	0.74	0.57
376	LEU-COMP-THERM-013-001_	0.98	0.91	0.97	0.92	0.89	0.92	0.91	0.94	0.84	0.89	0.94	0.87	0.60	0.76	0.63
377	LEU-COMP-THERM-013-002_	0.98	0.92	0.98	0.92	0.89	0.91	0.91	0.93	0.84	0.87	0.93	0.86	0.59	0.76	0.63
378	LEU-COMP-THERM-013-003_	0.98	0.91	0.97	0.91	0.88	0.91	0.90	0.93	0.83	0.88	0.94	0.87	0.60	0.76	0.63

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
379	LEU-COMP-THERM-013-004_	0.98	0.91	0.97	0.91	0.88	0.91	0.91	0.93	0.83	0.88	0.94	0.87	0.60	0.76	0.63
380	LEU-COMP-THERM-013-005_	0.98	0.92	0.98	0.92	0.89	0.91	0.91	0.93	0.84	0.87	0.93	0.86	0.59	0.76	0.63
381	LEU-COMP-THERM-013-006_	0.98	0.92	0.97	0.92	0.89	0.91	0.91	0.93	0.84	0.87	0.93	0.85	0.58	0.75	0.63
382	LEU-COMP-THERM-013-007_	0.98	0.92	0.97	0.91	0.89	0.91	0.91	0.93	0.83	0.88	0.93	0.86	0.59	0.76	0.63
383	LEU-COMP-THERM-014-001_	0.99	0.96	0.98	0.93	0.91	0.89	0.91	0.92	0.83	0.83	0.91	0.81	0.53	0.72	0.62
384	LEU-COMP-THERM-014-002_	0.99	0.94	0.99	0.91	0.89	0.89	0.89	0.91	0.82	0.84	0.91	0.83	0.56	0.74	0.63
385	LEU-COMP-THERM-014-005_	0.82	0.64	0.82	0.63	0.60	0.78	0.70	0.73	0.62	0.88	0.85	0.86	0.75	0.76	0.56
386	LEU-COMP-THERM-014-006_	0.98	0.91	0.97	0.88	0.85	0.87	0.86	0.89	0.78	0.84	0.90	0.83	0.60	0.77	0.65
387	LEU-COMP-THERM-014-007_	0.94	0.83	0.93	0.80	0.76	0.84	0.81	0.84	0.72	0.85	0.88	0.84	0.67	0.79	0.65
388	LEU-COMP-THERM-015-001_	0.99	0.93	0.98	0.92	0.89	0.90	0.90	0.92	0.82	0.86	0.92	0.84	0.57	0.74	0.61
389	LEU-COMP-THERM-015-002_	0.99	0.93	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.56	0.73	0.61
390	LEU-COMP-THERM-015-003_	0.99	0.94	0.98	0.92	0.90	0.89	0.90	0.91	0.82	0.84	0.91	0.82	0.55	0.73	0.61
391	LEU-COMP-THERM-015-004_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.84	0.91	0.82	0.56	0.73	0.61
392	LEU-COMP-THERM-015-005_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.84	0.91	0.82	0.55	0.73	0.61
393	LEU-COMP-THERM-015-006_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.82	0.84	0.91	0.82	0.55	0.73	0.61
394	LEU-COMP-THERM-015-007_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.84	0.91	0.82	0.55	0.73	0.61
395	LEU-COMP-THERM-015-008_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.84	0.91	0.82	0.55	0.73	0.61
396	LEU-COMP-THERM-015-009_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.61
397	LEU-COMP-THERM-015-010_	0.99	0.93	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.61
398	LEU-COMP-THERM-015-011_	0.99	0.94	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.61
399	LEU-COMP-THERM-015-012_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
400	LEU-COMP-THERM-015-013_	0.98	0.92	0.97	0.90	0.87	0.89	0.89	0.91	0.80	0.85	0.91	0.83	0.58	0.75	0.62
401	LEU-COMP-THERM-015-014_	0.98	0.92	0.97	0.90	0.87	0.89	0.89	0.91	0.80	0.85	0.91	0.83	0.58	0.75	0.62
402	LEU-COMP-THERM-015-015_	0.98	0.91	0.97	0.89	0.86	0.88	0.88	0.90	0.79	0.85	0.91	0.84	0.59	0.75	0.62
403	LEU-COMP-THERM-015-016_	0.96	0.86	0.95	0.84	0.81	0.88	0.85	0.88	0.77	0.89	0.92	0.87	0.65	0.77	0.61
404	LEU-COMP-THERM-015-017_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.77	0.62
405	LEU-COMP-THERM-015-018_	0.97	0.87	0.96	0.85	0.82	0.88	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.77	0.62
406	LEU-COMP-THERM-015-019_	0.97	0.87	0.96	0.85	0.82	0.88	0.86	0.88	0.77	0.87	0.91	0.86	0.63	0.77	0.62
407	LEU-COMP-THERM-015-020_	0.96	0.87	0.95	0.84	0.81	0.87	0.85	0.87	0.76	0.87	0.91	0.85	0.63	0.77	0.61
408	LEU-COMP-THERM-015-021_	0.97	0.87	0.96	0.85	0.82	0.88	0.86	0.88	0.77	0.87	0.91	0.85	0.63	0.77	0.62
409	LEU-COMP-THERM-015-022_	0.96	0.87	0.95	0.85	0.81	0.88	0.85	0.88	0.76	0.87	0.91	0.85	0.64	0.77	0.61
410	LEU-COMP-THERM-015-023_	0.97	0.87	0.96	0.85	0.82	0.88	0.85	0.88	0.76	0.87	0.91	0.85	0.63	0.77	0.62
411	LEU-COMP-THERM-015-024_	0.94	0.83	0.94	0.81	0.78	0.87	0.83	0.86	0.74	0.89	0.91	0.87	0.67	0.77	0.61
412	LEU-COMP-THERM-015-025_	0.94	0.82	0.93	0.80	0.77	0.86	0.82	0.85	0.73	0.89	0.91	0.86	0.67	0.77	0.61
413	LEU-COMP-THERM-015-026_	0.92	0.78	0.91	0.77	0.73	0.86	0.81	0.83	0.72	0.90	0.90	0.88	0.71	0.78	0.59
414	LEU-COMP-THERM-015-027_	0.92	0.78	0.91	0.77	0.73	0.86	0.80	0.83	0.71	0.90	0.90	0.87	0.70	0.78	0.59
415	LEU-COMP-THERM-015-028_	0.90	0.77	0.89	0.75	0.71	0.82	0.77	0.81	0.67	0.86	0.87	0.83	0.72	0.80	0.63
416	LEU-COMP-THERM-015-029_	0.90	0.77	0.89	0.75	0.70	0.82	0.77	0.80	0.67	0.85	0.86	0.83	0.72	0.80	0.63
417	LEU-COMP-THERM-015-030_	0.91	0.78	0.90	0.76	0.72	0.81	0.77	0.81	0.67	0.84	0.86	0.82	0.70	0.79	0.63
418	LEU-COMP-THERM-015-031_	0.91	0.78	0.90	0.76	0.72	0.82	0.77	0.81	0.68	0.85	0.86	0.83	0.70	0.79	0.63
419	LEU-COMP-THERM-015-032_	0.91	0.78	0.90	0.76	0.71	0.81	0.77	0.81	0.67	0.84	0.86	0.82	0.70	0.79	0.63
420	LEU-COMP-THERM-015-033_	0.90	0.78	0.89	0.75	0.71	0.81	0.77	0.80	0.67	0.84	0.86	0.82	0.71	0.79	0.63

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
421	LEU-COMP-THERM-015-034_	0.89	0.76	0.88	0.74	0.69	0.81	0.76	0.80	0.66	0.85	0.86	0.83	0.71	0.79	0.63
422	LEU-COMP-THERM-015-035_	0.90	0.77	0.89	0.75	0.70	0.81	0.76	0.80	0.66	0.84	0.86	0.82	0.70	0.79	0.63
423	LEU-COMP-THERM-015-036_	0.91	0.78	0.90	0.76	0.71	0.81	0.77	0.81	0.67	0.84	0.86	0.82	0.70	0.79	0.63
424	LEU-COMP-THERM-015-037_	0.88	0.74	0.87	0.72	0.67	0.79	0.74	0.78	0.64	0.84	0.84	0.82	0.72	0.79	0.62
425	LEU-COMP-THERM-015-038_	0.88	0.74	0.87	0.72	0.68	0.80	0.75	0.78	0.65	0.85	0.85	0.82	0.73	0.80	0.63
426	LEU-COMP-THERM-015-039_	0.98	0.96	0.97	0.95	0.93	0.90	0.92	0.92	0.86	0.82	0.90	0.80	0.49	0.67	0.57
427	LEU-COMP-THERM-015-040_	0.98	0.96	0.97	0.95	0.94	0.90	0.92	0.92	0.86	0.82	0.90	0.80	0.49	0.68	0.57
428	LEU-COMP-THERM-015-041_	0.98	0.96	0.97	0.95	0.94	0.90	0.92	0.92	0.86	0.82	0.90	0.80	0.49	0.68	0.57
429	LEU-COMP-THERM-015-042_	0.98	0.96	0.97	0.95	0.94	0.90	0.92	0.92	0.86	0.82	0.91	0.81	0.49	0.68	0.58
430	LEU-COMP-THERM-015-043_	0.98	0.96	0.97	0.95	0.94	0.90	0.92	0.93	0.86	0.82	0.91	0.81	0.50	0.69	0.58
431	LEU-COMP-THERM-015-044_	0.98	0.96	0.97	0.95	0.94	0.90	0.93	0.93	0.86	0.82	0.91	0.81	0.50	0.69	0.58
432	LEU-COMP-THERM-015-045_	0.98	0.96	0.97	0.95	0.93	0.91	0.93	0.93	0.86	0.83	0.91	0.81	0.50	0.69	0.58
433	LEU-COMP-THERM-015-046_	0.98	0.96	0.97	0.95	0.93	0.91	0.93	0.93	0.86	0.83	0.91	0.81	0.50	0.69	0.58
434	LEU-COMP-THERM-015-047_	0.99	0.96	0.97	0.95	0.93	0.91	0.93	0.93	0.86	0.83	0.91	0.81	0.50	0.69	0.58
435	LEU-COMP-THERM-015-048_	0.97	0.89	0.96	0.87	0.85	0.91	0.89	0.89	0.81	0.89	0.93	0.87	0.60	0.73	0.58
436	LEU-COMP-THERM-015-049_	0.97	0.90	0.96	0.88	0.86	0.91	0.89	0.90	0.81	0.89	0.93	0.87	0.59	0.73	0.58
437	LEU-COMP-THERM-015-050_	0.97	0.89	0.96	0.88	0.85	0.91	0.89	0.90	0.81	0.89	0.93	0.87	0.60	0.73	0.58
438	LEU-COMP-THERM-015-051_	0.97	0.89	0.96	0.87	0.85	0.91	0.89	0.89	0.81	0.89	0.93	0.87	0.60	0.73	0.58
439	LEU-COMP-THERM-015-052_	0.97	0.89	0.96	0.88	0.85	0.91	0.89	0.90	0.81	0.89	0.93	0.87	0.60	0.73	0.58
440	LEU-COMP-THERM-015-053_	0.97	0.89	0.96	0.88	0.85	0.91	0.89	0.90	0.81	0.89	0.93	0.87	0.60	0.73	0.58
441	LEU-COMP-THERM-015-054_	0.97	0.97	0.97	0.96	0.95	0.89	0.93	0.92	0.87	0.80	0.89	0.79	0.46	0.66	0.57
442	LEU-COMP-THERM-015-055_	0.97	0.97	0.97	0.96	0.95	0.89	0.93	0.92	0.87	0.80	0.89	0.78	0.46	0.66	0.57
443	LEU-COMP-THERM-015-056_	0.98	0.98	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.80	0.89	0.79	0.46	0.67	0.58
444	LEU-COMP-THERM-015-057_	0.98	0.98	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.80	0.89	0.79	0.47	0.67	0.58
445	LEU-COMP-THERM-015-058_	0.98	0.98	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.80	0.90	0.79	0.47	0.67	0.58
446	LEU-COMP-THERM-015-059_	0.98	0.98	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.80	0.90	0.79	0.47	0.68	0.58
447	LEU-COMP-THERM-015-060_	0.93	0.91	0.92	0.91	0.91	0.89	0.90	0.89	0.85	0.81	0.88	0.79	0.47	0.63	0.52
448	LEU-COMP-THERM-015-061_	0.93	0.91	0.92	0.91	0.91	0.89	0.90	0.89	0.85	0.81	0.89	0.80	0.47	0.63	0.52
449	LEU-COMP-THERM-015-062_	0.94	0.92	0.93	0.92	0.91	0.89	0.91	0.89	0.85	0.82	0.89	0.80	0.47	0.63	0.52
450	LEU-COMP-THERM-015-063_	0.94	0.92	0.93	0.92	0.91	0.89	0.91	0.89	0.85	0.82	0.89	0.80	0.48	0.64	0.52
451	LEU-COMP-THERM-015-064_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.85	0.82	0.89	0.80	0.47	0.64	0.53
452	LEU-COMP-THERM-015-065_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.85	0.82	0.90	0.81	0.48	0.64	0.53
453	LEU-COMP-THERM-015-066_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.85	0.83	0.90	0.81	0.48	0.64	0.53
454	LEU-COMP-THERM-015-067_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.85	0.83	0.90	0.81	0.48	0.64	0.53
455	LEU-COMP-THERM-015-068_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.85	0.83	0.90	0.81	0.48	0.65	0.53
456	LEU-COMP-THERM-015-069_	0.94	0.92	0.93	0.92	0.91	0.90	0.91	0.90	0.86	0.83	0.90	0.81	0.48	0.65	0.53
457	LEU-COMP-THERM-015-070_	0.93	0.82	0.91	0.81	0.77	0.87	0.82	0.84	0.72	0.87	0.89	0.84	0.65	0.74	0.56
458	LEU-COMP-THERM-015-071_	0.93	0.81	0.91	0.80	0.76	0.87	0.82	0.84	0.72	0.88	0.89	0.84	0.65	0.74	0.56
459	LEU-COMP-THERM-015-072_	0.92	0.79	0.90	0.78	0.74	0.86	0.80	0.82	0.71	0.88	0.89	0.85	0.68	0.75	0.57
460	LEU-COMP-THERM-015-073_	0.99	0.96	0.99	0.93	0.91	0.89	0.91	0.92	0.83	0.82	0.90	0.81	0.53	0.72	0.62
461	LEU-COMP-THERM-015-074_	0.99	0.96	0.99	0.94	0.92	0.90	0.91	0.93	0.84	0.84	0.91	0.82	0.54	0.73	0.62
462	LEU-COMP-THERM-015-075_	0.99	0.96	0.99	0.93	0.91	0.89	0.91	0.92	0.83	0.83	0.91	0.82	0.54	0.73	0.62

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
463	LEU-COMP-THERM-015-076_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.82	0.90	0.81	0.53	0.73	0.63
464	LEU-COMP-THERM-015-077_	0.96	0.86	0.95	0.84	0.81	0.87	0.85	0.87	0.76	0.88	0.91	0.86	0.65	0.78	0.63
465	LEU-COMP-THERM-015-078_	0.92	0.82	0.90	0.82	0.79	0.88	0.84	0.84	0.75	0.88	0.89	0.84	0.61	0.70	0.53
466	LEU-COMP-THERM-015-079_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.80	0.84	0.91	0.83	0.57	0.74	0.62
467	LEU-COMP-THERM-015-080_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
468	LEU-COMP-THERM-015-081_	0.99	0.92	0.97	0.90	0.87	0.89	0.89	0.91	0.80	0.85	0.91	0.83	0.58	0.75	0.62
469	LEU-COMP-THERM-015-082_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
470	LEU-COMP-THERM-015-083_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
471	LEU-COMP-THERM-015-084_	0.99	0.93	0.97	0.91	0.88	0.89	0.89	0.91	0.80	0.84	0.91	0.83	0.57	0.74	0.62
472	LEU-COMP-THERM-015-085_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
473	LEU-COMP-THERM-015-086_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
474	LEU-COMP-THERM-015-087_	0.99	0.93	0.97	0.90	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.58	0.74	0.62
475	LEU-COMP-THERM-015-088_	0.97	0.89	0.96	0.87	0.84	0.88	0.87	0.89	0.78	0.86	0.91	0.84	0.61	0.75	0.61
476	LEU-COMP-THERM-015-089_	0.97	0.88	0.96	0.86	0.83	0.88	0.87	0.88	0.78	0.87	0.91	0.85	0.61	0.75	0.61
477	LEU-COMP-THERM-015-090_	0.97	0.89	0.96	0.87	0.84	0.88	0.87	0.89	0.78	0.87	0.91	0.85	0.61	0.75	0.61
478	LEU-COMP-THERM-015-091_	0.95	0.84	0.94	0.82	0.79	0.87	0.84	0.86	0.75	0.88	0.91	0.86	0.65	0.76	0.60
479	LEU-COMP-THERM-015-092_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
480	LEU-COMP-THERM-015-093_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
481	LEU-COMP-THERM-015-094_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.76	0.61
482	LEU-COMP-THERM-015-095_	0.97	0.88	0.96	0.86	0.83	0.89	0.86	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
483	LEU-COMP-THERM-015-096_	0.95	0.84	0.94	0.83	0.79	0.88	0.84	0.86	0.75	0.89	0.91	0.87	0.66	0.77	0.61
484	LEU-COMP-THERM-015-097_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.76	0.61
485	LEU-COMP-THERM-015-098_	0.96	0.86	0.95	0.84	0.81	0.88	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.76	0.61
486	LEU-COMP-THERM-015-099_	0.96	0.86	0.95	0.85	0.81	0.88	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.77	0.61
487	LEU-COMP-THERM-015-100_	0.99	0.93	0.97	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.58	0.75	0.62
488	LEU-COMP-THERM-015-101_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.55	0.74	0.62
489	LEU-COMP-THERM-015-102_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
490	LEU-COMP-THERM-015-103_	0.99	0.93	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.62
491	LEU-COMP-THERM-015-104_	0.98	0.92	0.97	0.90	0.87	0.89	0.88	0.91	0.80	0.85	0.91	0.83	0.58	0.75	0.62
492	LEU-COMP-THERM-015-105_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.79	0.86	0.91	0.84	0.59	0.75	0.62
493	LEU-COMP-THERM-015-106_	0.93	0.82	0.92	0.80	0.76	0.84	0.80	0.83	0.71	0.85	0.88	0.83	0.68	0.79	0.63
494	LEU-COMP-THERM-015-107_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.79	0.86	0.92	0.84	0.60	0.75	0.62
495	LEU-COMP-THERM-015-108_	0.98	0.90	0.97	0.88	0.85	0.89	0.88	0.90	0.79	0.86	0.92	0.85	0.60	0.75	0.61
496	LEU-COMP-THERM-015-109_	0.98	0.89	0.97	0.87	0.84	0.89	0.87	0.89	0.79	0.87	0.92	0.85	0.62	0.76	0.62
497	LEU-COMP-THERM-015-110_	0.97	0.89	0.96	0.87	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.62	0.76	0.61
498	LEU-COMP-THERM-015-111_	0.97	0.89	0.96	0.87	0.84	0.89	0.87	0.89	0.78	0.87	0.92	0.85	0.62	0.76	0.62
499	LEU-COMP-THERM-015-112_	0.93	0.81	0.92	0.79	0.76	0.87	0.82	0.85	0.73	0.90	0.91	0.87	0.68	0.77	0.59
500	LEU-COMP-THERM-015-113_	0.99	0.93	0.98	0.91	0.89	0.89	0.90	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
501	LEU-COMP-THERM-015-114_	0.99	0.93	0.98	0.92	0.89	0.89	0.90	0.92	0.82	0.85	0.91	0.83	0.56	0.74	0.62
502	LEU-COMP-THERM-015-115_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.88	0.78	0.88	0.92	0.86	0.63	0.76	0.61
503	LEU-COMP-THERM-015-116_	0.94	0.81	0.93	0.80	0.77	0.88	0.83	0.85	0.74	0.90	0.92	0.88	0.68	0.77	0.59
504	LEU-COMP-THERM-015-117_	0.97	0.87	0.95	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.64	0.76	0.61

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
505	LEU-COMP-THERM-015-118_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
506	LEU-COMP-THERM-015-119_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
507	LEU-COMP-THERM-015-120_	0.97	0.88	0.96	0.86	0.83	0.89	0.87	0.89	0.78	0.88	0.92	0.86	0.63	0.76	0.61
508	LEU-COMP-THERM-015-121_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.63	0.76	0.61
509	LEU-COMP-THERM-015-122_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.78	0.89	0.92	0.87	0.64	0.76	0.60
510	LEU-COMP-THERM-015-123_	0.97	0.87	0.96	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.63	0.76	0.61
511	LEU-COMP-THERM-015-124_	0.97	0.87	0.96	0.86	0.83	0.89	0.86	0.88	0.78	0.89	0.92	0.86	0.63	0.76	0.60
512	LEU-COMP-THERM-015-125_	0.96	0.85	0.95	0.84	0.81	0.89	0.86	0.87	0.77	0.89	0.92	0.87	0.66	0.77	0.60
513	LEU-COMP-THERM-015-126_	0.99	0.96	0.98	0.94	0.92	0.90	0.91	0.92	0.84	0.83	0.91	0.81	0.52	0.71	0.60
514	LEU-COMP-THERM-015-127_	0.96	0.88	0.95	0.85	0.81	0.86	0.84	0.87	0.75	0.85	0.89	0.83	0.62	0.77	0.63
515	LEU-COMP-THERM-015-128_	0.99	0.94	0.98	0.92	0.89	0.90	0.90	0.92	0.82	0.85	0.92	0.83	0.56	0.73	0.61
516	LEU-COMP-THERM-015-129_	0.94	0.81	0.92	0.80	0.77	0.88	0.84	0.85	0.75	0.91	0.92	0.88	0.67	0.76	0.58
517	LEU-COMP-THERM-015-130_	0.99	0.95	0.98	0.93	0.91	0.90	0.91	0.92	0.83	0.84	0.91	0.83	0.54	0.72	0.61
518	LEU-COMP-THERM-015-131_	0.96	0.86	0.95	0.84	0.81	0.89	0.86	0.88	0.78	0.90	0.93	0.87	0.64	0.75	0.59
519	LEU-COMP-THERM-015-132_	0.94	0.83	0.93	0.81	0.78	0.88	0.84	0.86	0.75	0.90	0.92	0.88	0.67	0.76	0.59
520	LEU-COMP-THERM-015-133_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.92	0.82	0.84	0.91	0.83	0.55	0.73	0.61
521	LEU-COMP-THERM-015-134_	0.99	0.94	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.56	0.74	0.61
522	LEU-COMP-THERM-015-135_	0.95	0.84	0.94	0.83	0.80	0.89	0.85	0.87	0.77	0.90	0.92	0.88	0.65	0.76	0.59
523	LEU-COMP-THERM-015-136_	0.99	0.95	0.98	0.93	0.91	0.90	0.91	0.92	0.83	0.84	0.91	0.82	0.54	0.72	0.61
524	LEU-COMP-THERM-015-137_	0.99	0.94	0.98	0.92	0.89	0.90	0.90	0.92	0.82	0.85	0.92	0.83	0.56	0.73	0.61
525	LEU-COMP-THERM-015-138_	0.99	0.93	0.98	0.91	0.88	0.90	0.90	0.91	0.82	0.86	0.92	0.84	0.57	0.74	0.61
526	LEU-COMP-THERM-015-139_	0.98	0.92	0.97	0.90	0.87	0.90	0.89	0.91	0.81	0.86	0.92	0.85	0.58	0.74	0.61
527	LEU-COMP-THERM-015-140_	0.92	0.80	0.91	0.77	0.74	0.83	0.79	0.82	0.70	0.86	0.88	0.84	0.69	0.78	0.63
528	LEU-COMP-THERM-015-141_	0.92	0.80	0.91	0.77	0.73	0.83	0.79	0.82	0.70	0.86	0.88	0.84	0.69	0.78	0.63
529	LEU-COMP-THERM-015-142_	0.97	0.87	0.96	0.86	0.83	0.90	0.87	0.89	0.78	0.89	0.93	0.87	0.62	0.75	0.60
530	LEU-COMP-THERM-015-143_	0.99	0.94	0.98	0.93	0.91	0.91	0.91	0.92	0.84	0.85	0.92	0.83	0.55	0.73	0.60
531	LEU-COMP-THERM-015-144_	0.99	0.94	0.98	0.93	0.91	0.91	0.91	0.93	0.84	0.85	0.92	0.84	0.55	0.73	0.60
532	LEU-COMP-THERM-015-145_	0.98	0.93	0.97	0.92	0.89	0.90	0.90	0.91	0.83	0.86	0.92	0.84	0.55	0.72	0.59
533	LEU-COMP-THERM-015-146_	0.94	0.83	0.93	0.82	0.79	0.89	0.85	0.86	0.77	0.91	0.92	0.88	0.64	0.74	0.56
534	LEU-COMP-THERM-015-147_	0.99	0.94	0.98	0.93	0.91	0.91	0.91	0.92	0.84	0.86	0.93	0.84	0.55	0.72	0.59
535	LEU-COMP-THERM-015-148_	0.99	0.94	0.98	0.92	0.90	0.91	0.91	0.92	0.84	0.86	0.93	0.84	0.55	0.72	0.59
536	LEU-COMP-THERM-015-149_	0.96	0.86	0.94	0.85	0.82	0.90	0.87	0.88	0.79	0.90	0.93	0.88	0.63	0.74	0.57
537	LEU-COMP-THERM-015-150_	0.96	0.87	0.95	0.86	0.83	0.90	0.87	0.88	0.79	0.90	0.93	0.88	0.62	0.74	0.58
538	LEU-COMP-THERM-015-151_	0.92	0.79	0.90	0.78	0.76	0.88	0.82	0.83	0.74	0.91	0.91	0.88	0.66	0.73	0.55
539	LEU-COMP-THERM-015-152_	0.95	0.84	0.94	0.82	0.79	0.88	0.85	0.86	0.76	0.90	0.92	0.88	0.65	0.76	0.59
540	LEU-COMP-THERM-015-153_	0.99	0.93	0.98	0.91	0.89	0.91	0.91	0.92	0.83	0.87	0.93	0.85	0.57	0.73	0.60
541	LEU-COMP-THERM-015-154_	0.98	0.90	0.96	0.89	0.85	0.90	0.88	0.90	0.79	0.87	0.92	0.85	0.59	0.74	0.60
542	LEU-COMP-THERM-015-155_	0.98	0.91	0.97	0.90	0.87	0.90	0.89	0.91	0.81	0.86	0.92	0.84	0.58	0.73	0.59
543	LEU-COMP-THERM-015-156_	0.96	0.87	0.95	0.86	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.85	0.62	0.74	0.59
544	LEU-COMP-THERM-015-157_	0.96	0.86	0.94	0.85	0.82	0.89	0.86	0.88	0.77	0.88	0.92	0.86	0.62	0.74	0.58
545	LEU-COMP-THERM-015-158_	0.91	0.78	0.89	0.77	0.73	0.86	0.80	0.82	0.71	0.89	0.89	0.86	0.67	0.74	0.55
546	LEU-COMP-THERM-015-159_	0.99	0.94	0.98	0.93	0.90	0.90	0.91	0.92	0.83	0.85	0.92	0.83	0.56	0.74	0.62

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
547	LEU-COMP-THERM-015-160_	0.99	0.95	0.98	0.93	0.91	0.90	0.91	0.93	0.84	0.84	0.92	0.83	0.54	0.73	0.61
548	LEU-COMP-THERM-015-161_	0.99	0.94	0.98	0.92	0.90	0.90	0.90	0.92	0.83	0.85	0.92	0.83	0.56	0.74	0.62
549	LEU-COMP-THERM-015-162_	0.99	0.94	0.98	0.92	0.89	0.90	0.90	0.92	0.82	0.85	0.92	0.84	0.56	0.74	0.62
550	LEU-COMP-THERM-015-163_	0.99	0.92	0.98	0.90	0.87	0.90	0.89	0.91	0.81	0.86	0.92	0.85	0.59	0.75	0.62
551	LEU-COMP-THERM-015-164_	0.99	0.93	0.98	0.91	0.89	0.90	0.90	0.92	0.82	0.85	0.92	0.84	0.57	0.74	0.62
552	LEU-COMP-THERM-015-165_	0.98	0.92	0.97	0.90	0.87	0.90	0.89	0.91	0.81	0.86	0.92	0.84	0.58	0.74	0.61
553	LEU-COMP-THERM-016-001_	0.94	0.87	0.92	0.87	0.85	0.90	0.88	0.88	0.80	0.87	0.91	0.84	0.57	0.69	0.54
554	LEU-COMP-THERM-016-002_	0.94	0.85	0.92	0.86	0.83	0.90	0.87	0.87	0.79	0.87	0.91	0.84	0.58	0.69	0.53
555	LEU-COMP-THERM-016-003_	0.94	0.86	0.92	0.86	0.83	0.90	0.87	0.87	0.79	0.87	0.90	0.84	0.57	0.69	0.53
556	LEU-COMP-THERM-016-004_	0.94	0.86	0.92	0.87	0.84	0.90	0.87	0.88	0.80	0.87	0.91	0.84	0.57	0.69	0.54
557	LEU-COMP-THERM-016-005_	0.94	0.86	0.92	0.87	0.84	0.90	0.87	0.87	0.79	0.87	0.91	0.84	0.57	0.69	0.54
558	LEU-COMP-THERM-016-006_	0.95	0.87	0.93	0.87	0.85	0.90	0.88	0.88	0.80	0.87	0.91	0.84	0.56	0.69	0.54
559	LEU-COMP-THERM-016-007_	0.95	0.88	0.93	0.88	0.85	0.90	0.87	0.88	0.80	0.86	0.90	0.83	0.56	0.69	0.54
560	LEU-COMP-THERM-016-008_	0.94	0.85	0.92	0.85	0.83	0.89	0.86	0.86	0.78	0.87	0.90	0.84	0.58	0.69	0.53
561	LEU-COMP-THERM-016-009_	0.95	0.87	0.93	0.87	0.85	0.90	0.87	0.88	0.79	0.86	0.90	0.83	0.56	0.69	0.54
562	LEU-COMP-THERM-016-010_	0.95	0.87	0.93	0.87	0.84	0.90	0.87	0.87	0.79	0.87	0.90	0.84	0.57	0.69	0.54
563	LEU-COMP-THERM-016-011_	0.95	0.88	0.93	0.88	0.85	0.90	0.88	0.88	0.80	0.86	0.90	0.83	0.55	0.69	0.54
564	LEU-COMP-THERM-016-012_	0.95	0.87	0.93	0.87	0.85	0.90	0.87	0.88	0.79	0.86	0.90	0.83	0.56	0.69	0.54
565	LEU-COMP-THERM-016-013_	0.95	0.87	0.93	0.87	0.84	0.90	0.87	0.87	0.79	0.87	0.90	0.84	0.57	0.69	0.54
566	LEU-COMP-THERM-016-014_	0.95	0.87	0.93	0.87	0.85	0.90	0.87	0.88	0.79	0.86	0.90	0.83	0.56	0.69	0.54
567	LEU-COMP-THERM-016-015_	0.94	0.86	0.92	0.86	0.83	0.89	0.86	0.87	0.79	0.86	0.90	0.83	0.57	0.69	0.53
568	LEU-COMP-THERM-016-016_	0.94	0.87	0.92	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
569	LEU-COMP-THERM-016-017_	0.94	0.87	0.93	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
570	LEU-COMP-THERM-016-018_	0.94	0.87	0.93	0.87	0.85	0.90	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
571	LEU-COMP-THERM-016-019_	0.94	0.87	0.92	0.86	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
572	LEU-COMP-THERM-016-020_	0.94	0.87	0.92	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
573	LEU-COMP-THERM-016-021_	0.94	0.86	0.92	0.86	0.84	0.89	0.87	0.87	0.79	0.87	0.90	0.84	0.57	0.69	0.54
574	LEU-COMP-THERM-016-022_	0.95	0.87	0.93	0.87	0.85	0.90	0.87	0.88	0.79	0.86	0.90	0.83	0.56	0.69	0.54
575	LEU-COMP-THERM-016-023_	0.94	0.86	0.92	0.86	0.83	0.89	0.87	0.87	0.79	0.87	0.90	0.84	0.57	0.69	0.53
576	LEU-COMP-THERM-016-024_	0.95	0.88	0.93	0.87	0.85	0.90	0.87	0.88	0.79	0.86	0.90	0.83	0.56	0.69	0.54
577	LEU-COMP-THERM-016-025_	0.95	0.88	0.93	0.87	0.85	0.90	0.87	0.88	0.80	0.86	0.90	0.83	0.56	0.69	0.54
578	LEU-COMP-THERM-016-026_	0.95	0.88	0.93	0.88	0.86	0.90	0.88	0.88	0.80	0.86	0.90	0.83	0.55	0.69	0.54
579	LEU-COMP-THERM-016-027_	0.95	0.88	0.93	0.88	0.85	0.90	0.88	0.88	0.80	0.86	0.90	0.83	0.56	0.69	0.54
580	LEU-COMP-THERM-016-028_	0.94	0.86	0.92	0.86	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.53
581	LEU-COMP-THERM-016-029_	0.94	0.86	0.92	0.86	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.53
582	LEU-COMP-THERM-016-030_	0.94	0.87	0.92	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
583	LEU-COMP-THERM-016-031_	0.94	0.86	0.92	0.86	0.84	0.89	0.87	0.87	0.79	0.87	0.90	0.83	0.56	0.69	0.53
584	LEU-COMP-THERM-016-032_	0.94	0.87	0.92	0.87	0.84	0.89	0.87	0.87	0.79	0.86	0.90	0.83	0.56	0.69	0.54
585	LEU-COMP-THERM-017-001_	0.93	0.85	0.91	0.85	0.82	0.89	0.86	0.86	0.78	0.87	0.90	0.84	0.58	0.69	0.53
586	LEU-COMP-THERM-017-002_	0.93	0.85	0.92	0.85	0.83	0.89	0.86	0.86	0.78	0.87	0.90	0.84	0.57	0.69	0.53
587	LEU-COMP-THERM-017-003_	0.93	0.85	0.91	0.85	0.82	0.89	0.86	0.86	0.78	0.87	0.90	0.84	0.57	0.69	0.53
588	LEU-COMP-THERM-017-004_	0.88	0.75	0.86	0.76	0.73	0.86	0.80	0.80	0.71	0.88	0.88	0.84	0.65	0.70	0.50

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
589	LEU-COMP-THERM-017-005_	0.90	0.79	0.88	0.80	0.77	0.87	0.82	0.83	0.74	0.88	0.89	0.84	0.63	0.70	0.52
590	LEU-COMP-THERM-017-006_	0.91	0.80	0.89	0.81	0.78	0.88	0.83	0.83	0.75	0.88	0.89	0.84	0.61	0.70	0.52
591	LEU-COMP-THERM-017-007_	0.91	0.80	0.89	0.81	0.78	0.88	0.83	0.83	0.75	0.88	0.89	0.84	0.61	0.69	0.52
592	LEU-COMP-THERM-017-008_	0.92	0.83	0.90	0.83	0.80	0.88	0.84	0.85	0.76	0.87	0.89	0.84	0.59	0.69	0.52
593	LEU-COMP-THERM-017-009_	0.93	0.85	0.91	0.85	0.82	0.89	0.86	0.86	0.78	0.87	0.90	0.83	0.57	0.68	0.53
594	LEU-COMP-THERM-017-010_	0.92	0.82	0.90	0.84	0.81	0.91	0.87	0.88	0.80	0.90	0.92	0.87	0.61	0.71	0.53
595	LEU-COMP-THERM-017-011_	0.93	0.83	0.91	0.86	0.83	0.92	0.88	0.89	0.81	0.90	0.93	0.87	0.60	0.71	0.54
596	LEU-COMP-THERM-017-012_	0.93	0.83	0.91	0.85	0.82	0.91	0.87	0.87	0.79	0.90	0.92	0.86	0.60	0.70	0.53
597	LEU-COMP-THERM-017-013_	0.93	0.83	0.91	0.85	0.82	0.90	0.86	0.87	0.78	0.89	0.91	0.85	0.59	0.70	0.53
598	LEU-COMP-THERM-017-014_	0.93	0.84	0.91	0.85	0.82	0.89	0.86	0.87	0.78	0.88	0.91	0.85	0.58	0.69	0.53
599	LEU-COMP-THERM-017-015_	0.89	0.77	0.87	0.80	0.76	0.89	0.84	0.86	0.76	0.91	0.91	0.88	0.68	0.75	0.56
600	LEU-COMP-THERM-017-016_	0.91	0.79	0.89	0.82	0.78	0.90	0.85	0.87	0.77	0.91	0.92	0.88	0.66	0.75	0.56
601	LEU-COMP-THERM-017-017_	0.92	0.79	0.90	0.81	0.77	0.89	0.84	0.86	0.76	0.90	0.91	0.87	0.66	0.75	0.56
602	LEU-COMP-THERM-017-018_	0.92	0.80	0.90	0.81	0.77	0.89	0.84	0.86	0.75	0.90	0.91	0.87	0.66	0.75	0.56
603	LEU-COMP-THERM-017-019_	0.92	0.80	0.90	0.82	0.78	0.89	0.84	0.86	0.75	0.90	0.91	0.87	0.65	0.74	0.56
604	LEU-COMP-THERM-017-020_	0.93	0.81	0.91	0.82	0.78	0.89	0.84	0.86	0.75	0.89	0.91	0.86	0.64	0.74	0.56
605	LEU-COMP-THERM-017-021_	0.94	0.82	0.92	0.82	0.79	0.88	0.84	0.86	0.75	0.89	0.91	0.85	0.64	0.74	0.56
606	LEU-COMP-THERM-017-022_	0.94	0.83	0.92	0.83	0.79	0.88	0.84	0.85	0.74	0.88	0.90	0.84	0.62	0.73	0.56
607	LEU-COMP-THERM-017-023_	0.92	0.81	0.91	0.81	0.77	0.86	0.82	0.84	0.72	0.87	0.89	0.84	0.63	0.73	0.56
608	LEU-COMP-THERM-017-024_	0.93	0.82	0.91	0.81	0.77	0.87	0.82	0.84	0.73	0.87	0.89	0.84	0.63	0.73	0.56
609	LEU-COMP-THERM-017-025_	0.93	0.82	0.91	0.81	0.77	0.87	0.82	0.84	0.73	0.88	0.89	0.84	0.63	0.73	0.55
610	LEU-COMP-THERM-017-026_	0.82	0.66	0.80	0.66	0.62	0.80	0.71	0.73	0.62	0.86	0.83	0.82	0.71	0.72	0.50
611	LEU-COMP-THERM-017-027_	0.87	0.72	0.85	0.72	0.68	0.83	0.76	0.77	0.66	0.87	0.86	0.83	0.69	0.73	0.53
612	LEU-COMP-THERM-017-028_	0.89	0.75	0.87	0.75	0.71	0.84	0.78	0.79	0.68	0.88	0.87	0.84	0.68	0.73	0.53
613	LEU-COMP-THERM-017-029_	0.90	0.77	0.88	0.77	0.73	0.85	0.79	0.81	0.70	0.88	0.88	0.84	0.67	0.73	0.54
614	LEU-COMP-THERM-018-001_	0.95	0.98	0.95	0.99	0.99	0.92	0.96	0.96	0.93	0.79	0.90	0.79	0.46	0.67	0.59
615	LEU-COMP-THERM-020-001_	0.92	0.92	0.92	0.93	0.93	0.90	0.93	0.90	0.88	0.81	0.89	0.80	0.46	0.62	0.52
616	LEU-COMP-THERM-020-002_	0.91	0.93	0.91	0.93	0.93	0.88	0.91	0.89	0.87	0.78	0.87	0.77	0.43	0.60	0.51
617	LEU-COMP-THERM-020-003_	0.91	0.92	0.90	0.92	0.93	0.88	0.91	0.88	0.87	0.78	0.86	0.76	0.42	0.60	0.51
618	LEU-COMP-THERM-020-004_	0.91	0.92	0.90	0.92	0.93	0.87	0.91	0.88	0.87	0.77	0.86	0.76	0.42	0.59	0.50
619	LEU-COMP-THERM-020-005_	0.91	0.92	0.90	0.92	0.93	0.87	0.91	0.88	0.86	0.77	0.86	0.76	0.42	0.59	0.50
620	LEU-COMP-THERM-020-006_	0.91	0.92	0.90	0.92	0.93	0.87	0.90	0.88	0.86	0.77	0.85	0.75	0.42	0.59	0.50
621	LEU-COMP-THERM-020-007_	0.90	0.92	0.89	0.91	0.92	0.87	0.90	0.87	0.86	0.77	0.85	0.75	0.42	0.59	0.50
622	LEU-COMP-THERM-021-001_	0.98	0.95	0.97	0.93	0.93	0.91	0.93	0.92	0.87	0.85	0.92	0.84	0.52	0.69	0.58
623	LEU-COMP-THERM-021-002_	0.97	0.95	0.97	0.93	0.93	0.91	0.93	0.92	0.87	0.84	0.92	0.83	0.52	0.69	0.57
624	LEU-COMP-THERM-021-003_	0.97	0.95	0.97	0.93	0.93	0.91	0.93	0.92	0.87	0.85	0.92	0.83	0.52	0.69	0.57
625	LEU-COMP-THERM-021-004_	0.91	0.86	0.91	0.86	0.86	0.90	0.89	0.87	0.84	0.86	0.91	0.85	0.52	0.65	0.51
626	LEU-COMP-THERM-021-005_	0.91	0.87	0.91	0.87	0.87	0.90	0.89	0.87	0.84	0.86	0.91	0.84	0.52	0.64	0.51
627	LEU-COMP-THERM-021-006_	0.91	0.87	0.91	0.87	0.87	0.89	0.89	0.87	0.84	0.86	0.90	0.84	0.52	0.64	0.51
628	LEU-COMP-THERM-022-001_	0.93	0.92	0.93	0.96	0.94	0.96	0.98	0.99	0.96	0.88	0.95	0.88	0.62	0.78	0.68
629	LEU-COMP-THERM-022-002_	0.92	0.94	0.92	0.98	0.98	0.96	0.99	0.98	0.97	0.84	0.93	0.84	0.53	0.71	0.62
630	LEU-COMP-THERM-022-003_	0.88	0.92	0.88	0.96	0.97	0.93	0.97	0.95	0.97	0.80	0.89	0.80	0.46	0.63	0.55

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
631	LEU-COMP-THERM-022-004_	0.86	0.89	0.86	0.94	0.95	0.92	0.95	0.93	0.95	0.79	0.87	0.78	0.44	0.60	0.51
632	LEU-COMP-THERM-022-005_	0.84	0.87	0.84	0.92	0.93	0.91	0.94	0.91	0.94	0.79	0.87	0.79	0.44	0.59	0.49
633	LEU-COMP-THERM-022-006_	0.81	0.80	0.80	0.86	0.86	0.89	0.89	0.87	0.89	0.82	0.86	0.80	0.47	0.58	0.46
634	LEU-COMP-THERM-022-007_	0.81	0.79	0.80	0.85	0.86	0.90	0.89	0.87	0.89	0.82	0.87	0.81	0.47	0.58	0.46
635	LEU-COMP-THERM-023-001_	0.85	0.89	0.85	0.93	0.95	0.92	0.95	0.92	0.95	0.80	0.88	0.79	0.45	0.60	0.50
636	LEU-COMP-THERM-023-002_	0.85	0.89	0.85	0.93	0.95	0.91	0.95	0.92	0.95	0.79	0.87	0.78	0.44	0.59	0.50
637	LEU-COMP-THERM-023-003_	0.85	0.88	0.85	0.93	0.94	0.91	0.95	0.91	0.94	0.78	0.87	0.78	0.44	0.59	0.50
638	LEU-COMP-THERM-023-004_	0.85	0.88	0.85	0.93	0.94	0.91	0.94	0.91	0.94	0.78	0.86	0.78	0.43	0.59	0.50
639	LEU-COMP-THERM-023-005_	0.84	0.88	0.84	0.93	0.94	0.91	0.94	0.91	0.94	0.78	0.86	0.78	0.43	0.59	0.49
640	LEU-COMP-THERM-023-006_	0.84	0.88	0.84	0.92	0.94	0.91	0.94	0.91	0.94	0.78	0.86	0.78	0.44	0.59	0.49
641	LEU-COMP-THERM-024-001_	0.92	0.89	0.93	0.93	0.91	0.95	0.95	0.98	0.93	0.88	0.94	0.89	0.66	0.81	0.71
642	LEU-COMP-THERM-024-002_	0.89	0.91	0.89	0.96	0.97	0.94	0.98	0.96	0.97	0.82	0.91	0.82	0.49	0.65	0.56
643	LEU-COMP-THERM-026-001_	0.99	0.98	0.98	0.95	0.94	0.89	0.92	0.93	0.85	0.80	0.90	0.79	0.50	0.71	0.62
644	LEU-COMP-THERM-026-002_	0.99	0.96	0.99	0.94	0.91	0.89	0.90	0.92	0.83	0.82	0.90	0.81	0.54	0.73	0.63
645	LEU-COMP-THERM-026-003_	0.93	0.83	0.93	0.80	0.76	0.83	0.80	0.84	0.71	0.83	0.87	0.82	0.68	0.80	0.68
646	LEU-COMP-THERM-026-004_	0.88	0.76	0.88	0.73	0.69	0.80	0.75	0.79	0.66	0.84	0.85	0.82	0.75	0.82	0.68
647	LEU-COMP-THERM-026-005_	0.99	0.94	0.98	0.91	0.89	0.89	0.90	0.92	0.82	0.84	0.91	0.83	0.58	0.76	0.65
648	LEU-COMP-THERM-026-006_	0.98	0.92	0.98	0.90	0.87	0.89	0.89	0.91	0.81	0.85	0.91	0.84	0.61	0.77	0.66
649	LEU-COMP-THERM-027-001_	0.91	0.90	0.91	0.90	0.89	0.86	0.88	0.87	0.83	0.78	0.86	0.77	0.47	0.64	0.54
650	LEU-COMP-THERM-027-002_	0.92	0.91	0.92	0.91	0.90	0.87	0.89	0.88	0.84	0.79	0.87	0.78	0.47	0.65	0.54
651	LEU-COMP-THERM-027-003_	0.93	0.92	0.92	0.92	0.91	0.88	0.90	0.89	0.85	0.80	0.88	0.79	0.48	0.65	0.55
652	LEU-COMP-THERM-027-004_	0.94	0.92	0.93	0.92	0.92	0.89	0.91	0.90	0.86	0.81	0.89	0.80	0.49	0.66	0.55
653	LEU-COMP-THERM-028-001_	0.92	0.88	0.91	0.94	0.91	0.98	0.97	0.98	0.94	0.91	0.96	0.90	0.60	0.74	0.60
654	LEU-COMP-THERM-028-002_	0.91	0.86	0.91	0.92	0.89	0.98	0.96	0.98	0.93	0.93	0.97	0.92	0.63	0.75	0.60
655	LEU-COMP-THERM-028-003_	0.90	0.83	0.90	0.89	0.86	0.98	0.94	0.97	0.92	0.95	0.97	0.93	0.66	0.77	0.60
656	LEU-COMP-THERM-028-004_	0.89	0.80	0.88	0.87	0.84	0.97	0.93	0.95	0.90	0.96	0.97	0.95	0.69	0.77	0.59
657	LEU-COMP-THERM-028-005_	0.91	0.86	0.90	0.92	0.89	0.97	0.95	0.97	0.93	0.92	0.96	0.91	0.62	0.75	0.60
658	LEU-COMP-THERM-028-006_	0.87	0.80	0.87	0.86	0.83	0.95	0.91	0.93	0.89	0.92	0.94	0.91	0.65	0.74	0.58
659	LEU-COMP-THERM-028-007_	0.90	0.84	0.89	0.90	0.88	0.96	0.94	0.96	0.92	0.93	0.96	0.93	0.62	0.74	0.59
660	LEU-COMP-THERM-028-008_	0.85	0.79	0.85	0.85	0.82	0.92	0.89	0.91	0.87	0.92	0.94	0.94	0.62	0.72	0.57
661	LEU-COMP-THERM-028-009_	0.80	0.73	0.80	0.79	0.76	0.88	0.84	0.86	0.82	0.90	0.91	0.92	0.61	0.69	0.54
662	LEU-COMP-THERM-028-010_	0.89	0.86	0.89	0.93	0.92	0.98	0.97	0.97	0.95	0.91	0.95	0.89	0.57	0.70	0.55
663	LEU-COMP-THERM-028-011_	0.89	0.84	0.88	0.91	0.89	0.98	0.96	0.96	0.94	0.94	0.96	0.92	0.61	0.71	0.55
664	LEU-COMP-THERM-028-012_	0.86	0.78	0.86	0.86	0.84	0.98	0.93	0.94	0.91	0.96	0.97	0.94	0.65	0.73	0.54
665	LEU-COMP-THERM-028-013_	0.86	0.81	0.86	0.88	0.86	0.95	0.93	0.93	0.91	0.93	0.95	0.93	0.59	0.69	0.54
666	LEU-COMP-THERM-028-014_	0.77	0.69	0.76	0.76	0.74	0.86	0.82	0.83	0.81	0.89	0.89	0.92	0.58	0.64	0.48
667	LEU-COMP-THERM-028-015_	0.85	0.79	0.84	0.87	0.86	0.96	0.92	0.92	0.91	0.92	0.94	0.90	0.58	0.67	0.51
668	LEU-COMP-THERM-028-016_	0.84	0.77	0.83	0.85	0.84	0.95	0.91	0.91	0.90	0.93	0.94	0.91	0.60	0.67	0.51
669	LEU-COMP-THERM-028-017_	0.80	0.69	0.79	0.78	0.76	0.93	0.86	0.87	0.85	0.95	0.93	0.92	0.64	0.68	0.48
670	LEU-COMP-THERM-028-018_	0.82	0.73	0.81	0.81	0.79	0.94	0.89	0.89	0.87	0.94	0.93	0.92	0.63	0.68	0.50
671	LEU-COMP-THERM-028-019_	0.82	0.75	0.81	0.83	0.81	0.94	0.89	0.89	0.88	0.93	0.94	0.93	0.59	0.66	0.50
672	LEU-COMP-THERM-028-020_	0.78	0.69	0.77	0.77	0.75	0.90	0.84	0.85	0.83	0.92	0.91	0.93	0.59	0.64	0.47

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
673	LEU-COMP-THERM-029-001_	0.96	0.96	0.95	0.96	0.96	0.90	0.93	0.92	0.88	0.79	0.89	0.78	0.46	0.66	0.56
674	LEU-COMP-THERM-029-002_	0.96	0.96	0.95	0.96	0.96	0.90	0.93	0.92	0.88	0.79	0.89	0.78	0.46	0.66	0.56
675	LEU-COMP-THERM-029-003_	0.96	0.96	0.95	0.96	0.96	0.90	0.93	0.92	0.88	0.79	0.89	0.78	0.46	0.66	0.56
676	LEU-COMP-THERM-029-004_	0.96	0.96	0.95	0.96	0.96	0.90	0.93	0.92	0.88	0.79	0.89	0.79	0.46	0.66	0.56
677	LEU-COMP-THERM-029-005_	0.96	0.96	0.95	0.96	0.96	0.90	0.93	0.92	0.88	0.80	0.89	0.79	0.46	0.66	0.57
678	LEU-COMP-THERM-029-006_	0.96	0.96	0.95	0.95	0.95	0.90	0.93	0.92	0.88	0.80	0.89	0.79	0.47	0.67	0.57
679	LEU-COMP-THERM-029-007_	0.96	0.96	0.95	0.95	0.95	0.90	0.93	0.92	0.88	0.80	0.89	0.79	0.47	0.66	0.57
680	LEU-COMP-THERM-029-008_	0.95	0.96	0.95	0.95	0.95	0.90	0.93	0.92	0.88	0.80	0.89	0.79	0.47	0.66	0.56
681	LEU-COMP-THERM-029-009_	0.95	0.96	0.95	0.96	0.96	0.89	0.93	0.92	0.88	0.78	0.88	0.78	0.45	0.65	0.56
682	LEU-COMP-THERM-029-010_	0.95	0.96	0.94	0.96	0.96	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.45	0.65	0.56
683	LEU-COMP-THERM-029-011_	0.95	0.96	0.94	0.96	0.96	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.45	0.65	0.56
684	LEU-COMP-THERM-029-012_	0.95	0.96	0.94	0.96	0.96	0.89	0.93	0.91	0.88	0.78	0.88	0.77	0.45	0.65	0.56
685	LEU-COMP-THERM-030-001_	0.98	0.92	0.97	0.90	0.87	0.89	0.88	0.91	0.80	0.84	0.91	0.83	0.57	0.74	0.62
686	LEU-COMP-THERM-030-002_	0.99	0.93	0.97	0.91	0.88	0.88	0.89	0.91	0.80	0.84	0.90	0.82	0.56	0.74	0.61
687	LEU-COMP-THERM-030-003_	0.99	0.93	0.98	0.91	0.88	0.88	0.89	0.91	0.80	0.83	0.90	0.82	0.55	0.73	0.61
688	LEU-COMP-THERM-030-004_	0.99	0.94	0.98	0.91	0.89	0.88	0.89	0.91	0.81	0.83	0.90	0.81	0.55	0.73	0.61
689	LEU-COMP-THERM-030-005_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.90	0.82	0.55	0.73	0.61
690	LEU-COMP-THERM-030-006_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.90	0.82	0.55	0.73	0.61
691	LEU-COMP-THERM-030-007_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.90	0.81	0.55	0.73	0.61
692	LEU-COMP-THERM-030-008_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.91	0.82	0.55	0.73	0.61
693	LEU-COMP-THERM-030-009_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.90	0.81	0.54	0.73	0.61
694	LEU-COMP-THERM-030-010_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.90	0.82	0.55	0.73	0.61
695	LEU-COMP-THERM-030-011_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.83	0.91	0.82	0.55	0.73	0.61
696	LEU-COMP-THERM-030-012_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.55	0.73	0.61
697	LEU-COMP-THERM-031-001_	0.99	0.95	0.98	0.93	0.91	0.89	0.90	0.92	0.83	0.83	0.91	0.82	0.55	0.74	0.63
698	LEU-COMP-THERM-031-002_	0.99	0.95	0.98	0.93	0.90	0.89	0.90	0.92	0.83	0.83	0.91	0.82	0.55	0.74	0.63
699	LEU-COMP-THERM-031-003_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.83	0.82	0.90	0.81	0.54	0.73	0.63
700	LEU-COMP-THERM-031-004_	0.99	0.96	0.98	0.93	0.91	0.89	0.91	0.92	0.83	0.82	0.90	0.81	0.54	0.73	0.63
701	LEU-COMP-THERM-031-005_	0.99	0.96	0.98	0.93	0.91	0.89	0.91	0.92	0.83	0.82	0.91	0.81	0.54	0.73	0.63
702	LEU-COMP-THERM-031-006_	0.99	0.96	0.98	0.93	0.91	0.89	0.90	0.92	0.83	0.82	0.91	0.81	0.54	0.73	0.63
703	LEU-COMP-THERM-032-001_	0.93	0.92	0.93	0.96	0.95	0.96	0.97	0.99	0.95	0.87	0.94	0.87	0.61	0.77	0.68
704	LEU-COMP-THERM-032-002_	0.93	0.91	0.93	0.95	0.94	0.95	0.97	0.98	0.95	0.87	0.94	0.88	0.62	0.79	0.69
705	LEU-COMP-THERM-032-003_	0.92	0.88	0.92	0.92	0.91	0.95	0.95	0.97	0.93	0.89	0.94	0.89	0.67	0.81	0.72
706	LEU-COMP-THERM-032-004_	0.84	0.87	0.84	0.92	0.94	0.91	0.94	0.91	0.94	0.79	0.87	0.79	0.44	0.59	0.49
707	LEU-COMP-THERM-032-005_	0.84	0.88	0.84	0.93	0.95	0.91	0.95	0.92	0.95	0.78	0.86	0.78	0.44	0.59	0.50
708	LEU-COMP-THERM-032-006_	0.85	0.89	0.85	0.94	0.95	0.91	0.95	0.92	0.95	0.78	0.86	0.78	0.44	0.59	0.51
709	LEU-COMP-THERM-032-007_	0.80	0.79	0.80	0.85	0.86	0.90	0.89	0.87	0.89	0.83	0.87	0.81	0.48	0.58	0.46
710	LEU-COMP-THERM-032-008_	0.81	0.82	0.81	0.87	0.89	0.90	0.91	0.88	0.91	0.81	0.87	0.80	0.46	0.58	0.47
711	LEU-COMP-THERM-032-009_	0.82	0.84	0.82	0.89	0.90	0.91	0.92	0.89	0.92	0.81	0.87	0.80	0.46	0.58	0.47
712	LEU-COMP-THERM-033-001_	0.74	0.57	0.72	0.58	0.53	0.72	0.64	0.65	0.53	0.80	0.76	0.76	0.73	0.75	0.54
713	LEU-COMP-THERM-033-002_	0.74	0.58	0.73	0.59	0.54	0.73	0.65	0.66	0.54	0.80	0.76	0.76	0.74	0.77	0.55
714	LEU-COMP-THERM-033-003_	0.75	0.58	0.73	0.59	0.54	0.73	0.64	0.66	0.54	0.80	0.76	0.76	0.73	0.77	0.55

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
715	LEU-COMP-THERM-033-004_	0.74	0.58	0.72	0.58	0.54	0.72	0.64	0.66	0.53	0.80	0.76	0.76	0.74	0.77	0.55
716	LEU-COMP-THERM-033-005_	0.80	0.67	0.78	0.68	0.64	0.78	0.72	0.73	0.62	0.82	0.81	0.78	0.68	0.76	0.56
717	LEU-COMP-THERM-033-006_	0.80	0.67	0.78	0.67	0.63	0.78	0.72	0.72	0.62	0.82	0.81	0.78	0.69	0.76	0.56
718	LEU-COMP-THERM-033-007_	0.80	0.66	0.78	0.67	0.63	0.78	0.72	0.72	0.61	0.82	0.81	0.78	0.69	0.76	0.55
719	LEU-COMP-THERM-033-008_	0.81	0.69	0.80	0.70	0.67	0.79	0.74	0.74	0.65	0.82	0.82	0.79	0.65	0.74	0.55
720	LEU-COMP-THERM-033-009_	0.81	0.69	0.79	0.70	0.67	0.79	0.74	0.74	0.65	0.83	0.82	0.79	0.65	0.74	0.54
721	LEU-COMP-THERM-033-010_	0.80	0.69	0.79	0.70	0.68	0.80	0.75	0.74	0.66	0.82	0.82	0.79	0.63	0.70	0.51
722	LEU-COMP-THERM-033-011_	0.80	0.69	0.79	0.70	0.67	0.79	0.74	0.74	0.65	0.82	0.82	0.79	0.63	0.71	0.52
723	LEU-COMP-THERM-033-012_	0.81	0.69	0.79	0.70	0.68	0.80	0.75	0.74	0.66	0.82	0.82	0.79	0.63	0.72	0.53
724	LEU-COMP-THERM-033-013_	0.78	0.67	0.77	0.68	0.65	0.78	0.73	0.72	0.65	0.81	0.81	0.78	0.61	0.68	0.50
725	LEU-COMP-THERM-033-014_	0.66	0.52	0.65	0.53	0.51	0.68	0.61	0.60	0.53	0.76	0.72	0.73	0.59	0.59	0.39
726	LEU-COMP-THERM-033-015_	0.67	0.53	0.66	0.55	0.52	0.69	0.62	0.61	0.54	0.76	0.73	0.73	0.59	0.60	0.40
727	LEU-COMP-THERM-033-016_	0.67	0.54	0.66	0.55	0.53	0.69	0.63	0.62	0.55	0.77	0.73	0.73	0.58	0.60	0.40
728	LEU-COMP-THERM-033-017_	0.84	0.72	0.83	0.72	0.69	0.80	0.75	0.77	0.66	0.82	0.83	0.80	0.70	0.81	0.63
729	LEU-COMP-THERM-033-018_	0.84	0.73	0.83	0.72	0.69	0.80	0.75	0.77	0.65	0.82	0.83	0.79	0.69	0.81	0.64
730	LEU-COMP-THERM-033-019_	0.85	0.74	0.83	0.73	0.70	0.80	0.76	0.77	0.66	0.81	0.83	0.79	0.68	0.82	0.65
731	LEU-COMP-THERM-033-020_	0.85	0.73	0.84	0.73	0.69	0.80	0.76	0.77	0.66	0.82	0.83	0.80	0.69	0.81	0.64
732	LEU-COMP-THERM-033-021_	0.84	0.72	0.83	0.72	0.68	0.79	0.75	0.76	0.65	0.82	0.83	0.79	0.70	0.82	0.64
733	LEU-COMP-THERM-033-022_	0.88	0.82	0.87	0.83	0.81	0.84	0.84	0.83	0.76	0.80	0.85	0.79	0.58	0.75	0.60
734	LEU-COMP-THERM-033-023_	0.69	0.51	0.67	0.52	0.46	0.67	0.58	0.60	0.47	0.76	0.71	0.72	0.74	0.77	0.55
735	LEU-COMP-THERM-033-024_	0.70	0.53	0.68	0.53	0.48	0.68	0.59	0.61	0.49	0.76	0.72	0.73	0.74	0.78	0.56
736	LEU-COMP-THERM-033-025_	0.69	0.51	0.67	0.52	0.46	0.67	0.58	0.60	0.47	0.76	0.71	0.72	0.75	0.77	0.55
737	LEU-COMP-THERM-033-026_	0.77	0.63	0.75	0.63	0.59	0.75	0.68	0.69	0.58	0.81	0.79	0.77	0.70	0.77	0.56
738	LEU-COMP-THERM-033-027_	0.76	0.62	0.75	0.62	0.58	0.74	0.67	0.68	0.57	0.79	0.77	0.76	0.70	0.78	0.57
739	LEU-COMP-THERM-033-028_	0.76	0.61	0.74	0.61	0.57	0.73	0.66	0.67	0.55	0.79	0.77	0.76	0.70	0.77	0.57
740	LEU-COMP-THERM-033-029_	0.77	0.62	0.75	0.63	0.59	0.75	0.68	0.69	0.58	0.80	0.78	0.77	0.70	0.77	0.56
741	LEU-COMP-THERM-033-030_	0.79	0.66	0.78	0.67	0.63	0.78	0.72	0.72	0.62	0.83	0.81	0.79	0.67	0.73	0.53
742	LEU-COMP-THERM-033-031_	0.78	0.64	0.76	0.65	0.61	0.77	0.70	0.71	0.60	0.82	0.80	0.78	0.67	0.74	0.54
743	LEU-COMP-THERM-033-032_	0.81	0.68	0.79	0.69	0.66	0.78	0.73	0.74	0.64	0.82	0.81	0.78	0.66	0.75	0.56
744	LEU-COMP-THERM-033-033_	0.80	0.67	0.78	0.68	0.64	0.77	0.72	0.73	0.62	0.81	0.81	0.78	0.66	0.76	0.57
745	LEU-COMP-THERM-033-034_	0.80	0.68	0.79	0.69	0.65	0.78	0.73	0.73	0.63	0.81	0.81	0.78	0.66	0.76	0.57
746	LEU-COMP-THERM-033-035_	0.78	0.65	0.77	0.66	0.63	0.78	0.72	0.72	0.63	0.82	0.81	0.79	0.65	0.71	0.51
747	LEU-COMP-THERM-033-036_	0.78	0.66	0.77	0.66	0.63	0.78	0.72	0.72	0.63	0.82	0.81	0.79	0.65	0.72	0.52
748	LEU-COMP-THERM-033-037_	0.79	0.66	0.77	0.67	0.64	0.78	0.72	0.72	0.63	0.82	0.81	0.79	0.65	0.73	0.53
749	LEU-COMP-THERM-033-038_	0.79	0.66	0.77	0.67	0.64	0.77	0.72	0.72	0.62	0.81	0.81	0.78	0.65	0.73	0.54
750	LEU-COMP-THERM-033-039_	0.80	0.68	0.78	0.69	0.66	0.78	0.73	0.73	0.64	0.81	0.81	0.78	0.64	0.74	0.55
751	LEU-COMP-THERM-033-040_	0.80	0.69	0.79	0.69	0.66	0.78	0.73	0.73	0.64	0.81	0.81	0.78	0.64	0.73	0.55
752	LEU-COMP-THERM-033-041_	0.77	0.66	0.76	0.67	0.64	0.78	0.72	0.71	0.64	0.81	0.80	0.78	0.63	0.68	0.49
753	LEU-COMP-THERM-033-042_	0.77	0.64	0.75	0.65	0.62	0.76	0.70	0.70	0.62	0.81	0.80	0.78	0.63	0.70	0.51
754	LEU-COMP-THERM-033-043_	0.77	0.65	0.76	0.66	0.63	0.77	0.72	0.71	0.63	0.82	0.80	0.78	0.63	0.68	0.49
755	LEU-COMP-THERM-033-044_	0.66	0.51	0.65	0.53	0.50	0.68	0.60	0.60	0.53	0.76	0.72	0.73	0.59	0.60	0.40
756	LEU-COMP-THERM-033-045_	0.68	0.54	0.67	0.56	0.53	0.69	0.63	0.62	0.55	0.77	0.73	0.73	0.59	0.60	0.41

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
757	LEU-COMP-THERM-033-046_	0.66	0.52	0.65	0.53	0.51	0.68	0.61	0.60	0.53	0.76	0.72	0.73	0.59	0.60	0.40
758	LEU-COMP-THERM-033-047_	0.80	0.68	0.79	0.67	0.63	0.74	0.70	0.72	0.60	0.78	0.78	0.75	0.70	0.83	0.66
759	LEU-COMP-THERM-033-048_	0.77	0.63	0.75	0.62	0.58	0.72	0.66	0.68	0.56	0.77	0.76	0.74	0.71	0.83	0.65
760	LEU-COMP-THERM-033-049_	0.79	0.67	0.78	0.66	0.62	0.73	0.68	0.71	0.58	0.76	0.77	0.74	0.69	0.83	0.67
761	LEU-COMP-THERM-033-050_	0.87	0.80	0.86	0.80	0.78	0.83	0.82	0.81	0.73	0.82	0.85	0.80	0.61	0.76	0.61
762	LEU-COMP-THERM-033-051_	0.85	0.78	0.84	0.78	0.76	0.81	0.79	0.79	0.71	0.79	0.83	0.77	0.60	0.78	0.63
763	LEU-COMP-THERM-033-052_	0.87	0.79	0.86	0.80	0.77	0.83	0.81	0.81	0.73	0.82	0.85	0.80	0.61	0.77	0.61
764	LEU-COMP-THERM-034-001_	0.98	0.96	0.98	0.95	0.94	0.92	0.94	0.94	0.88	0.84	0.92	0.83	0.51	0.69	0.58
765	LEU-COMP-THERM-034-002_	0.98	0.95	0.97	0.94	0.94	0.92	0.94	0.93	0.88	0.85	0.93	0.84	0.52	0.69	0.58
766	LEU-COMP-THERM-034-003_	0.98	0.95	0.97	0.94	0.93	0.92	0.94	0.93	0.88	0.85	0.93	0.84	0.52	0.70	0.58
767	LEU-COMP-THERM-034-004_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.85	0.92	0.84	0.52	0.69	0.58
768	LEU-COMP-THERM-034-005_	0.98	0.95	0.97	0.94	0.94	0.92	0.94	0.93	0.87	0.84	0.92	0.83	0.51	0.69	0.58
769	LEU-COMP-THERM-034-006_	0.98	0.96	0.97	0.94	0.94	0.92	0.93	0.93	0.87	0.84	0.92	0.83	0.51	0.69	0.57
770	LEU-COMP-THERM-034-007_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.84	0.92	0.82	0.50	0.68	0.57
771	LEU-COMP-THERM-034-008_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.50	0.68	0.57
772	LEU-COMP-THERM-034-009_	0.98	0.95	0.98	0.93	0.92	0.92	0.93	0.92	0.86	0.85	0.92	0.84	0.53	0.70	0.58
773	LEU-COMP-THERM-034-010_	0.98	0.94	0.98	0.93	0.92	0.92	0.92	0.92	0.86	0.86	0.92	0.84	0.53	0.70	0.58
774	LEU-COMP-THERM-034-011_	0.98	0.95	0.98	0.93	0.92	0.91	0.93	0.92	0.86	0.85	0.92	0.84	0.53	0.69	0.58
775	LEU-COMP-THERM-034-012_	0.98	0.95	0.98	0.93	0.92	0.91	0.92	0.92	0.86	0.85	0.92	0.84	0.53	0.70	0.58
776	LEU-COMP-THERM-034-013_	0.98	0.95	0.98	0.93	0.92	0.91	0.93	0.92	0.86	0.85	0.92	0.84	0.52	0.69	0.58
777	LEU-COMP-THERM-034-014_	0.98	0.95	0.98	0.93	0.92	0.91	0.93	0.92	0.86	0.85	0.92	0.84	0.52	0.69	0.57
778	LEU-COMP-THERM-034-015_	0.98	0.96	0.98	0.95	0.94	0.92	0.94	0.94	0.88	0.85	0.93	0.84	0.52	0.70	0.58
779	LEU-COMP-THERM-034-016_	0.98	0.95	0.98	0.94	0.93	0.92	0.94	0.94	0.88	0.85	0.93	0.84	0.52	0.70	0.58
780	LEU-COMP-THERM-034-017_	0.98	0.95	0.97	0.94	0.93	0.92	0.94	0.93	0.87	0.85	0.93	0.84	0.52	0.70	0.58
781	LEU-COMP-THERM-034-018_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.85	0.93	0.84	0.52	0.70	0.58
782	LEU-COMP-THERM-034-019_	0.98	0.95	0.98	0.93	0.93	0.92	0.93	0.93	0.87	0.85	0.93	0.84	0.53	0.70	0.58
783	LEU-COMP-THERM-034-020_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.85	0.93	0.84	0.52	0.69	0.58
784	LEU-COMP-THERM-034-021_	0.98	0.95	0.97	0.94	0.93	0.92	0.93	0.93	0.87	0.85	0.92	0.84	0.52	0.69	0.58
785	LEU-COMP-THERM-034-022_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.85	0.92	0.84	0.52	0.69	0.58
786	LEU-COMP-THERM-034-023_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.84	0.92	0.83	0.51	0.69	0.58
787	LEU-COMP-THERM-034-024_	0.98	0.95	0.98	0.94	0.93	0.92	0.93	0.93	0.87	0.84	0.92	0.83	0.51	0.69	0.57
788	LEU-COMP-THERM-035-001_	0.98	0.91	0.96	0.89	0.85	0.88	0.87	0.89	0.78	0.84	0.90	0.82	0.57	0.73	0.59
789	LEU-COMP-THERM-035-002_	0.98	0.90	0.96	0.88	0.85	0.88	0.87	0.89	0.78	0.85	0.90	0.82	0.57	0.73	0.59
790	LEU-COMP-THERM-035-003_	0.95	0.88	0.94	0.86	0.83	0.86	0.85	0.87	0.76	0.85	0.90	0.85	0.57	0.72	0.58
791	LEU-COMP-THERM-036-001_	0.98	0.91	0.97	0.92	0.88	0.93	0.92	0.94	0.84	0.89	0.94	0.87	0.62	0.77	0.63
792	LEU-COMP-THERM-036-002_	0.97	0.89	0.96	0.90	0.87	0.92	0.91	0.93	0.83	0.89	0.94	0.87	0.63	0.77	0.63
793	LEU-COMP-THERM-036-003_	0.96	0.88	0.95	0.89	0.86	0.91	0.90	0.93	0.83	0.89	0.94	0.87	0.63	0.77	0.62
794	LEU-COMP-THERM-036-004_	0.98	0.91	0.97	0.91	0.88	0.91	0.90	0.93	0.83	0.88	0.93	0.86	0.60	0.76	0.62
795	LEU-COMP-THERM-036-005_	0.99	0.94	0.98	0.91	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.61
796	LEU-COMP-THERM-036-006_	0.98	0.92	0.97	0.91	0.88	0.90	0.90	0.92	0.82	0.86	0.92	0.84	0.58	0.75	0.62
797	LEU-COMP-THERM-036-007_	0.98	0.91	0.97	0.91	0.88	0.90	0.90	0.92	0.82	0.86	0.92	0.85	0.59	0.76	0.62
798	LEU-COMP-THERM-036-008_	0.97	0.90	0.96	0.90	0.87	0.90	0.90	0.92	0.82	0.87	0.93	0.86	0.61	0.77	0.63

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
799	LEU-COMP-THERM-036-009_	0.97	0.91	0.96	0.91	0.87	0.91	0.90	0.93	0.82	0.87	0.93	0.86	0.60	0.76	0.63
800	LEU-COMP-THERM-036-010_	0.98	0.92	0.97	0.91	0.88	0.91	0.91	0.93	0.83	0.87	0.93	0.85	0.60	0.76	0.63
801	LEU-COMP-THERM-036-011_	0.98	0.92	0.97	0.91	0.88	0.91	0.91	0.93	0.83	0.87	0.93	0.85	0.59	0.76	0.63
802	LEU-COMP-THERM-036-012_	0.97	0.88	0.96	0.88	0.85	0.91	0.89	0.91	0.81	0.89	0.93	0.87	0.64	0.78	0.62
803	LEU-COMP-THERM-036-013_	0.98	0.89	0.97	0.88	0.85	0.89	0.88	0.90	0.80	0.88	0.92	0.86	0.62	0.76	0.62
804	LEU-COMP-THERM-036-014_	0.96	0.87	0.95	0.86	0.83	0.90	0.88	0.90	0.79	0.89	0.93	0.87	0.64	0.77	0.62
805	LEU-COMP-THERM-036-015_	0.95	0.86	0.94	0.86	0.83	0.90	0.88	0.90	0.80	0.90	0.93	0.88	0.66	0.78	0.62
806	LEU-COMP-THERM-036-016_	0.91	0.78	0.89	0.77	0.73	0.85	0.79	0.82	0.69	0.87	0.88	0.83	0.66	0.74	0.55
807	LEU-COMP-THERM-036-017_	0.91	0.78	0.89	0.77	0.72	0.84	0.79	0.81	0.69	0.87	0.87	0.83	0.65	0.74	0.55
808	LEU-COMP-THERM-036-018_	0.92	0.80	0.90	0.79	0.75	0.85	0.80	0.83	0.70	0.87	0.88	0.83	0.64	0.74	0.56
809	LEU-COMP-THERM-036-019_	0.92	0.81	0.90	0.80	0.75	0.85	0.81	0.83	0.71	0.87	0.88	0.83	0.64	0.74	0.56
810	LEU-COMP-THERM-036-020_	0.93	0.81	0.90	0.80	0.75	0.85	0.80	0.83	0.70	0.86	0.88	0.83	0.64	0.73	0.56
811	LEU-COMP-THERM-036-021_	0.93	0.81	0.90	0.80	0.75	0.85	0.81	0.83	0.71	0.87	0.88	0.83	0.64	0.73	0.56
812	LEU-COMP-THERM-036-022_	0.93	0.81	0.90	0.80	0.76	0.85	0.81	0.83	0.71	0.87	0.88	0.83	0.64	0.73	0.56
813	LEU-COMP-THERM-036-023_	0.92	0.80	0.90	0.79	0.74	0.85	0.80	0.82	0.70	0.87	0.88	0.83	0.64	0.74	0.56
814	LEU-COMP-THERM-036-024_	0.95	0.84	0.93	0.83	0.79	0.86	0.83	0.85	0.73	0.86	0.89	0.83	0.62	0.74	0.57
815	LEU-COMP-THERM-036-025_	0.88	0.77	0.86	0.78	0.75	0.85	0.80	0.80	0.72	0.87	0.88	0.83	0.58	0.66	0.49
816	LEU-COMP-THERM-036-026_	0.88	0.77	0.86	0.78	0.75	0.85	0.80	0.80	0.72	0.87	0.87	0.83	0.58	0.66	0.49
817	LEU-COMP-THERM-036-027_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
818	LEU-COMP-THERM-036-028_	0.99	0.93	0.97	0.90	0.88	0.89	0.89	0.91	0.80	0.85	0.91	0.83	0.57	0.74	0.62
819	LEU-COMP-THERM-036-029_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.84	0.59	0.75	0.62
820	LEU-COMP-THERM-036-030_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.62
821	LEU-COMP-THERM-036-031_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
822	LEU-COMP-THERM-036-032_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.56	0.74	0.62
823	LEU-COMP-THERM-036-033_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.57	0.74	0.62
824	LEU-COMP-THERM-036-034_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.56	0.74	0.62
825	LEU-COMP-THERM-036-035_	0.98	0.92	0.97	0.89	0.87	0.89	0.88	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.62
826	LEU-COMP-THERM-036-036_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.84	0.58	0.75	0.62
827	LEU-COMP-THERM-036-037_	0.99	0.93	0.97	0.91	0.88	0.89	0.89	0.91	0.80	0.85	0.91	0.83	0.57	0.74	0.62
828	LEU-COMP-THERM-036-038_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.62
829	LEU-COMP-THERM-036-039_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.62
830	LEU-COMP-THERM-036-040_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.80	0.84	0.91	0.83	0.57	0.74	0.62
831	LEU-COMP-THERM-036-041_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.79	0.86	0.92	0.85	0.59	0.75	0.62
832	LEU-COMP-THERM-036-042_	0.98	0.91	0.97	0.89	0.86	0.89	0.88	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.62
833	LEU-COMP-THERM-036-043_	0.99	0.92	0.97	0.90	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.58	0.75	0.62
834	LEU-COMP-THERM-036-044_	0.99	0.93	0.97	0.90	0.88	0.89	0.89	0.91	0.81	0.85	0.92	0.84	0.57	0.74	0.62
835	LEU-COMP-THERM-036-045_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.62
836	LEU-COMP-THERM-036-046_	0.93	0.81	0.91	0.80	0.76	0.86	0.81	0.83	0.71	0.87	0.89	0.83	0.64	0.73	0.56
837	LEU-COMP-THERM-036-047_	0.92	0.80	0.90	0.79	0.74	0.85	0.80	0.83	0.70	0.87	0.88	0.83	0.64	0.74	0.56
838	LEU-COMP-THERM-036-048_	0.95	0.86	0.93	0.84	0.80	0.87	0.84	0.86	0.74	0.86	0.89	0.83	0.61	0.74	0.58
839	LEU-COMP-THERM-036-049_	0.94	0.84	0.92	0.82	0.78	0.86	0.83	0.85	0.73	0.86	0.89	0.83	0.62	0.74	0.57
840	LEU-COMP-THERM-036-050_	0.98	0.89	0.96	0.88	0.85	0.90	0.88	0.90	0.80	0.88	0.93	0.86	0.62	0.76	0.61

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
841	LEU-COMP-THERM-036-051_	0.98	0.91	0.97	0.90	0.87	0.90	0.89	0.91	0.81	0.87	0.92	0.85	0.60	0.75	0.61
842	LEU-COMP-THERM-036-052_	0.97	0.89	0.96	0.88	0.85	0.90	0.88	0.90	0.80	0.88	0.93	0.86	0.62	0.75	0.60
843	LEU-COMP-THERM-036-053_	0.98	0.92	0.97	0.91	0.88	0.91	0.90	0.92	0.82	0.87	0.93	0.85	0.59	0.74	0.61
844	LEU-COMP-THERM-036-054_	0.99	0.92	0.97	0.91	0.89	0.91	0.90	0.92	0.82	0.87	0.93	0.85	0.58	0.75	0.61
845	LEU-COMP-THERM-036-055_	0.99	0.93	0.98	0.92	0.89	0.91	0.91	0.92	0.83	0.86	0.93	0.84	0.58	0.74	0.62
846	LEU-COMP-THERM-036-056_	0.97	0.89	0.96	0.88	0.85	0.90	0.88	0.89	0.80	0.88	0.93	0.86	0.62	0.75	0.60
847	LEU-COMP-THERM-036-057_	0.98	0.89	0.96	0.88	0.85	0.90	0.88	0.90	0.80	0.88	0.92	0.86	0.61	0.75	0.61
848	LEU-COMP-THERM-036-058_	0.98	0.91	0.97	0.89	0.87	0.90	0.89	0.90	0.80	0.87	0.92	0.85	0.60	0.75	0.61
849	LEU-COMP-THERM-036-059_	0.98	0.91	0.97	0.90	0.87	0.90	0.89	0.90	0.80	0.86	0.92	0.85	0.59	0.75	0.61
850	LEU-COMP-THERM-036-060_	0.98	0.91	0.97	0.89	0.87	0.90	0.89	0.90	0.80	0.87	0.92	0.85	0.60	0.75	0.61
851	LEU-COMP-THERM-036-061_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.84	0.91	0.83	0.56	0.74	0.62
852	LEU-COMP-THERM-036-062_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.55	0.73	0.61
853	LEU-COMP-THERM-036-063_	0.99	0.94	0.98	0.92	0.89	0.89	0.89	0.91	0.81	0.84	0.91	0.82	0.56	0.74	0.61
854	LEU-COMP-THERM-036-064_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.82	0.84	0.91	0.83	0.56	0.73	0.61
855	LEU-COMP-THERM-036-065_	0.99	0.93	0.98	0.91	0.88	0.89	0.89	0.91	0.81	0.85	0.91	0.83	0.57	0.74	0.61
856	LEU-COMP-THERM-036-066_	0.99	0.93	0.98	0.92	0.89	0.89	0.90	0.91	0.81	0.85	0.91	0.83	0.56	0.73	0.61
857	LEU-COMP-THERM-036-067_	0.99	0.95	0.98	0.93	0.91	0.90	0.91	0.92	0.84	0.84	0.92	0.82	0.53	0.71	0.60
858	LEU-COMP-THERM-036-068_	0.97	0.89	0.96	0.88	0.86	0.91	0.89	0.90	0.81	0.89	0.93	0.87	0.59	0.72	0.57
859	LEU-COMP-THERM-036-069_	0.98	0.93	0.97	0.92	0.90	0.90	0.90	0.91	0.83	0.86	0.92	0.84	0.54	0.71	0.58
860	LEU-COMP-THERM-037-001_	0.96	0.98	0.95	0.96	0.96	0.89	0.93	0.92	0.87	0.77	0.88	0.77	0.43	0.64	0.56
861	LEU-COMP-THERM-037-002_	0.96	0.98	0.96	0.96	0.96	0.88	0.93	0.92	0.87	0.77	0.87	0.76	0.43	0.64	0.56
862	LEU-COMP-THERM-037-003_	0.96	0.97	0.95	0.96	0.95	0.89	0.93	0.92	0.87	0.77	0.88	0.77	0.44	0.64	0.56
863	LEU-COMP-THERM-037-004_	0.96	0.98	0.95	0.96	0.95	0.89	0.93	0.92	0.87	0.77	0.88	0.77	0.44	0.64	0.56
864	LEU-COMP-THERM-037-005_	0.96	0.97	0.96	0.95	0.95	0.89	0.93	0.92	0.87	0.78	0.88	0.77	0.44	0.64	0.56
865	LEU-COMP-THERM-037-006_	0.96	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.44	0.64	0.56
866	LEU-COMP-THERM-037-007_	0.96	0.97	0.96	0.95	0.95	0.89	0.93	0.92	0.87	0.78	0.88	0.78	0.45	0.64	0.56
867	LEU-COMP-THERM-037-008_	0.96	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.44	0.64	0.56
868	LEU-COMP-THERM-037-009_	0.96	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.44	0.64	0.56
869	LEU-COMP-THERM-037-010_	0.96	0.97	0.96	0.95	0.95	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.44	0.64	0.56
870	LEU-COMP-THERM-037-011_	0.96	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.88	0.78	0.88	0.77	0.44	0.64	0.56
871	LEU-COMP-THERM-038-001_	0.96	0.98	0.96	0.96	0.96	0.89	0.93	0.92	0.88	0.77	0.88	0.77	0.43	0.64	0.56
872	LEU-COMP-THERM-038-002_	0.96	0.98	0.96	0.96	0.96	0.89	0.93	0.92	0.87	0.78	0.88	0.77	0.44	0.64	0.56
873	LEU-COMP-THERM-038-003_	0.96	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.87	0.78	0.88	0.77	0.45	0.65	0.56
874	LEU-COMP-THERM-038-004_	0.97	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.87	0.79	0.89	0.78	0.45	0.65	0.56
875	LEU-COMP-THERM-038-005_	0.97	0.97	0.96	0.96	0.95	0.89	0.93	0.92	0.87	0.79	0.88	0.78	0.45	0.65	0.56
876	LEU-COMP-THERM-038-006_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.49	0.68	0.57
877	LEU-COMP-THERM-038-007_	0.97	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.82	0.90	0.81	0.48	0.67	0.57
878	LEU-COMP-THERM-038-008_	0.97	0.97	0.96	0.95	0.95	0.90	0.93	0.92	0.87	0.80	0.90	0.80	0.47	0.66	0.57
879	LEU-COMP-THERM-038-009_	0.97	0.96	0.96	0.95	0.94	0.90	0.93	0.92	0.87	0.81	0.90	0.80	0.48	0.66	0.56
880	LEU-COMP-THERM-038-010_	0.97	0.97	0.96	0.96	0.95	0.90	0.93	0.92	0.87	0.80	0.89	0.79	0.46	0.66	0.56
881	LEU-COMP-THERM-038-011_	0.97	0.96	0.96	0.95	0.95	0.90	0.93	0.92	0.87	0.80	0.89	0.79	0.47	0.66	0.56
882	LEU-COMP-THERM-038-012_	0.97	0.97	0.96	0.96	0.95	0.90	0.93	0.92	0.87	0.79	0.89	0.78	0.46	0.65	0.56

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
883	LEU-COMP-THERM-038-013_	0.97	0.97	0.96	0.95	0.95	0.90	0.93	0.92	0.87	0.80	0.89	0.79	0.46	0.65	0.56
884	LEU-COMP-THERM-038-014_	0.97	0.97	0.96	0.96	0.96	0.89	0.93	0.92	0.87	0.78	0.88	0.78	0.45	0.65	0.56
885	LEU-COMP-THERM-039-001_	0.99	0.98	0.98	0.95	0.94	0.88	0.91	0.92	0.85	0.79	0.89	0.78	0.48	0.69	0.61
886	LEU-COMP-THERM-039-002_	0.99	0.98	0.98	0.95	0.94	0.88	0.92	0.92	0.85	0.79	0.89	0.78	0.48	0.69	0.60
887	LEU-COMP-THERM-039-003_	0.98	0.98	0.98	0.96	0.95	0.88	0.92	0.92	0.85	0.78	0.88	0.77	0.46	0.68	0.60
888	LEU-COMP-THERM-039-004_	0.98	0.98	0.98	0.96	0.95	0.88	0.92	0.92	0.86	0.78	0.88	0.77	0.46	0.68	0.59
889	LEU-COMP-THERM-039-005_	0.97	0.98	0.96	0.96	0.96	0.89	0.92	0.92	0.87	0.78	0.88	0.77	0.44	0.65	0.57
890	LEU-COMP-THERM-039-006_	0.97	0.98	0.97	0.96	0.96	0.88	0.92	0.92	0.87	0.77	0.88	0.77	0.44	0.66	0.58
891	LEU-COMP-THERM-039-007_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.78	0.88	0.77	0.47	0.68	0.60
892	LEU-COMP-THERM-039-008_	0.98	0.98	0.98	0.96	0.95	0.88	0.92	0.92	0.85	0.78	0.88	0.77	0.46	0.68	0.60
893	LEU-COMP-THERM-039-009_	0.98	0.98	0.98	0.96	0.95	0.88	0.92	0.92	0.85	0.78	0.88	0.77	0.46	0.68	0.60
894	LEU-COMP-THERM-039-010_	0.98	0.99	0.97	0.96	0.95	0.88	0.92	0.92	0.86	0.78	0.88	0.77	0.45	0.67	0.59
895	LEU-COMP-THERM-039-011_	0.99	0.98	0.98	0.95	0.94	0.88	0.91	0.92	0.85	0.79	0.89	0.78	0.48	0.69	0.61
896	LEU-COMP-THERM-039-012_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.79	0.88	0.78	0.47	0.69	0.60
897	LEU-COMP-THERM-039-013_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.79	0.88	0.78	0.47	0.69	0.60
898	LEU-COMP-THERM-039-014_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.78	0.88	0.78	0.47	0.68	0.60
899	LEU-COMP-THERM-039-015_	0.98	0.98	0.98	0.96	0.95	0.88	0.92	0.92	0.85	0.78	0.88	0.77	0.46	0.68	0.60
900	LEU-COMP-THERM-039-016_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.78	0.88	0.78	0.47	0.68	0.60
901	LEU-COMP-THERM-039-017_	0.99	0.98	0.98	0.96	0.94	0.88	0.92	0.92	0.85	0.78	0.88	0.78	0.47	0.68	0.60
902	LEU-COMP-THERM-040-001_	0.98	0.96	0.98	0.94	0.94	0.92	0.94	0.93	0.88	0.85	0.92	0.84	0.52	0.69	0.58
903	LEU-COMP-THERM-040-002_	0.98	0.94	0.97	0.94	0.93	0.92	0.94	0.93	0.88	0.86	0.93	0.85	0.53	0.70	0.58
904	LEU-COMP-THERM-040-003_	0.98	0.95	0.97	0.94	0.93	0.92	0.94	0.93	0.88	0.86	0.93	0.85	0.53	0.70	0.58
905	LEU-COMP-THERM-040-004_	0.98	0.95	0.98	0.94	0.93	0.92	0.94	0.93	0.88	0.86	0.93	0.84	0.53	0.70	0.58
906	LEU-COMP-THERM-040-005_	0.98	0.95	0.98	0.93	0.92	0.91	0.93	0.92	0.86	0.85	0.92	0.84	0.52	0.69	0.58
907	LEU-COMP-THERM-040-006_	0.98	0.94	0.97	0.92	0.91	0.92	0.92	0.92	0.86	0.86	0.93	0.85	0.54	0.70	0.58
908	LEU-COMP-THERM-040-007_	0.98	0.94	0.98	0.92	0.92	0.92	0.92	0.92	0.86	0.86	0.92	0.84	0.53	0.70	0.57
909	LEU-COMP-THERM-040-008_	0.98	0.94	0.98	0.93	0.92	0.91	0.92	0.92	0.86	0.85	0.92	0.84	0.53	0.70	0.58
910	LEU-COMP-THERM-040-009_	0.97	0.92	0.96	0.92	0.91	0.93	0.93	0.93	0.87	0.88	0.94	0.86	0.55	0.71	0.58
911	LEU-COMP-THERM-040-010_	0.98	0.94	0.97	0.92	0.91	0.92	0.93	0.92	0.86	0.86	0.93	0.85	0.54	0.70	0.58
912	LEU-COMP-THERM-042-001_	0.91	0.79	0.89	0.82	0.77	0.91	0.85	0.88	0.77	0.92	0.92	0.89	0.68	0.76	0.57
913	LEU-COMP-THERM-042-002_	0.90	0.77	0.88	0.80	0.75	0.89	0.84	0.86	0.75	0.92	0.91	0.88	0.68	0.76	0.56
914	LEU-COMP-THERM-042-003_	0.90	0.76	0.88	0.79	0.74	0.89	0.83	0.85	0.75	0.92	0.91	0.88	0.69	0.76	0.56
915	LEU-COMP-THERM-042-004_	0.89	0.76	0.88	0.78	0.74	0.89	0.83	0.85	0.74	0.92	0.91	0.88	0.69	0.76	0.56
916	LEU-COMP-THERM-042-005_	0.90	0.76	0.88	0.79	0.74	0.89	0.83	0.85	0.74	0.92	0.91	0.88	0.69	0.76	0.56
917	LEU-COMP-THERM-042-006_	0.90	0.78	0.89	0.80	0.76	0.89	0.84	0.86	0.75	0.91	0.91	0.88	0.67	0.75	0.56
918	LEU-COMP-THERM-042-007_	0.90	0.77	0.88	0.79	0.75	0.89	0.83	0.86	0.75	0.91	0.91	0.88	0.68	0.75	0.56
919	LEU-COMP-THERM-043-001_	0.86	0.81	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.94	0.96	0.92	0.63	0.73	0.56
920	LEU-COMP-THERM-043-002_	0.86	0.80	0.85	0.89	0.87	0.98	0.96	0.96	0.95	0.94	0.96	0.93	0.64	0.73	0.56
921	LEU-COMP-THERM-043-003_	0.86	0.81	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.94	0.96	0.93	0.63	0.73	0.56
922	LEU-COMP-THERM-043-004_	0.86	0.80	0.86	0.89	0.87	0.98	0.96	0.96	0.95	0.94	0.96	0.93	0.64	0.73	0.56
923	LEU-COMP-THERM-043-005_	0.86	0.80	0.86	0.89	0.87	0.98	0.96	0.96	0.95	0.94	0.96	0.93	0.64	0.73	0.56
924	LEU-COMP-THERM-043-006_	0.85	0.80	0.85	0.89	0.87	0.98	0.95	0.96	0.94	0.94	0.96	0.93	0.64	0.73	0.56

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
925	LEU-COMP-THERM-043-007_	0.86	0.81	0.86	0.89	0.87	0.98	0.95	0.96	0.94	0.94	0.96	0.92	0.64	0.73	0.56
926	LEU-COMP-THERM-043-008_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
927	LEU-COMP-THERM-043-009_	0.86	0.81	0.86	0.90	0.87	0.98	0.95	0.96	0.94	0.94	0.96	0.92	0.63	0.73	0.56
928	LEU-COMP-THERM-044-001_	0.86	0.82	0.86	0.90	0.88	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.62	0.72	0.56
929	LEU-COMP-THERM-044-002_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.94	0.93	0.96	0.92	0.63	0.73	0.56
930	LEU-COMP-THERM-044-003_	0.87	0.82	0.86	0.90	0.89	0.98	0.96	0.96	0.95	0.92	0.95	0.91	0.62	0.72	0.56
931	LEU-COMP-THERM-044-004_	0.86	0.81	0.86	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.96	0.92	0.63	0.72	0.56
932	LEU-COMP-THERM-044-005_	0.86	0.81	0.86	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.92	0.63	0.72	0.56
933	LEU-COMP-THERM-044-006_	0.86	0.81	0.86	0.90	0.88	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.62	0.72	0.56
934	LEU-COMP-THERM-044-007_	0.86	0.81	0.86	0.90	0.88	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.63	0.72	0.56
935	LEU-COMP-THERM-044-008_	0.86	0.81	0.86	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.92	0.63	0.72	0.56
936	LEU-COMP-THERM-044-009_	0.87	0.82	0.86	0.90	0.89	0.98	0.96	0.97	0.95	0.93	0.95	0.91	0.62	0.72	0.56
937	LEU-COMP-THERM-044-010_	0.86	0.81	0.85	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.92	0.63	0.72	0.56
938	LEU-COMP-THERM-045-001_	0.97	0.89	0.96	0.87	0.84	0.87	0.85	0.88	0.77	0.85	0.90	0.84	0.60	0.76	0.64
939	LEU-COMP-THERM-045-002_	0.97	0.88	0.96	0.86	0.83	0.87	0.85	0.88	0.77	0.86	0.90	0.84	0.60	0.76	0.64
940	LEU-COMP-THERM-045-003_	0.88	0.74	0.87	0.71	0.67	0.78	0.73	0.78	0.64	0.82	0.83	0.81	0.73	0.81	0.67
941	LEU-COMP-THERM-045-004_	0.87	0.74	0.87	0.71	0.66	0.77	0.73	0.77	0.63	0.82	0.83	0.81	0.73	0.81	0.67
942	LEU-COMP-THERM-045-005_	0.92	0.81	0.92	0.78	0.74	0.82	0.78	0.82	0.69	0.84	0.87	0.83	0.68	0.79	0.66
943	LEU-COMP-THERM-045-006_	0.94	0.83	0.93	0.82	0.79	0.86	0.82	0.85	0.74	0.87	0.90	0.85	0.64	0.77	0.63
944	LEU-COMP-THERM-045-007_	0.82	0.72	0.82	0.80	0.76	0.93	0.87	0.90	0.85	0.94	0.93	0.92	0.72	0.78	0.60
945	LEU-COMP-THERM-045-008_	0.82	0.71	0.82	0.79	0.76	0.93	0.86	0.90	0.84	0.94	0.93	0.92	0.73	0.78	0.60
946	LEU-COMP-THERM-045-009_	0.92	0.81	0.91	0.85	0.82	0.93	0.89	0.92	0.84	0.94	0.95	0.92	0.70	0.80	0.64
947	LEU-COMP-THERM-045-010_	0.81	0.68	0.81	0.74	0.69	0.88	0.81	0.85	0.77	0.92	0.90	0.91	0.80	0.83	0.65
948	LEU-COMP-THERM-045-011_	0.96	0.87	0.95	0.85	0.82	0.87	0.84	0.87	0.76	0.87	0.91	0.85	0.62	0.76	0.63
949	LEU-COMP-THERM-045-012_	0.96	0.87	0.95	0.85	0.82	0.87	0.85	0.87	0.76	0.86	0.91	0.85	0.62	0.76	0.63
950	LEU-COMP-THERM-045-013_	0.96	0.87	0.95	0.84	0.81	0.87	0.85	0.88	0.77	0.87	0.91	0.86	0.63	0.77	0.64
951	LEU-COMP-THERM-045-014_	0.96	0.86	0.95	0.84	0.81	0.87	0.85	0.87	0.77	0.87	0.91	0.86	0.64	0.77	0.63
952	LEU-COMP-THERM-045-015_	0.81	0.66	0.81	0.62	0.58	0.74	0.68	0.71	0.59	0.81	0.80	0.80	0.79	0.81	0.65
953	LEU-COMP-THERM-045-016_	0.80	0.64	0.80	0.61	0.57	0.74	0.67	0.71	0.58	0.81	0.79	0.80	0.80	0.81	0.65
954	LEU-COMP-THERM-045-017_	0.82	0.67	0.82	0.64	0.60	0.76	0.69	0.73	0.61	0.84	0.82	0.82	0.79	0.81	0.65
955	LEU-COMP-THERM-045-018_	0.93	0.82	0.92	0.79	0.76	0.86	0.82	0.85	0.74	0.88	0.90	0.87	0.67	0.77	0.62
956	LEU-COMP-THERM-045-019_	0.93	0.81	0.92	0.79	0.76	0.86	0.81	0.84	0.73	0.88	0.90	0.86	0.67	0.77	0.62
957	LEU-COMP-THERM-045-020_	0.81	0.69	0.80	0.77	0.73	0.92	0.85	0.88	0.83	0.94	0.92	0.93	0.75	0.78	0.59
958	LEU-COMP-THERM-045-021_	0.81	0.69	0.80	0.76	0.73	0.92	0.85	0.88	0.83	0.94	0.92	0.93	0.75	0.78	0.59
959	LEU-COMP-THERM-046-001_	0.88	0.84	0.87	0.92	0.90	0.98	0.97	0.97	0.95	0.92	0.95	0.90	0.60	0.72	0.57
960	LEU-COMP-THERM-046-002_	0.88	0.84	0.87	0.92	0.90	0.98	0.97	0.97	0.95	0.92	0.95	0.90	0.60	0.72	0.57
961	LEU-COMP-THERM-046-003_	0.88	0.84	0.88	0.92	0.90	0.98	0.97	0.97	0.95	0.91	0.95	0.90	0.60	0.72	0.57
962	LEU-COMP-THERM-046-004_	0.88	0.84	0.87	0.92	0.90	0.98	0.97	0.97	0.95	0.92	0.95	0.90	0.60	0.72	0.57
963	LEU-COMP-THERM-046-005_	0.88	0.84	0.87	0.92	0.90	0.98	0.96	0.97	0.95	0.92	0.95	0.90	0.61	0.72	0.57
964	LEU-COMP-THERM-046-006_	0.88	0.84	0.87	0.92	0.90	0.98	0.96	0.97	0.95	0.92	0.95	0.90	0.61	0.72	0.57
965	LEU-COMP-THERM-046-007_	0.88	0.84	0.87	0.92	0.90	0.98	0.96	0.97	0.95	0.92	0.95	0.90	0.61	0.72	0.57
966	LEU-COMP-THERM-046-008_	0.88	0.84	0.87	0.92	0.90	0.98	0.97	0.97	0.95	0.92	0.95	0.90	0.60	0.72	0.57

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
967	LEU-COMP-THERM-046-009_	0.88	0.84	0.87	0.92	0.90	0.98	0.96	0.97	0.95	0.92	0.95	0.90	0.61	0.72	0.57
968	LEU-COMP-THERM-046-010_	0.88	0.84	0.88	0.92	0.90	0.98	0.97	0.97	0.95	0.91	0.95	0.90	0.60	0.72	0.57
969	LEU-COMP-THERM-046-011_	0.88	0.84	0.88	0.92	0.90	0.98	0.96	0.97	0.95	0.92	0.95	0.90	0.61	0.72	0.57
970	LEU-COMP-THERM-046-012_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
971	LEU-COMP-THERM-046-013_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
972	LEU-COMP-THERM-046-014_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
973	LEU-COMP-THERM-046-015_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
974	LEU-COMP-THERM-046-016_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
975	LEU-COMP-THERM-046-017_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
976	LEU-COMP-THERM-046-018_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.95	0.91	0.61	0.72	0.57
977	LEU-COMP-THERM-046-019_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.95	0.91	0.61	0.72	0.57
978	LEU-COMP-THERM-046-020_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.95	0.91	0.61	0.72	0.57
979	LEU-COMP-THERM-046-021_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.95	0.91	0.62	0.72	0.57
980	LEU-COMP-THERM-046-022_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.95	0.91	0.61	0.72	0.57
981	LEU-COMP-THERM-047-001_	0.84	0.69	0.82	0.75	0.71	0.92	0.84	0.85	0.79	0.97	0.94	0.94	0.73	0.75	0.53
982	LEU-COMP-THERM-047-002_	0.94	0.87	0.94	0.91	0.89	0.98	0.95	0.96	0.91	0.95	0.98	0.94	0.65	0.75	0.58
983	LEU-COMP-THERM-047-003_	0.91	0.81	0.91	0.86	0.84	0.97	0.92	0.93	0.88	0.97	0.98	0.95	0.68	0.76	0.57
984	LEU-COMP-THERM-048-001_	0.86	0.72	0.85	0.75	0.70	0.87	0.80	0.84	0.73	0.91	0.89	0.88	0.76	0.81	0.61
985	LEU-COMP-THERM-048-002_	0.86	0.72	0.85	0.75	0.70	0.87	0.80	0.84	0.73	0.91	0.89	0.88	0.76	0.81	0.61
986	LEU-COMP-THERM-048-003_	0.86	0.72	0.84	0.75	0.70	0.87	0.80	0.84	0.73	0.90	0.89	0.88	0.76	0.81	0.61
987	LEU-COMP-THERM-048-004_	0.86	0.72	0.84	0.75	0.70	0.87	0.80	0.84	0.73	0.91	0.89	0.88	0.76	0.81	0.61
988	LEU-COMP-THERM-048-005_	0.86	0.72	0.85	0.75	0.70	0.87	0.80	0.84	0.73	0.90	0.89	0.88	0.76	0.81	0.61
989	LEU-COMP-THERM-049-001_	0.78	0.62	0.78	0.59	0.55	0.71	0.65	0.68	0.55	0.79	0.77	0.78	0.81	0.82	0.66
990	LEU-COMP-THERM-049-002_	0.78	0.62	0.78	0.60	0.56	0.71	0.65	0.68	0.55	0.79	0.77	0.78	0.80	0.82	0.66
991	LEU-COMP-THERM-049-003_	0.76	0.59	0.76	0.57	0.53	0.70	0.63	0.66	0.54	0.79	0.76	0.77	0.82	0.81	0.65
992	LEU-COMP-THERM-049-004_	0.75	0.58	0.75	0.56	0.52	0.69	0.62	0.65	0.52	0.78	0.75	0.77	0.82	0.81	0.64
993	LEU-COMP-THERM-049-005_	0.88	0.76	0.88	0.73	0.69	0.79	0.75	0.79	0.66	0.82	0.84	0.81	0.73	0.82	0.67
994	LEU-COMP-THERM-049-006_	0.88	0.75	0.87	0.73	0.69	0.79	0.75	0.78	0.65	0.82	0.84	0.81	0.74	0.82	0.67
995	LEU-COMP-THERM-049-007_	0.88	0.77	0.88	0.74	0.70	0.79	0.76	0.79	0.66	0.82	0.84	0.81	0.73	0.82	0.67
996	LEU-COMP-THERM-049-008_	0.87	0.74	0.86	0.71	0.67	0.78	0.74	0.77	0.64	0.83	0.84	0.81	0.75	0.82	0.67
997	LEU-COMP-THERM-049-009_	0.93	0.83	0.92	0.80	0.77	0.83	0.81	0.84	0.72	0.83	0.87	0.82	0.68	0.80	0.67
998	LEU-COMP-THERM-049-010_	0.93	0.83	0.92	0.81	0.77	0.83	0.81	0.84	0.72	0.83	0.87	0.82	0.68	0.80	0.67
999	LEU-COMP-THERM-049-011_	0.93	0.83	0.92	0.81	0.77	0.83	0.81	0.84	0.72	0.83	0.87	0.82	0.68	0.80	0.67
1000	LEU-COMP-THERM-049-012_	0.92	0.81	0.92	0.79	0.75	0.83	0.80	0.83	0.71	0.84	0.87	0.82	0.70	0.81	0.67
1001	LEU-COMP-THERM-049-013_	0.88	0.76	0.87	0.73	0.69	0.78	0.74	0.78	0.65	0.81	0.83	0.80	0.73	0.81	0.67
1002	LEU-COMP-THERM-049-014_	0.87	0.74	0.87	0.71	0.67	0.78	0.73	0.77	0.64	0.82	0.83	0.80	0.74	0.82	0.67
1003	LEU-COMP-THERM-049-015_	0.87	0.75	0.87	0.72	0.68	0.78	0.74	0.78	0.64	0.82	0.83	0.80	0.73	0.82	0.67
1004	LEU-COMP-THERM-049-016_	0.89	0.77	0.88	0.74	0.70	0.80	0.76	0.79	0.66	0.82	0.84	0.81	0.73	0.82	0.67
1005	LEU-COMP-THERM-049-017_	0.87	0.74	0.87	0.71	0.68	0.79	0.74	0.77	0.65	0.83	0.84	0.81	0.75	0.82	0.67
1006	LEU-COMP-THERM-049-018_	0.83	0.68	0.83	0.66	0.63	0.77	0.71	0.74	0.62	0.84	0.83	0.83	0.78	0.81	0.64
1007	LEU-COMP-THERM-050-001_	0.99	0.98	0.98	0.95	0.94	0.89	0.92	0.92	0.85	0.79	0.89	0.79	0.48	0.68	0.60
1008	LEU-COMP-THERM-050-002_	0.98	0.98	0.98	0.95	0.94	0.89	0.92	0.92	0.85	0.80	0.89	0.79	0.47	0.68	0.60

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1009	LEU-COMP-THERM-050-003_	0.99	0.97	0.98	0.95	0.94	0.89	0.92	0.93	0.85	0.81	0.90	0.80	0.49	0.70	0.60
1010	LEU-COMP-THERM-050-004_	0.99	0.97	0.98	0.95	0.93	0.89	0.92	0.93	0.85	0.81	0.90	0.80	0.50	0.70	0.60
1011	LEU-COMP-THERM-050-005_	0.99	0.97	0.99	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.51	0.71	0.61
1012	LEU-COMP-THERM-050-006_	0.99	0.97	0.99	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1013	LEU-COMP-THERM-050-007_	0.99	0.96	0.99	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1014	LEU-COMP-THERM-050-008_	0.99	0.97	0.98	0.95	0.94	0.89	0.92	0.93	0.85	0.80	0.90	0.79	0.49	0.69	0.60
1015	LEU-COMP-THERM-050-009_	0.99	0.97	0.98	0.95	0.94	0.89	0.92	0.93	0.85	0.81	0.90	0.80	0.49	0.69	0.60
1016	LEU-COMP-THERM-050-010_	0.99	0.97	0.98	0.95	0.94	0.89	0.92	0.92	0.85	0.81	0.90	0.80	0.49	0.69	0.60
1017	LEU-COMP-THERM-050-011_	0.99	0.97	0.98	0.95	0.93	0.89	0.92	0.93	0.85	0.81	0.90	0.80	0.50	0.70	0.61
1018	LEU-COMP-THERM-050-012_	0.99	0.97	0.98	0.95	0.93	0.90	0.92	0.93	0.85	0.82	0.90	0.81	0.50	0.70	0.60
1019	LEU-COMP-THERM-050-013_	0.99	0.97	0.98	0.95	0.93	0.90	0.92	0.93	0.85	0.82	0.90	0.81	0.50	0.70	0.60
1020	LEU-COMP-THERM-050-014_	0.99	0.97	0.98	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1021	LEU-COMP-THERM-050-015_	0.99	0.96	0.98	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1022	LEU-COMP-THERM-050-016_	0.99	0.97	0.98	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.51	0.71	0.61
1023	LEU-COMP-THERM-050-017_	0.99	0.96	0.98	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1024	LEU-COMP-THERM-050-018_	0.99	0.97	0.98	0.94	0.93	0.90	0.92	0.93	0.85	0.82	0.91	0.81	0.52	0.71	0.61
1025	LEU-COMP-THERM-051-001_	0.83	0.67	0.81	0.68	0.64	0.81	0.73	0.74	0.64	0.88	0.85	0.84	0.66	0.69	0.49
1026	LEU-COMP-THERM-051-002_	0.79	0.61	0.77	0.65	0.61	0.86	0.75	0.77	0.69	0.94	0.88	0.90	0.76	0.74	0.50
1027	LEU-COMP-THERM-051-003_	0.79	0.62	0.78	0.66	0.62	0.86	0.76	0.78	0.69	0.94	0.89	0.90	0.76	0.74	0.50
1028	LEU-COMP-THERM-051-004_	0.80	0.62	0.78	0.67	0.62	0.86	0.76	0.78	0.69	0.94	0.89	0.90	0.76	0.74	0.51
1029	LEU-COMP-THERM-051-005_	0.81	0.64	0.79	0.68	0.64	0.87	0.77	0.79	0.71	0.94	0.89	0.91	0.76	0.75	0.51
1030	LEU-COMP-THERM-051-006_	0.81	0.64	0.79	0.68	0.64	0.87	0.77	0.79	0.70	0.94	0.89	0.91	0.76	0.75	0.51
1031	LEU-COMP-THERM-051-007_	0.80	0.63	0.79	0.67	0.63	0.87	0.77	0.79	0.70	0.94	0.89	0.91	0.76	0.74	0.51
1032	LEU-COMP-THERM-051-008_	0.82	0.66	0.81	0.70	0.66	0.88	0.79	0.81	0.72	0.95	0.90	0.91	0.75	0.75	0.52
1033	LEU-COMP-THERM-051-009_	0.81	0.64	0.79	0.69	0.65	0.87	0.78	0.79	0.71	0.94	0.89	0.91	0.75	0.74	0.50
1034	LEU-COMP-THERM-051-010_	0.82	0.65	0.80	0.65	0.61	0.80	0.71	0.73	0.62	0.88	0.84	0.84	0.71	0.72	0.50
1035	LEU-COMP-THERM-051-011_	0.82	0.64	0.80	0.65	0.61	0.80	0.71	0.73	0.62	0.88	0.84	0.84	0.71	0.71	0.50
1036	LEU-COMP-THERM-051-012_	0.82	0.64	0.80	0.64	0.61	0.80	0.71	0.73	0.62	0.88	0.84	0.85	0.71	0.71	0.50
1037	LEU-COMP-THERM-051-013_	0.81	0.64	0.80	0.64	0.60	0.80	0.71	0.72	0.61	0.88	0.84	0.85	0.71	0.71	0.49
1038	LEU-COMP-THERM-051-014_	0.83	0.66	0.81	0.66	0.62	0.81	0.72	0.74	0.63	0.89	0.85	0.85	0.70	0.71	0.49
1039	LEU-COMP-THERM-051-015_	0.81	0.63	0.79	0.63	0.59	0.79	0.70	0.72	0.61	0.88	0.84	0.84	0.71	0.71	0.49
1040	LEU-COMP-THERM-051-016_	0.82	0.65	0.81	0.66	0.62	0.81	0.72	0.73	0.63	0.88	0.85	0.85	0.70	0.71	0.49
1041	LEU-COMP-THERM-051-017_	0.81	0.63	0.79	0.63	0.59	0.79	0.70	0.72	0.61	0.88	0.84	0.84	0.71	0.71	0.49
1042	LEU-COMP-THERM-051-018_	0.82	0.65	0.80	0.65	0.61	0.80	0.71	0.73	0.62	0.88	0.85	0.85	0.69	0.70	0.49
1043	LEU-COMP-THERM-051-019_	0.84	0.68	0.82	0.69	0.65	0.82	0.74	0.75	0.65	0.88	0.86	0.84	0.67	0.70	0.49
1044	LEU-COMP-THERM-052-001_	0.78	0.72	0.78	0.70	0.67	0.71	0.70	0.72	0.63	0.75	0.78	0.79	0.50	0.62	0.51
1045	LEU-COMP-THERM-052-002_	0.57	0.51	0.57	0.51	0.50	0.55	0.53	0.53	0.49	0.62	0.63	0.68	0.37	0.44	0.34
1046	LEU-COMP-THERM-052-003_	0.55	0.48	0.55	0.48	0.48	0.55	0.52	0.51	0.48	0.64	0.63	0.69	0.37	0.42	0.30
1047	LEU-COMP-THERM-052-004_	0.78	0.72	0.78	0.69	0.67	0.71	0.69	0.71	0.63	0.75	0.78	0.79	0.50	0.62	0.51
1048	LEU-COMP-THERM-052-005_	0.56	0.50	0.56	0.50	0.49	0.54	0.52	0.52	0.48	0.61	0.62	0.67	0.37	0.43	0.33
1049	LEU-COMP-THERM-052-006_	0.53	0.46	0.53	0.47	0.46	0.54	0.50	0.50	0.47	0.63	0.62	0.68	0.36	0.40	0.30
1050	LEU-COMP-THERM-053-001_	0.98	0.94	0.98	0.92	0.89	0.88	0.89	0.92	0.82	0.83	0.90	0.82	0.56	0.75	0.64

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1051	LEU-COMP-THERM-053-002_	0.98	0.94	0.98	0.91	0.89	0.88	0.89	0.92	0.81	0.83	0.90	0.82	0.56	0.75	0.64
1052	LEU-COMP-THERM-053-003_	0.99	0.94	0.98	0.92	0.89	0.88	0.89	0.91	0.81	0.82	0.90	0.81	0.55	0.74	0.63
1053	LEU-COMP-THERM-053-004_	0.99	0.95	0.98	0.92	0.90	0.88	0.90	0.92	0.82	0.82	0.90	0.81	0.54	0.73	0.63
1054	LEU-COMP-THERM-053-005_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.81	0.89	0.80	0.52	0.72	0.63
1055	LEU-COMP-THERM-053-006_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.81	0.89	0.80	0.52	0.72	0.63
1056	LEU-COMP-THERM-053-007_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.81	0.89	0.80	0.52	0.72	0.62
1057	LEU-COMP-THERM-053-008_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.81	0.89	0.80	0.52	0.72	0.62
1058	LEU-COMP-THERM-053-009_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.83	0.81	0.90	0.80	0.52	0.72	0.62
1059	LEU-COMP-THERM-053-010_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.82	0.81	0.90	0.80	0.52	0.72	0.62
1060	LEU-COMP-THERM-053-011_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.83	0.81	0.90	0.80	0.52	0.72	0.62
1061	LEU-COMP-THERM-053-012_	0.99	0.96	0.98	0.93	0.91	0.89	0.90	0.92	0.83	0.82	0.90	0.81	0.53	0.72	0.62
1062	LEU-COMP-THERM-053-013_	0.99	0.96	0.98	0.94	0.92	0.88	0.90	0.92	0.83	0.81	0.90	0.80	0.52	0.72	0.62
1063	LEU-COMP-THERM-053-014_	0.99	0.96	0.98	0.93	0.91	0.88	0.90	0.92	0.83	0.81	0.90	0.80	0.52	0.72	0.62
1064	LEU-COMP-THERM-054-001_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.94	0.94	0.96	0.92	0.63	0.73	0.57
1065	LEU-COMP-THERM-054-002_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1066	LEU-COMP-THERM-054-003_	0.87	0.82	0.87	0.90	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1067	LEU-COMP-THERM-054-004_	0.87	0.82	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1068	LEU-COMP-THERM-054-005_	0.87	0.82	0.87	0.90	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1069	LEU-COMP-THERM-054-006_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1070	LEU-COMP-THERM-054-007_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.94	0.94	0.96	0.92	0.63	0.73	0.57
1071	LEU-COMP-THERM-054-008_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1072	LEU-COMP-THERM-055-001_	0.72	0.53	0.71	0.57	0.52	0.77	0.67	0.71	0.60	0.87	0.81	0.84	0.84	0.79	0.57
1073	LEU-COMP-THERM-055-002_	0.69	0.50	0.68	0.55	0.50	0.76	0.66	0.69	0.59	0.86	0.79	0.83	0.85	0.78	0.56
1074	LEU-COMP-THERM-057-001_	0.98	0.96	0.98	0.94	0.93	0.90	0.92	0.92	0.85	0.83	0.91	0.81	0.51	0.70	0.59
1075	LEU-COMP-THERM-057-002_	0.98	0.95	0.97	0.94	0.93	0.90	0.92	0.92	0.85	0.83	0.91	0.82	0.51	0.70	0.59
1076	LEU-COMP-THERM-057-003_	0.98	0.94	0.97	0.93	0.92	0.90	0.91	0.92	0.85	0.84	0.91	0.82	0.52	0.70	0.59
1077	LEU-COMP-THERM-057-004_	0.98	0.94	0.97	0.93	0.92	0.90	0.91	0.92	0.85	0.84	0.91	0.82	0.52	0.70	0.59
1078	LEU-COMP-THERM-057-005_	0.98	0.95	0.97	0.94	0.92	0.91	0.92	0.92	0.85	0.84	0.91	0.82	0.51	0.70	0.59
1079	LEU-COMP-THERM-057-006_	0.98	0.95	0.97	0.94	0.92	0.91	0.92	0.92	0.85	0.84	0.91	0.82	0.51	0.70	0.59
1080	LEU-COMP-THERM-057-007_	0.98	0.96	0.97	0.94	0.93	0.91	0.92	0.93	0.86	0.83	0.91	0.82	0.51	0.69	0.59
1081	LEU-COMP-THERM-057-008_	0.98	0.96	0.98	0.95	0.94	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.50	0.69	0.59
1082	LEU-COMP-THERM-057-009_	0.98	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.48	0.69	0.59
1083	LEU-COMP-THERM-057-010_	0.98	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.48	0.69	0.60
1084	LEU-COMP-THERM-057-011_	0.99	0.98	0.98	0.97	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.48	0.69	0.60
1085	LEU-COMP-THERM-057-012_	0.99	0.98	0.98	0.97	0.95	0.90	0.93	0.94	0.87	0.80	0.90	0.79	0.48	0.69	0.60
1086	LEU-COMP-THERM-057-013_	0.99	0.98	0.98	0.97	0.95	0.89	0.93	0.94	0.87	0.79	0.89	0.79	0.47	0.69	0.60
1087	LEU-COMP-THERM-057-014_	0.99	0.98	0.98	0.97	0.95	0.90	0.93	0.94	0.87	0.80	0.90	0.79	0.48	0.69	0.61
1088	LEU-COMP-THERM-057-015_	0.99	0.98	0.98	0.96	0.95	0.89	0.93	0.94	0.86	0.80	0.89	0.79	0.48	0.70	0.61
1089	LEU-COMP-THERM-057-016_	0.98	0.96	0.98	0.94	0.93	0.90	0.92	0.92	0.85	0.82	0.91	0.81	0.50	0.69	0.59
1090	LEU-COMP-THERM-057-017_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.61
1091	LEU-COMP-THERM-057-018_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.91	0.81	0.49	0.70	0.60
1092	LEU-COMP-THERM-057-019_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.80	0.90	0.80	0.49	0.70	0.61

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1093	LEU-COMP-THERM-057-020_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.60
1094	LEU-COMP-THERM-057-021_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.60
1095	LEU-COMP-THERM-057-022_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.80	0.90	0.80	0.48	0.70	0.61
1096	LEU-COMP-THERM-057-023_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.61
1097	LEU-COMP-THERM-057-024_	0.98	0.96	0.97	0.94	0.93	0.91	0.92	0.93	0.86	0.83	0.91	0.82	0.51	0.70	0.59
1098	LEU-COMP-THERM-057-025_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.50	0.70	0.61
1099	LEU-COMP-THERM-057-026_	0.99	0.96	0.98	0.95	0.94	0.91	0.93	0.93	0.86	0.83	0.91	0.82	0.51	0.70	0.60
1100	LEU-COMP-THERM-057-027_	0.99	0.97	0.98	0.96	0.94	0.91	0.93	0.93	0.87	0.82	0.91	0.81	0.50	0.70	0.60
1101	LEU-COMP-THERM-057-028_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.60
1102	LEU-COMP-THERM-057-029_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.81	0.90	0.80	0.49	0.70	0.61
1103	LEU-COMP-THERM-057-030_	0.98	0.95	0.97	0.94	0.92	0.90	0.92	0.92	0.85	0.83	0.91	0.82	0.51	0.70	0.59
1104	LEU-COMP-THERM-057-031_	0.99	0.98	0.98	0.96	0.95	0.90	0.93	0.94	0.87	0.82	0.91	0.81	0.50	0.70	0.61
1105	LEU-COMP-THERM-057-032_	0.98	0.94	0.97	0.93	0.92	0.91	0.91	0.92	0.85	0.84	0.91	0.83	0.52	0.70	0.59
1106	LEU-COMP-THERM-057-033_	0.98	0.95	0.97	0.94	0.93	0.91	0.92	0.92	0.85	0.84	0.91	0.82	0.52	0.70	0.59
1107	LEU-COMP-THERM-057-034_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.85	0.84	0.91	0.83	0.52	0.70	0.59
1108	LEU-COMP-THERM-057-035_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.85	0.84	0.91	0.83	0.52	0.70	0.59
1109	LEU-COMP-THERM-057-036_	0.98	0.97	0.98	0.95	0.94	0.91	0.93	0.93	0.86	0.82	0.91	0.81	0.50	0.70	0.59
1110	LEU-COMP-THERM-058-001_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1111	LEU-COMP-THERM-058-002_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1112	LEU-COMP-THERM-058-003_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1113	LEU-COMP-THERM-058-004_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.94	0.96	0.92	0.63	0.73	0.57
1114	LEU-COMP-THERM-058-005_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1115	LEU-COMP-THERM-058-006_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.94	0.96	0.92	0.63	0.73	0.57
1116	LEU-COMP-THERM-058-007_	0.88	0.84	0.87	0.92	0.90	0.98	0.97	0.97	0.95	0.92	0.95	0.91	0.61	0.72	0.57
1117	LEU-COMP-THERM-058-008_	0.88	0.83	0.87	0.91	0.90	0.98	0.96	0.97	0.95	0.92	0.96	0.91	0.61	0.72	0.57
1118	LEU-COMP-THERM-058-009_	0.88	0.83	0.87	0.91	0.90	0.98	0.96	0.97	0.95	0.92	0.96	0.91	0.61	0.72	0.57
1119	LEU-COMP-THERM-061-001_	0.99	0.94	0.98	0.92	0.89	0.90	0.90	0.91	0.82	0.85	0.92	0.83	0.57	0.74	0.62
1120	LEU-COMP-THERM-061-002_	0.99	0.93	0.98	0.91	0.89	0.90	0.90	0.91	0.82	0.85	0.92	0.84	0.57	0.74	0.62
1121	LEU-COMP-THERM-061-003_	0.99	0.94	0.98	0.91	0.89	0.89	0.90	0.91	0.82	0.85	0.91	0.83	0.57	0.74	0.62
1122	LEU-COMP-THERM-061-004_	0.99	0.94	0.98	0.91	0.89	0.89	0.90	0.91	0.82	0.85	0.91	0.83	0.57	0.74	0.62
1123	LEU-COMP-THERM-061-005_	0.99	0.94	0.98	0.92	0.90	0.89	0.90	0.91	0.82	0.84	0.91	0.83	0.56	0.74	0.62
1124	LEU-COMP-THERM-061-006_	0.99	0.94	0.98	0.92	0.89	0.89	0.90	0.91	0.82	0.84	0.91	0.83	0.56	0.74	0.62
1125	LEU-COMP-THERM-061-007_	0.99	0.95	0.98	0.92	0.90	0.89	0.90	0.92	0.82	0.84	0.91	0.83	0.55	0.74	0.62
1126	LEU-COMP-THERM-061-008_	0.99	0.94	0.98	0.92	0.90	0.89	0.90	0.92	0.82	0.84	0.91	0.83	0.56	0.74	0.62
1127	LEU-COMP-THERM-061-009_	0.99	0.95	0.98	0.93	0.91	0.90	0.91	0.92	0.84	0.85	0.92	0.84	0.55	0.73	0.61
1128	LEU-COMP-THERM-061-010_	0.95	0.85	0.93	0.85	0.82	0.89	0.86	0.87	0.78	0.88	0.92	0.86	0.60	0.72	0.58
1129	LEU-COMP-THERM-062-001_	0.98	0.91	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.90	0.83	0.57	0.73	0.59
1130	LEU-COMP-THERM-062-002_	0.98	0.91	0.96	0.90	0.86	0.90	0.88	0.90	0.80	0.86	0.91	0.84	0.58	0.73	0.59
1131	LEU-COMP-THERM-062-003_	0.98	0.90	0.96	0.89	0.86	0.90	0.88	0.90	0.80	0.86	0.91	0.84	0.58	0.73	0.59
1132	LEU-COMP-THERM-062-004_	0.98	0.91	0.96	0.89	0.86	0.90	0.88	0.90	0.80	0.86	0.91	0.83	0.58	0.73	0.59
1133	LEU-COMP-THERM-062-005_	0.98	0.91	0.96	0.90	0.86	0.89	0.88	0.90	0.80	0.85	0.91	0.83	0.57	0.73	0.59
1134	LEU-COMP-THERM-062-006_	0.98	0.90	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.91	0.83	0.58	0.73	0.59

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1135	LEU-COMP-THERM-062-007_	0.97	0.90	0.96	0.88	0.85	0.89	0.87	0.89	0.78	0.86	0.91	0.83	0.58	0.73	0.59
1136	LEU-COMP-THERM-062-008_	0.98	0.90	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.91	0.83	0.58	0.73	0.59
1137	LEU-COMP-THERM-062-009_	0.98	0.91	0.96	0.89	0.86	0.89	0.88	0.90	0.79	0.85	0.91	0.83	0.57	0.73	0.59
1138	LEU-COMP-THERM-062-010_	0.98	0.90	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.91	0.83	0.58	0.73	0.59
1139	LEU-COMP-THERM-062-011_	0.98	0.91	0.96	0.89	0.86	0.89	0.88	0.90	0.79	0.85	0.91	0.83	0.57	0.73	0.59
1140	LEU-COMP-THERM-062-012_	0.98	0.90	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.91	0.83	0.58	0.73	0.59
1141	LEU-COMP-THERM-062-013_	0.97	0.90	0.96	0.89	0.85	0.89	0.87	0.89	0.79	0.86	0.91	0.83	0.58	0.73	0.59
1142	LEU-COMP-THERM-062-014_	0.98	0.91	0.96	0.89	0.86	0.89	0.88	0.90	0.79	0.85	0.91	0.83	0.57	0.73	0.59
1143	LEU-COMP-THERM-062-015_	0.98	0.90	0.96	0.89	0.86	0.89	0.88	0.89	0.79	0.85	0.91	0.83	0.57	0.73	0.59
1144	LEU-COMP-THERM-065-001_	0.97	0.89	0.95	0.87	0.84	0.89	0.87	0.88	0.78	0.86	0.91	0.84	0.59	0.73	0.58
1145	LEU-COMP-THERM-065-002_	0.96	0.87	0.95	0.88	0.84	0.91	0.88	0.90	0.80	0.89	0.93	0.86	0.62	0.75	0.59
1146	LEU-COMP-THERM-065-003_	0.97	0.88	0.95	0.86	0.83	0.89	0.86	0.88	0.77	0.87	0.91	0.84	0.61	0.74	0.58
1147	LEU-COMP-THERM-065-004_	0.96	0.87	0.95	0.86	0.82	0.89	0.86	0.88	0.77	0.87	0.91	0.84	0.61	0.74	0.58
1148	LEU-COMP-THERM-065-005_	0.97	0.88	0.95	0.87	0.84	0.89	0.87	0.88	0.78	0.86	0.91	0.84	0.59	0.73	0.58
1149	LEU-COMP-THERM-065-006_	0.97	0.89	0.95	0.88	0.85	0.91	0.88	0.90	0.80	0.88	0.92	0.85	0.60	0.74	0.59
1150	LEU-COMP-THERM-065-007_	0.97	0.88	0.95	0.88	0.84	0.90	0.88	0.89	0.79	0.88	0.92	0.85	0.61	0.74	0.59
1151	LEU-COMP-THERM-065-008_	0.97	0.88	0.95	0.88	0.84	0.91	0.88	0.90	0.80	0.89	0.92	0.86	0.61	0.75	0.59
1152	LEU-COMP-THERM-065-009_	0.97	0.88	0.95	0.88	0.84	0.90	0.88	0.90	0.79	0.88	0.92	0.85	0.61	0.74	0.59
1153	LEU-COMP-THERM-065-010_	0.97	0.89	0.95	0.87	0.84	0.89	0.87	0.89	0.78	0.86	0.91	0.84	0.59	0.74	0.59
1154	LEU-COMP-THERM-065-011_	0.97	0.88	0.95	0.87	0.83	0.89	0.86	0.88	0.77	0.87	0.91	0.84	0.60	0.74	0.58
1155	LEU-COMP-THERM-065-012_	0.97	0.88	0.95	0.87	0.84	0.89	0.87	0.89	0.78	0.87	0.91	0.84	0.60	0.74	0.58
1156	LEU-COMP-THERM-065-013_	0.97	0.89	0.95	0.87	0.84	0.89	0.87	0.89	0.78	0.86	0.91	0.84	0.59	0.74	0.59
1157	LEU-COMP-THERM-065-014_	0.97	0.88	0.95	0.87	0.83	0.89	0.86	0.88	0.77	0.87	0.91	0.84	0.60	0.74	0.58
1158	LEU-COMP-THERM-065-015_	0.97	0.88	0.95	0.87	0.84	0.89	0.87	0.88	0.78	0.87	0.91	0.84	0.60	0.74	0.58
1159	LEU-COMP-THERM-065-016_	0.97	0.88	0.95	0.87	0.84	0.89	0.87	0.89	0.78	0.87	0.91	0.84	0.60	0.74	0.59
1160	LEU-COMP-THERM-065-017_	0.97	0.88	0.95	0.87	0.83	0.89	0.86	0.88	0.77	0.87	0.91	0.84	0.60	0.74	0.58
1161	LEU-COMP-THERM-066-004_	0.92	0.92	0.93	0.89	0.90	0.87	0.91	0.89	0.87	0.79	0.87	0.80	0.65	0.77	0.71
1162	LEU-COMP-THERM-066-005_	0.94	0.96	0.95	0.93	0.94	0.86	0.92	0.91	0.89	0.76	0.86	0.77	0.55	0.73	0.69
1163	LEU-COMP-THERM-066-006_	0.91	0.97	0.92	0.94	0.96	0.83	0.91	0.89	0.89	0.69	0.82	0.71	0.44	0.65	0.64
1164	LEU-COMP-THERM-066-007_	0.93	0.90	0.94	0.89	0.89	0.91	0.92	0.91	0.88	0.85	0.91	0.85	0.67	0.77	0.67
1165	LEU-COMP-THERM-066-008_	0.95	0.95	0.96	0.94	0.94	0.91	0.94	0.93	0.90	0.82	0.91	0.83	0.58	0.74	0.65
1166	LEU-COMP-THERM-066-009_	0.96	0.95	0.96	0.94	0.94	0.91	0.94	0.93	0.90	0.82	0.91	0.83	0.57	0.73	0.65
1167	LEU-COMP-THERM-066-010_	0.93	0.97	0.93	0.95	0.97	0.88	0.94	0.92	0.91	0.76	0.87	0.76	0.45	0.65	0.59
1168	LEU-COMP-THERM-068-004_	0.03	0.03	0.03	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1169	LEU-COMP-THERM-068-005_	0.03	0.03	0.03	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1170	LEU-COMP-THERM-068-006_	0.04	0.04	0.04	0.02	0.02	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1171	LEU-COMP-THERM-068-007_	0.04	0.04	0.04	0.02	0.02	0.00	0.00	0.00	0.00	0.01	0.02	0.02	0.00	0.00	0.00
1172	LEU-COMP-THERM-068-008_	0.05	0.05	0.05	0.01	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.00	0.00	0.00
1173	LEU-COMP-THERM-068-009_	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1174	LEU-COMP-THERM-068-010_	0.02	0.03	0.03	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1175	LEU-COMP-THERM-068-011_	0.03	0.03	0.03	0.02	0.02	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.00	0.00	0.00
1176	LEU-COMP-THERM-068-012_	0.05	0.05	0.05	0.02	0.01	0.00	0.00	0.00	0.01	0.02	0.02	0.02	0.00	0.00	0.00

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1177	LEU-COMP-THERM-068-013_	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1178	LEU-COMP-THERM-068-014_	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1179	LEU-COMP-THERM-068-015_	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1180	LEU-COMP-THERM-068-016_	0.04	0.04	0.04	0.02	0.02	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1181	LEU-COMP-THERM-068-017_	0.03	0.04	0.04	0.02	0.02	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
1182	LEU-COMP-THERM-069-001_	0.97	0.90	0.96	0.88	0.85	0.88	0.86	0.89	0.78	0.85	0.91	0.84	0.59	0.75	0.63
1183	LEU-COMP-THERM-069-002_	0.90	0.77	0.89	0.75	0.70	0.80	0.76	0.80	0.66	0.83	0.85	0.82	0.72	0.81	0.67
1184	LEU-COMP-THERM-069-003_	0.90	0.77	0.89	0.74	0.70	0.80	0.76	0.80	0.66	0.83	0.85	0.82	0.72	0.81	0.67
1185	LEU-COMP-THERM-069-004_	0.98	0.91	0.97	0.90	0.87	0.89	0.88	0.90	0.80	0.86	0.91	0.84	0.59	0.75	0.63
1186	LEU-COMP-THERM-069-005_	0.94	0.85	0.94	0.82	0.79	0.85	0.82	0.85	0.73	0.84	0.88	0.83	0.67	0.79	0.66
1187	LEU-COMP-THERM-070-001_	0.95	0.87	0.95	0.83	0.80	0.82	0.82	0.86	0.74	0.81	0.87	0.81	0.64	0.80	0.71
1188	LEU-COMP-THERM-070-002_	0.95	0.87	0.95	0.83	0.80	0.83	0.82	0.86	0.74	0.82	0.87	0.81	0.65	0.80	0.71
1189	LEU-COMP-THERM-070-003_	0.95	0.88	0.95	0.84	0.81	0.83	0.82	0.86	0.74	0.81	0.87	0.81	0.64	0.80	0.71
1190	LEU-COMP-THERM-070-004_	0.95	0.87	0.95	0.83	0.80	0.83	0.82	0.86	0.74	0.81	0.87	0.81	0.65	0.80	0.71
1191	LEU-COMP-THERM-070-005_	0.95	0.88	0.95	0.84	0.81	0.83	0.82	0.86	0.74	0.81	0.87	0.81	0.65	0.80	0.71
1192	LEU-COMP-THERM-070-006_	0.95	0.88	0.95	0.83	0.81	0.82	0.82	0.86	0.74	0.81	0.87	0.80	0.64	0.80	0.71
1193	LEU-COMP-THERM-070-007_	0.95	0.87	0.95	0.83	0.81	0.83	0.82	0.86	0.74	0.82	0.87	0.81	0.65	0.80	0.71
1194	LEU-COMP-THERM-070-008_	0.95	0.88	0.95	0.84	0.81	0.83	0.83	0.86	0.75	0.81	0.87	0.81	0.64	0.80	0.71
1195	LEU-COMP-THERM-070-009_	0.95	0.87	0.95	0.83	0.80	0.83	0.82	0.86	0.74	0.82	0.87	0.82	0.66	0.80	0.71
1196	LEU-COMP-THERM-070-010_	0.95	0.87	0.95	0.83	0.80	0.83	0.82	0.86	0.74	0.82	0.87	0.81	0.65	0.80	0.71
1197	LEU-COMP-THERM-070-011_	0.95	0.88	0.95	0.84	0.81	0.83	0.83	0.86	0.75	0.81	0.87	0.81	0.64	0.80	0.71
1198	LEU-COMP-THERM-070-012_	0.95	0.88	0.95	0.84	0.81	0.83	0.83	0.86	0.75	0.82	0.87	0.81	0.65	0.80	0.71
1199	LEU-COMP-THERM-071-001_	0.96	0.89	0.96	0.85	0.82	0.85	0.84	0.87	0.75	0.83	0.88	0.82	0.62	0.78	0.66
1200	LEU-COMP-THERM-071-002_	0.97	0.90	0.96	0.86	0.83	0.85	0.84	0.88	0.76	0.82	0.88	0.81	0.61	0.77	0.66
1201	LEU-COMP-THERM-071-003_	0.97	0.89	0.96	0.86	0.83	0.85	0.84	0.88	0.76	0.83	0.89	0.82	0.61	0.77	0.66
1202	LEU-COMP-THERM-071-004_	0.95	0.86	0.94	0.83	0.79	0.84	0.82	0.86	0.73	0.83	0.88	0.82	0.65	0.79	0.67
1203	LEU-COMP-THERM-072-001_	0.96	0.98	0.95	0.96	0.96	0.88	0.93	0.92	0.87	0.77	0.87	0.76	0.43	0.63	0.56
1204	LEU-COMP-THERM-072-002_	0.96	0.97	0.95	0.96	0.96	0.88	0.92	0.91	0.87	0.77	0.87	0.76	0.43	0.63	0.55
1205	LEU-COMP-THERM-072-003_	0.96	0.97	0.95	0.96	0.96	0.88	0.93	0.91	0.87	0.77	0.87	0.76	0.43	0.63	0.55
1206	LEU-COMP-THERM-072-004_	0.96	0.97	0.96	0.96	0.96	0.89	0.93	0.92	0.88	0.78	0.88	0.78	0.44	0.65	0.56
1207	LEU-COMP-THERM-072-005_	0.96	0.97	0.95	0.96	0.96	0.89	0.93	0.92	0.87	0.78	0.88	0.78	0.44	0.65	0.56
1208	LEU-COMP-THERM-072-006_	0.96	0.97	0.95	0.96	0.96	0.89	0.93	0.92	0.88	0.78	0.88	0.78	0.44	0.65	0.56
1209	LEU-COMP-THERM-072-007_	0.95	0.87	0.95	0.85	0.81	0.84	0.83	0.87	0.75	0.83	0.88	0.82	0.62	0.78	0.66
1210	LEU-COMP-THERM-072-008_	0.95	0.87	0.95	0.84	0.81	0.84	0.83	0.86	0.74	0.83	0.88	0.82	0.62	0.78	0.66
1211	LEU-COMP-THERM-072-009_	0.93	0.84	0.93	0.81	0.78	0.82	0.80	0.84	0.72	0.83	0.87	0.82	0.65	0.79	0.67
1212	LEU-COMP-THERM-073-001_	0.97	0.89	0.96	0.86	0.83	0.86	0.85	0.88	0.76	0.85	0.90	0.83	0.61	0.77	0.65
1213	LEU-COMP-THERM-073-002_	0.97	0.89	0.96	0.86	0.83	0.87	0.85	0.88	0.77	0.85	0.90	0.84	0.61	0.77	0.65
1214	LEU-COMP-THERM-073-003_	0.97	0.89	0.96	0.87	0.84	0.87	0.85	0.88	0.77	0.85	0.90	0.84	0.60	0.76	0.64
1215	LEU-COMP-THERM-073-004_	0.97	0.91	0.97	0.88	0.85	0.86	0.85	0.89	0.77	0.82	0.89	0.81	0.59	0.76	0.66
1216	LEU-COMP-THERM-073-005_	0.98	0.92	0.97	0.89	0.86	0.86	0.86	0.89	0.78	0.82	0.89	0.81	0.57	0.75	0.65
1217	LEU-COMP-THERM-073-006_	0.98	0.91	0.97	0.88	0.85	0.86	0.86	0.89	0.78	0.84	0.90	0.82	0.59	0.76	0.65
1218	LEU-COMP-THERM-073-007_	0.98	0.90	0.97	0.88	0.84	0.86	0.86	0.89	0.77	0.84	0.90	0.83	0.59	0.76	0.65

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1219	LEU-COMP-THERM-073-008_	0.98	0.91	0.97	0.88	0.85	0.87	0.86	0.89	0.78	0.84	0.90	0.82	0.59	0.76	0.64
1220	LEU-COMP-THERM-073-009_	0.98	0.93	0.98	0.90	0.88	0.87	0.87	0.90	0.80	0.82	0.90	0.81	0.55	0.74	0.64
1221	LEU-COMP-THERM-073-010_	0.98	0.93	0.98	0.90	0.87	0.87	0.87	0.90	0.80	0.83	0.90	0.82	0.56	0.74	0.64
1222	LEU-COMP-THERM-073-011_	0.99	0.93	0.98	0.90	0.88	0.87	0.88	0.90	0.80	0.83	0.90	0.82	0.55	0.74	0.63
1223	LEU-COMP-THERM-073-012_	0.97	0.88	0.96	0.86	0.83	0.87	0.85	0.88	0.77	0.86	0.91	0.85	0.62	0.76	0.63
1224	LEU-COMP-THERM-073-013_	0.97	0.88	0.96	0.86	0.83	0.87	0.85	0.88	0.77	0.86	0.91	0.85	0.62	0.76	0.63
1225	LEU-COMP-THERM-073-014_	0.97	0.88	0.96	0.86	0.83	0.87	0.85	0.88	0.77	0.87	0.91	0.85	0.62	0.76	0.63
1226	LEU-COMP-THERM-074-001_	0.95	0.94	0.95	0.93	0.92	0.89	0.91	0.90	0.85	0.80	0.89	0.79	0.47	0.65	0.55
1227	LEU-COMP-THERM-074-002_	0.95	0.93	0.95	0.92	0.91	0.89	0.91	0.90	0.85	0.82	0.89	0.81	0.49	0.66	0.55
1228	LEU-COMP-THERM-074-003_	0.95	0.97	0.95	0.95	0.95	0.88	0.92	0.91	0.87	0.77	0.87	0.76	0.43	0.63	0.55
1229	LEU-COMP-THERM-074-004_	0.95	0.96	0.94	0.95	0.95	0.88	0.92	0.91	0.87	0.77	0.87	0.76	0.43	0.63	0.54
1230	LEU-COMP-THERM-075-001_	0.94	0.86	0.94	0.82	0.79	0.82	0.81	0.85	0.73	0.82	0.87	0.81	0.67	0.81	0.71
1231	LEU-COMP-THERM-075-002_	0.94	0.85	0.94	0.81	0.78	0.82	0.81	0.84	0.73	0.83	0.87	0.82	0.68	0.81	0.71
1232	LEU-COMP-THERM-075-003_	0.94	0.85	0.94	0.81	0.78	0.83	0.81	0.85	0.73	0.83	0.88	0.83	0.69	0.82	0.72
1233	LEU-COMP-THERM-075-004_	0.95	0.88	0.95	0.84	0.81	0.82	0.82	0.86	0.74	0.81	0.87	0.80	0.64	0.80	0.71
1234	LEU-COMP-THERM-075-005_	0.95	0.88	0.95	0.84	0.81	0.82	0.82	0.86	0.74	0.81	0.87	0.80	0.64	0.80	0.71
1235	LEU-COMP-THERM-075-006_	0.95	0.88	0.95	0.84	0.81	0.83	0.83	0.86	0.75	0.81	0.87	0.81	0.64	0.80	0.71
1236	LEU-COMP-THERM-076-001_	0.61	0.40	0.60	0.46	0.41	0.71	0.58	0.61	0.52	0.83	0.74	0.80	0.87	0.75	0.51
1237	LEU-COMP-THERM-076-002_	0.61	0.40	0.60	0.46	0.42	0.72	0.59	0.62	0.53	0.84	0.75	0.81	0.86	0.75	0.51
1238	LEU-COMP-THERM-076-003_	0.59	0.38	0.58	0.44	0.39	0.70	0.58	0.60	0.52	0.83	0.73	0.80	0.87	0.74	0.50
1239	LEU-COMP-THERM-076-004_	0.55	0.34	0.54	0.40	0.36	0.67	0.54	0.57	0.49	0.81	0.70	0.78	0.87	0.73	0.48
1240	LEU-COMP-THERM-076-005_	0.66	0.46	0.65	0.52	0.47	0.75	0.64	0.67	0.58	0.86	0.78	0.83	0.87	0.78	0.54
1241	LEU-COMP-THERM-076-006_	0.63	0.43	0.62	0.49	0.44	0.73	0.61	0.64	0.55	0.84	0.76	0.82	0.86	0.76	0.53
1242	LEU-COMP-THERM-076-007_	0.73	0.54	0.72	0.60	0.55	0.80	0.70	0.73	0.64	0.90	0.84	0.87	0.86	0.81	0.58
1243	LEU-COMP-THERM-077-001_	0.87	0.82	0.86	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1244	LEU-COMP-THERM-077-002_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.96	0.91	0.61	0.73	0.57
1245	LEU-COMP-THERM-077-003_	0.86	0.81	0.85	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.95	0.92	0.63	0.73	0.57
1246	LEU-COMP-THERM-077-004_	0.86	0.81	0.85	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.95	0.92	0.63	0.73	0.57
1247	LEU-COMP-THERM-077-005_	0.86	0.81	0.85	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.95	0.92	0.63	0.73	0.57
1248	LEU-COMP-THERM-078-001_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1249	LEU-COMP-THERM-078-002_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1250	LEU-COMP-THERM-078-003_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1251	LEU-COMP-THERM-078-004_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1252	LEU-COMP-THERM-078-005_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1253	LEU-COMP-THERM-078-006_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1254	LEU-COMP-THERM-078-007_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.44	0.68	0.62
1255	LEU-COMP-THERM-078-008_	0.97	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.44	0.68	0.62
1256	LEU-COMP-THERM-078-009_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1257	LEU-COMP-THERM-078-010_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1258	LEU-COMP-THERM-078-011_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1259	LEU-COMP-THERM-078-012_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1260	LEU-COMP-THERM-078-013_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1261	LEU-COMP-THERM-078-014_	0.98	0.99	0.97	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.45	0.68	0.62
1262	LEU-COMP-THERM-078-015_	0.97	1.00	0.97	0.97	0.96	0.86	0.92	0.92	0.86	0.74	0.86	0.74	0.43	0.66	0.60
1263	LEU-COMP-THERM-079-001_	0.99	0.96	0.98	0.93	0.91	0.87	0.89	0.91	0.82	0.79	0.88	0.78	0.50	0.71	0.62
1264	LEU-COMP-THERM-079-002_	0.99	0.96	0.98	0.93	0.91	0.87	0.89	0.91	0.81	0.79	0.88	0.78	0.50	0.71	0.62
1265	LEU-COMP-THERM-079-003_	0.99	0.96	0.98	0.93	0.91	0.87	0.89	0.91	0.81	0.80	0.89	0.79	0.50	0.71	0.62
1266	LEU-COMP-THERM-079-004_	0.99	0.96	0.98	0.93	0.91	0.87	0.89	0.91	0.81	0.80	0.89	0.79	0.51	0.71	0.62
1267	LEU-COMP-THERM-079-005_	0.99	0.96	0.98	0.93	0.90	0.87	0.89	0.91	0.81	0.81	0.89	0.80	0.52	0.72	0.62
1268	LEU-COMP-THERM-079-006_	0.96	0.96	0.95	0.95	0.95	0.88	0.92	0.91	0.86	0.78	0.88	0.77	0.43	0.63	0.55
1269	LEU-COMP-THERM-079-007_	0.96	0.96	0.95	0.95	0.94	0.88	0.92	0.91	0.86	0.78	0.88	0.77	0.43	0.63	0.55
1270	LEU-COMP-THERM-079-008_	0.96	0.96	0.95	0.95	0.94	0.89	0.92	0.91	0.86	0.79	0.88	0.78	0.44	0.64	0.55
1271	LEU-COMP-THERM-079-009_	0.96	0.96	0.95	0.94	0.94	0.89	0.92	0.91	0.86	0.79	0.88	0.78	0.44	0.64	0.55
1272	LEU-COMP-THERM-079-010_	0.96	0.95	0.95	0.94	0.93	0.89	0.91	0.91	0.86	0.81	0.89	0.79	0.46	0.65	0.55
1273	LEU-COMP-THERM-080-001_	0.98	0.98	0.98	0.94	0.93	0.86	0.89	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1274	LEU-COMP-THERM-080-002_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1275	LEU-COMP-THERM-080-003_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1276	LEU-COMP-THERM-080-004_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1277	LEU-COMP-THERM-080-005_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1278	LEU-COMP-THERM-080-006_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1279	LEU-COMP-THERM-080-007_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1280	LEU-COMP-THERM-080-008_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1281	LEU-COMP-THERM-080-009_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1282	LEU-COMP-THERM-080-010_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.91	0.83	0.76	0.87	0.76	0.48	0.71	0.65
1283	LEU-COMP-THERM-080-011_	0.98	0.99	0.98	0.96	0.95	0.86	0.91	0.92	0.85	0.75	0.86	0.75	0.46	0.69	0.63
1284	LEU-COMP-THERM-082-002_	0.88	0.84	0.87	0.91	0.90	0.98	0.96	0.97	0.95	0.92	0.96	0.91	0.61	0.72	0.57
1285	LEU-COMP-THERM-082-003_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.96	0.92	0.63	0.73	0.56
1286	LEU-COMP-THERM-082-004_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.56
1287	LEU-COMP-THERM-082-005_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.96	0.92	0.63	0.73	0.56
1288	LEU-COMP-THERM-082-006_	0.87	0.81	0.86	0.90	0.88	0.98	0.96	0.96	0.94	0.94	0.96	0.92	0.63	0.73	0.56
1289	LEU-COMP-THERM-083-001_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1290	LEU-COMP-THERM-083-002_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.92	0.96	0.91	0.62	0.72	0.57
1291	LEU-COMP-THERM-083-003_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.72	0.57
1292	LEU-COMP-THERM-084-001_	0.84	0.79	0.84	0.88	0.86	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.63	0.72	0.56
1293	LEU-COMP-THERM-085-001_	0.98	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.83	0.79	0.88	0.78	0.50	0.72	0.65
1294	LEU-COMP-THERM-085-002_	0.98	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.83	0.79	0.89	0.79	0.51	0.73	0.65
1295	LEU-COMP-THERM-085-003_	0.99	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.83	0.79	0.89	0.79	0.51	0.73	0.65
1296	LEU-COMP-THERM-085-004_	0.98	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.84	0.79	0.88	0.78	0.50	0.72	0.65
1297	LEU-COMP-THERM-085-005_	0.98	0.97	0.98	0.94	0.92	0.87	0.90	0.92	0.83	0.79	0.88	0.78	0.50	0.72	0.65
1298	LEU-COMP-THERM-085-006_	0.98	0.98	0.98	0.94	0.93	0.86	0.90	0.92	0.84	0.78	0.88	0.78	0.49	0.71	0.65
1299	LEU-COMP-THERM-085-007_	0.99	0.98	0.98	0.94	0.93	0.87	0.90	0.92	0.84	0.78	0.88	0.78	0.49	0.72	0.64
1300	LEU-COMP-THERM-085-008_	0.99	0.98	0.98	0.95	0.93	0.87	0.90	0.92	0.84	0.78	0.88	0.78	0.49	0.71	0.64
1301	LEU-COMP-THERM-085-009_	0.99	0.98	0.98	0.95	0.94	0.87	0.91	0.92	0.84	0.78	0.88	0.78	0.49	0.71	0.64
1302	LEU-COMP-THERM-085-010_	0.99	0.98	0.99	0.95	0.94	0.87	0.91	0.92	0.84	0.78	0.89	0.78	0.49	0.71	0.64

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1303	LEU-COMP-THERM-085-011_	0.99	0.98	0.98	0.95	0.94	0.87	0.91	0.92	0.84	0.78	0.88	0.78	0.49	0.71	0.64
1304	LEU-COMP-THERM-085-012_	0.99	0.98	0.99	0.95	0.94	0.88	0.91	0.92	0.85	0.79	0.89	0.79	0.50	0.71	0.64
1305	LEU-COMP-THERM-085-013_	0.99	0.98	0.98	0.95	0.94	0.87	0.91	0.92	0.85	0.78	0.89	0.78	0.49	0.71	0.64
1306	LEU-COMP-THERM-089-001_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1307	LEU-COMP-THERM-089-002_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.94	0.96	0.92	0.63	0.73	0.57
1308	LEU-COMP-THERM-089-003_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1309	LEU-COMP-THERM-089-004_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1310	LEU-COMP-THERM-090-001_	0.85	0.80	0.84	0.89	0.87	0.98	0.95	0.96	0.95	0.92	0.95	0.91	0.62	0.71	0.55
1311	LEU-COMP-THERM-090-002_	0.84	0.80	0.84	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.62	0.72	0.55
1312	LEU-COMP-THERM-090-003_	0.85	0.80	0.84	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.63	0.72	0.55
1313	LEU-COMP-THERM-090-004_	0.85	0.80	0.85	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.92	0.63	0.72	0.56
1314	LEU-COMP-THERM-090-005_	0.85	0.80	0.85	0.89	0.87	0.98	0.95	0.96	0.95	0.93	0.95	0.91	0.63	0.72	0.56
1315	LEU-COMP-THERM-090-006_	0.85	0.80	0.84	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.63	0.72	0.55
1316	LEU-COMP-THERM-090-007_	0.84	0.79	0.84	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.95	0.91	0.63	0.72	0.55
1317	LEU-COMP-THERM-090-008_	0.85	0.80	0.85	0.89	0.87	0.98	0.95	0.96	0.95	0.93	0.95	0.91	0.62	0.72	0.56
1318	LEU-COMP-THERM-090-009_	0.86	0.81	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.95	0.91	0.62	0.72	0.56
1319	LEU-COMP-THERM-091-001_	0.87	0.81	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.96	0.92	0.63	0.73	0.56
1320	LEU-COMP-THERM-091-002_	0.88	0.83	0.87	0.91	0.89	0.99	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1321	LEU-COMP-THERM-091-003_	0.87	0.83	0.87	0.91	0.89	0.99	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1322	LEU-COMP-THERM-091-004_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.57
1323	LEU-COMP-THERM-091-005_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.63	0.73	0.56
1324	LEU-COMP-THERM-091-006_	0.86	0.81	0.85	0.89	0.87	0.98	0.95	0.96	0.94	0.93	0.96	0.92	0.62	0.72	0.55
1325	LEU-COMP-THERM-091-007_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.96	0.92	0.62	0.72	0.55
1326	LEU-COMP-THERM-091-008_	0.87	0.82	0.86	0.90	0.88	0.98	0.96	0.96	0.95	0.93	0.96	0.92	0.62	0.71	0.55
1327	LEU-COMP-THERM-091-009_	0.87	0.82	0.86	0.91	0.89	0.98	0.96	0.96	0.95	0.93	0.96	0.91	0.61	0.71	0.56
1328	LEU-COMP-THERM-092-001_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1329	LEU-COMP-THERM-092-002_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1330	LEU-COMP-THERM-092-003_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1331	LEU-COMP-THERM-092-004_	0.87	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.91	0.62	0.73	0.57
1332	LEU-COMP-THERM-092-005_	0.87	0.82	0.87	0.90	0.88	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1333	LEU-COMP-THERM-092-006_	0.88	0.83	0.87	0.91	0.89	0.98	0.96	0.97	0.95	0.93	0.96	0.92	0.62	0.73	0.57
1334	LEU-COMP-THERM-094-001_	0.90	0.80	0.90	0.76	0.73	0.80	0.77	0.81	0.69	0.82	0.85	0.81	0.71	0.82	0.71
1335	LEU-COMP-THERM-094-002_	0.90	0.79	0.90	0.76	0.72	0.79	0.76	0.81	0.68	0.82	0.85	0.81	0.71	0.82	0.70
1336	LEU-COMP-THERM-094-003_	0.91	0.81	0.91	0.78	0.74	0.80	0.78	0.82	0.69	0.81	0.85	0.80	0.69	0.81	0.71
1337	LEU-COMP-THERM-094-004_	0.91	0.82	0.91	0.78	0.74	0.80	0.78	0.82	0.70	0.82	0.85	0.81	0.69	0.81	0.71
1338	LEU-COMP-THERM-094-005_	0.92	0.83	0.92	0.79	0.75	0.80	0.78	0.83	0.70	0.81	0.85	0.80	0.68	0.81	0.70
1339	LEU-COMP-THERM-094-006_	0.93	0.84	0.93	0.80	0.77	0.81	0.79	0.84	0.71	0.81	0.86	0.80	0.67	0.81	0.71
1340	LEU-COMP-THERM-094-007_	0.93	0.85	0.93	0.81	0.77	0.81	0.80	0.84	0.71	0.80	0.85	0.80	0.66	0.80	0.71
1341	LEU-COMP-THERM-094-008_	0.93	0.85	0.93	0.81	0.78	0.81	0.80	0.84	0.72	0.80	0.86	0.80	0.65	0.80	0.71
1342	LEU-COMP-THERM-094-009_	0.93	0.85	0.93	0.81	0.78	0.81	0.80	0.84	0.72	0.80	0.86	0.80	0.66	0.80	0.71
1343	LEU-COMP-THERM-094-010_	0.94	0.86	0.94	0.82	0.78	0.81	0.81	0.84	0.72	0.81	0.86	0.80	0.66	0.80	0.71
1344	LEU-COMP-THERM-094-011_	0.94	0.86	0.94	0.82	0.79	0.82	0.81	0.85	0.73	0.81	0.86	0.80	0.65	0.80	0.71

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1345	LEU-MET-THERM-001-001_E	0.41	0.22	0.38	0.23	0.19	0.44	0.33	0.33	0.24	0.55	0.46	0.50	0.55	0.43	0.22
1346	LEU-MET-THERM-002-001_E	0.52	0.40	0.51	0.38	0.36	0.51	0.45	0.46	0.40	0.58	0.54	0.56	0.43	0.41	0.26
1347	LEU-MET-THERM-002-002_E	0.50	0.39	0.49	0.37	0.35	0.50	0.44	0.44	0.39	0.55	0.52	0.53	0.41	0.39	0.26
1348	LEU-MET-THERM-002-003_E	0.51	0.40	0.50	0.38	0.36	0.51	0.45	0.45	0.40	0.57	0.54	0.55	0.42	0.40	0.26
1349	LEU-MET-THERM-002-004_E	0.51	0.41	0.50	0.39	0.37	0.51	0.45	0.46	0.40	0.56	0.53	0.54	0.43	0.41	0.27
1350	LEU-MET-THERM-002-005_E	0.55	0.42	0.54	0.41	0.39	0.55	0.48	0.49	0.43	0.62	0.58	0.59	0.46	0.43	0.28
1351	LEU-MET-THERM-002-006_E	0.53	0.40	0.52	0.39	0.36	0.53	0.47	0.47	0.40	0.60	0.56	0.57	0.50	0.46	0.30
1352	LEU-MET-THERM-002-007_E	0.55	0.43	0.54	0.41	0.39	0.55	0.49	0.49	0.43	0.61	0.58	0.59	0.46	0.44	0.28
1353	LEU-MET-THERM-002-008_E	0.50	0.40	0.49	0.38	0.36	0.50	0.44	0.45	0.39	0.54	0.52	0.52	0.41	0.40	0.26
1354	LEU-MET-THERM-002-009_E	0.52	0.41	0.51	0.39	0.37	0.52	0.46	0.46	0.41	0.57	0.54	0.55	0.43	0.41	0.27
1355	LEU-MET-THERM-002-010_E	0.58	0.45	0.57	0.44	0.42	0.58	0.51	0.51	0.45	0.64	0.60	0.61	0.48	0.46	0.30
1356	LEU-MET-THERM-002-011_E	0.57	0.45	0.55	0.43	0.41	0.56	0.50	0.50	0.44	0.62	0.59	0.59	0.47	0.45	0.30
1357	LEU-MET-THERM-002-012_E	0.59	0.45	0.58	0.44	0.42	0.59	0.52	0.52	0.46	0.67	0.63	0.64	0.49	0.47	0.30
1358	LEU-MET-THERM-004-001_E	0.93	0.87	0.93	0.84	0.80	0.78	0.79	0.84	0.71	0.76	0.83	0.75	0.50	0.71	0.63
1359	LEU-MET-THERM-004-002_E	0.93	0.87	0.93	0.84	0.80	0.78	0.78	0.84	0.70	0.75	0.82	0.74	0.48	0.70	0.63
1360	LEU-MET-THERM-004-003_E	0.95	0.90	0.94	0.87	0.84	0.81	0.82	0.86	0.74	0.77	0.85	0.76	0.48	0.69	0.62
1361	LEU-MET-THERM-004-004_E	0.95	0.90	0.94	0.87	0.84	0.81	0.81	0.86	0.74	0.76	0.84	0.75	0.47	0.69	0.61
1362	LEU-MET-THERM-004-005_E	0.95	0.90	0.95	0.87	0.84	0.83	0.83	0.87	0.76	0.80	0.87	0.78	0.49	0.69	0.60
1363	LEU-MET-THERM-004-006_E	0.96	0.90	0.95	0.88	0.85	0.83	0.83	0.87	0.76	0.79	0.86	0.78	0.48	0.69	0.60
1364	LEU-MET-THERM-004-007_E	0.92	0.83	0.91	0.82	0.80	0.83	0.81	0.84	0.74	0.83	0.87	0.81	0.52	0.67	0.56
1365	LEU-MET-THERM-004-008_E	0.92	0.84	0.91	0.82	0.80	0.83	0.81	0.84	0.74	0.83	0.87	0.81	0.52	0.67	0.56
1366	LEU-MET-THERM-006-001_E	0.48	0.24	0.46	0.27	0.22	0.51	0.37	0.39	0.28	0.68	0.56	0.63	0.69	0.54	0.31
1367	LEU-MET-THERM-006-002_E	0.46	0.23	0.44	0.25	0.20	0.50	0.35	0.37	0.27	0.67	0.55	0.62	0.69	0.53	0.30
1368	LEU-MET-THERM-006-003_E	0.48	0.24	0.45	0.27	0.21	0.51	0.37	0.39	0.28	0.68	0.56	0.63	0.69	0.54	0.31
1369	LEU-MET-THERM-006-004_E	0.57	0.34	0.54	0.36	0.31	0.58	0.45	0.47	0.36	0.73	0.63	0.68	0.70	0.59	0.35
1370	LEU-MET-THERM-006-005_E	0.58	0.35	0.55	0.37	0.31	0.58	0.45	0.48	0.36	0.73	0.63	0.68	0.69	0.59	0.36
1371	LEU-MET-THERM-006-006_E	0.63	0.41	0.60	0.43	0.38	0.63	0.51	0.53	0.41	0.77	0.68	0.71	0.69	0.61	0.39
1372	LEU-MET-THERM-006-007_E	0.65	0.43	0.62	0.45	0.39	0.64	0.52	0.55	0.42	0.77	0.69	0.72	0.69	0.62	0.40
1373	LEU-MET-THERM-006-008_E	0.63	0.41	0.60	0.43	0.37	0.63	0.50	0.53	0.41	0.76	0.68	0.71	0.69	0.61	0.38
1374	LEU-MET-THERM-006-009_E	0.64	0.42	0.61	0.44	0.38	0.64	0.51	0.54	0.42	0.77	0.68	0.72	0.69	0.62	0.39
1375	LEU-MET-THERM-006-010_E	0.64	0.42	0.61	0.44	0.39	0.64	0.51	0.54	0.42	0.77	0.69	0.72	0.69	0.62	0.39
1376	LEU-MET-THERM-006-011_E	0.62	0.40	0.59	0.42	0.36	0.62	0.49	0.52	0.40	0.76	0.67	0.71	0.69	0.61	0.38
1377	LEU-MET-THERM-006-012_E	0.64	0.42	0.61	0.44	0.39	0.64	0.52	0.54	0.42	0.77	0.69	0.72	0.68	0.61	0.38
1378	LEU-MET-THERM-006-013_E	0.65	0.43	0.62	0.45	0.40	0.65	0.52	0.55	0.43	0.77	0.69	0.72	0.68	0.61	0.39
1379	LEU-MET-THERM-006-014_E	0.64	0.42	0.61	0.45	0.40	0.64	0.52	0.54	0.43	0.77	0.69	0.72	0.67	0.60	0.38
1380	LEU-MET-THERM-006-015_E	0.62	0.40	0.59	0.43	0.37	0.63	0.50	0.52	0.41	0.76	0.68	0.71	0.67	0.59	0.36
1381	LEU-MET-THERM-006-016_E	0.62	0.41	0.59	0.43	0.38	0.63	0.50	0.53	0.41	0.76	0.68	0.71	0.67	0.59	0.37
1382	LEU-MET-THERM-006-017_E	0.58	0.36	0.55	0.39	0.34	0.61	0.47	0.49	0.39	0.75	0.65	0.69	0.65	0.56	0.34
1383	LEU-MET-THERM-006-018_E	0.58	0.36	0.55	0.39	0.34	0.60	0.47	0.49	0.39	0.74	0.65	0.69	0.65	0.56	0.33
1384	LEU-MET-THERM-006-019_E	0.47	0.23	0.45	0.26	0.21	0.51	0.36	0.38	0.28	0.68	0.56	0.62	0.68	0.53	0.30
1385	LEU-MET-THERM-006-020_E	0.49	0.25	0.46	0.28	0.22	0.52	0.37	0.40	0.29	0.68	0.57	0.63	0.68	0.54	0.31
1386	LEU-MET-THERM-006-021_E	0.57	0.35	0.55	0.37	0.32	0.59	0.45	0.48	0.37	0.74	0.64	0.68	0.69	0.58	0.35

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1387	LEU-MET-THERM-006-022_E	0.55	0.32	0.53	0.35	0.29	0.57	0.44	0.46	0.35	0.72	0.62	0.67	0.68	0.57	0.34
1388	LEU-MET-THERM-006-023_E	0.55	0.32	0.52	0.34	0.29	0.57	0.43	0.45	0.34	0.72	0.62	0.67	0.68	0.57	0.34
1389	LEU-MET-THERM-006-024_E	0.55	0.32	0.52	0.34	0.29	0.57	0.43	0.46	0.34	0.72	0.62	0.67	0.69	0.57	0.34
1390	LEU-MET-THERM-006-025_E	0.58	0.35	0.55	0.38	0.33	0.60	0.46	0.49	0.38	0.74	0.65	0.69	0.68	0.58	0.35
1391	LEU-MET-THERM-006-026_E	0.58	0.36	0.56	0.38	0.33	0.60	0.47	0.49	0.38	0.74	0.65	0.69	0.68	0.58	0.35
1392	LEU-MET-THERM-006-027_E	0.59	0.37	0.57	0.39	0.34	0.61	0.47	0.50	0.38	0.75	0.65	0.69	0.68	0.59	0.36
1393	LEU-MET-THERM-006-028_E	0.57	0.35	0.54	0.37	0.32	0.59	0.46	0.48	0.37	0.74	0.64	0.68	0.68	0.58	0.35
1394	LEU-MET-THERM-006-029_E	0.57	0.35	0.54	0.38	0.33	0.60	0.46	0.48	0.38	0.74	0.64	0.69	0.67	0.57	0.34
1395	LEU-MET-THERM-006-030_E	0.56	0.34	0.53	0.36	0.31	0.59	0.45	0.47	0.37	0.73	0.63	0.68	0.67	0.56	0.33
1396	LEU-MET-THERM-007-001_E	0.96	0.94	0.96	0.90	0.88	0.82	0.84	0.88	0.77	0.75	0.84	0.74	0.47	0.70	0.63
1397	LEU-MET-THERM-007-002_E	0.97	0.98	0.97	0.95	0.93	0.85	0.89	0.91	0.82	0.75	0.86	0.74	0.43	0.67	0.60
1398	LEU-MET-THERM-007-003_E	0.97	0.99	0.96	0.96	0.96	0.86	0.91	0.92	0.85	0.75	0.86	0.74	0.41	0.64	0.58
1399	LEU-MET-THERM-007-004_E	0.96	0.98	0.95	0.96	0.96	0.87	0.91	0.91	0.86	0.76	0.86	0.75	0.41	0.63	0.56
1400	LEU-MET-THERM-007-005_E	0.94	0.94	0.93	0.93	0.93	0.87	0.90	0.89	0.85	0.78	0.87	0.76	0.42	0.61	0.53
1401	LEU-MET-THERM-007-006_E	0.88	0.84	0.87	0.85	0.84	0.85	0.84	0.83	0.79	0.80	0.85	0.78	0.46	0.60	0.48
1402	LEU-MET-THERM-015-001_E	0.53	0.41	0.52	0.40	0.37	0.53	0.47	0.47	0.40	0.58	0.55	0.56	0.47	0.45	0.29
1403	LEU-MET-THERM-015-002_E	0.53	0.42	0.52	0.40	0.38	0.53	0.47	0.47	0.41	0.58	0.55	0.56	0.47	0.44	0.29
1404	LEU-MET-THERM-015-003_E	0.53	0.41	0.52	0.40	0.37	0.53	0.46	0.47	0.40	0.58	0.55	0.56	0.47	0.44	0.29
1405	LEU-MET-THERM-015-004_E	0.53	0.42	0.52	0.40	0.38	0.53	0.47	0.47	0.41	0.58	0.55	0.56	0.47	0.44	0.29
1406	LEU-MET-THERM-015-005_E	0.53	0.42	0.52	0.40	0.38	0.53	0.47	0.47	0.41	0.58	0.55	0.56	0.47	0.44	0.29
1407	LEU-MET-THERM-015-006_E	0.53	0.41	0.52	0.40	0.38	0.53	0.47	0.47	0.41	0.58	0.55	0.55	0.46	0.44	0.29
1408	LEU-MET-THERM-015-007_E	0.53	0.41	0.51	0.40	0.38	0.52	0.46	0.47	0.41	0.57	0.54	0.55	0.46	0.44	0.29
1409	LEU-MET-THERM-015-008_E	0.56	0.44	0.55	0.42	0.40	0.56	0.50	0.50	0.44	0.63	0.59	0.61	0.46	0.44	0.28
1410	LEU-MET-THERM-015-009_E	0.56	0.43	0.55	0.42	0.40	0.56	0.50	0.50	0.44	0.63	0.60	0.61	0.46	0.44	0.28
1411	LEU-MET-THERM-015-010_E	0.56	0.43	0.55	0.42	0.40	0.56	0.49	0.50	0.44	0.64	0.60	0.61	0.46	0.44	0.28
1412	LEU-MET-THERM-015-011_E	0.56	0.43	0.55	0.42	0.39	0.56	0.49	0.50	0.44	0.63	0.59	0.61	0.46	0.44	0.28
1413	LEU-MET-THERM-015-012_E	0.56	0.44	0.55	0.42	0.40	0.57	0.50	0.50	0.44	0.63	0.60	0.61	0.46	0.44	0.28
1414	LEU-MET-THERM-015-013_E	0.56	0.43	0.55	0.41	0.39	0.56	0.49	0.49	0.43	0.63	0.59	0.60	0.46	0.44	0.28
1415	LEU-MET-THERM-015-014_E	0.56	0.43	0.55	0.42	0.40	0.56	0.49	0.50	0.44	0.63	0.59	0.60	0.46	0.44	0.28
1416	LEU-MET-THERM-015-015_E	0.53	0.41	0.52	0.39	0.37	0.52	0.46	0.47	0.41	0.59	0.55	0.57	0.43	0.41	0.26
1417	LEU-MET-THERM-015-016_E	0.53	0.41	0.52	0.39	0.37	0.53	0.46	0.47	0.41	0.59	0.55	0.57	0.43	0.41	0.27
1418	LEU-MET-THERM-015-017_E	0.53	0.41	0.52	0.39	0.37	0.53	0.47	0.47	0.41	0.59	0.56	0.57	0.43	0.41	0.27
1419	LEU-MET-THERM-015-018_E	0.53	0.41	0.52	0.40	0.37	0.53	0.47	0.47	0.41	0.59	0.56	0.57	0.44	0.42	0.27
1420	LEU-MET-THERM-015-019_E	0.53	0.42	0.52	0.40	0.38	0.53	0.47	0.47	0.42	0.60	0.56	0.57	0.44	0.42	0.27
1421	LEU-MET-THERM-015-020_E	0.54	0.42	0.53	0.40	0.38	0.54	0.47	0.48	0.42	0.60	0.56	0.58	0.44	0.42	0.27
1422	LEU-MET-THERM-015-021_E	0.53	0.41	0.52	0.40	0.38	0.53	0.47	0.47	0.42	0.60	0.56	0.57	0.44	0.42	0.27
1423	LEU-MET-THERM-015-022_E	0.53	0.41	0.52	0.39	0.37	0.53	0.47	0.47	0.41	0.59	0.56	0.57	0.43	0.41	0.27
1424	LEU-MISC-THERM-001-001_E	0.93	0.93	0.93	0.93	0.93	0.90	0.92	0.90	0.87	0.80	0.89	0.79	0.46	0.64	0.53
1425	LEU-MISC-THERM-001-002_E	0.93	0.93	0.93	0.93	0.93	0.89	0.92	0.90	0.87	0.80	0.88	0.79	0.46	0.63	0.53
1426	LEU-MISC-THERM-001-003_E	0.93	0.93	0.92	0.92	0.93	0.89	0.92	0.90	0.87	0.80	0.88	0.78	0.45	0.63	0.53
1427	LEU-MISC-THERM-001-004_E	0.93	0.93	0.92	0.92	0.93	0.88	0.91	0.89	0.86	0.79	0.87	0.78	0.45	0.62	0.52
1428	LEU-MISC-THERM-001-005_E	0.93	0.93	0.92	0.92	0.92	0.88	0.91	0.89	0.86	0.79	0.87	0.78	0.44	0.62	0.52

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1429	LEU-MISC-THERM-002-001_	0.94	0.95	0.93	0.94	0.94	0.89	0.92	0.90	0.87	0.78	0.87	0.77	0.45	0.63	0.54
1430	LEU-MISC-THERM-002-002_	0.94	0.95	0.93	0.93	0.94	0.89	0.92	0.90	0.87	0.78	0.87	0.77	0.44	0.63	0.53
1431	LEU-MISC-THERM-002-003_	0.93	0.94	0.93	0.93	0.93	0.89	0.92	0.90	0.87	0.79	0.87	0.77	0.45	0.62	0.53
1432	LEU-MISC-THERM-002-004_	0.93	0.94	0.92	0.93	0.93	0.88	0.91	0.89	0.87	0.79	0.87	0.77	0.44	0.62	0.53
1433	LEU-MISC-THERM-002-005_	0.93	0.93	0.92	0.93	0.93	0.88	0.91	0.89	0.86	0.78	0.87	0.77	0.44	0.62	0.52
1434	LEU-MISC-THERM-002-006_	0.93	0.93	0.92	0.92	0.93	0.88	0.91	0.89	0.86	0.78	0.87	0.77	0.44	0.61	0.52
1435	LEU-MISC-THERM-003-001_	0.98	0.97	0.97	0.95	0.94	0.90	0.93	0.93	0.87	0.80	0.90	0.80	0.49	0.68	0.59
1436	LEU-MISC-THERM-003-002_	0.98	0.97	0.97	0.95	0.94	0.90	0.93	0.93	0.87	0.80	0.90	0.79	0.48	0.68	0.59
1437	LEU-MISC-THERM-003-003_	0.98	0.97	0.97	0.95	0.95	0.90	0.93	0.93	0.87	0.80	0.90	0.79	0.48	0.68	0.59
1438	LEU-MISC-THERM-003-004_	0.98	0.97	0.97	0.95	0.95	0.90	0.93	0.93	0.87	0.80	0.90	0.79	0.48	0.68	0.59
1439	LEU-MISC-THERM-003-005_	0.98	0.98	0.97	0.96	0.95	0.89	0.93	0.93	0.87	0.80	0.89	0.79	0.47	0.68	0.59
1440	LEU-MISC-THERM-003-006_	0.98	0.98	0.97	0.96	0.95	0.89	0.93	0.93	0.87	0.79	0.89	0.79	0.47	0.67	0.58
1441	LEU-MISC-THERM-003-007_	0.98	0.98	0.97	0.96	0.95	0.89	0.93	0.93	0.87	0.79	0.89	0.78	0.46	0.67	0.59
1442	LEU-MISC-THERM-003-008_	0.98	0.98	0.97	0.96	0.95	0.89	0.93	0.92	0.87	0.78	0.89	0.78	0.45	0.67	0.58
1443	LEU-MISC-THERM-003-009_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.50	0.69	0.59
1444	LEU-MISC-THERM-003-010_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.82	0.91	0.81	0.50	0.69	0.59
1445	LEU-MISC-THERM-003-011_	0.98	0.97	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.82	0.91	0.81	0.49	0.69	0.59
1446	LEU-MISC-THERM-003-012_	0.98	0.97	0.97	0.95	0.94	0.90	0.93	0.93	0.87	0.82	0.91	0.81	0.49	0.68	0.59
1447	LEU-MISC-THERM-003-013_	0.98	0.97	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.81	0.90	0.80	0.48	0.68	0.59
1448	LEU-MISC-THERM-003-014_	0.98	0.98	0.97	0.96	0.95	0.90	0.93	0.93	0.87	0.80	0.89	0.79	0.47	0.67	0.59
1449	LEU-MISC-THERM-003-015_	0.98	0.98	0.97	0.96	0.95	0.89	0.93	0.93	0.87	0.79	0.89	0.78	0.46	0.67	0.58
1450	LEU-MISC-THERM-005-001_	0.98	0.96	0.97	0.95	0.94	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.51	0.69	0.59
1451	LEU-MISC-THERM-005-002_	0.98	0.96	0.97	0.94	0.93	0.91	0.93	0.93	0.87	0.83	0.91	0.82	0.52	0.70	0.59
1452	LEU-MISC-THERM-005-003_	0.98	0.95	0.97	0.94	0.93	0.91	0.93	0.93	0.86	0.84	0.92	0.83	0.52	0.70	0.59
1453	LEU-MISC-THERM-005-004_	0.98	0.95	0.97	0.94	0.93	0.91	0.93	0.93	0.86	0.84	0.92	0.83	0.52	0.70	0.59
1454	LEU-MISC-THERM-005-005_	0.98	0.95	0.97	0.94	0.93	0.91	0.93	0.93	0.86	0.84	0.92	0.83	0.52	0.70	0.59
1455	LEU-MISC-THERM-005-006_	0.98	0.95	0.97	0.93	0.92	0.91	0.93	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1456	LEU-MISC-THERM-005-007_	0.98	0.95	0.97	0.93	0.92	0.91	0.93	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1457	LEU-MISC-THERM-005-008_	0.98	0.95	0.97	0.93	0.92	0.91	0.93	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1458	LEU-MISC-THERM-005-009_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1459	LEU-MISC-THERM-005-010_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1460	LEU-MISC-THERM-005-011_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1461	LEU-MISC-THERM-005-012_	0.98	0.95	0.97	0.93	0.92	0.91	0.92	0.92	0.86	0.84	0.92	0.83	0.53	0.70	0.59
1462	LEU-MISC-THERM-006-001_	0.97	0.96	0.97	0.94	0.93	0.91	0.93	0.93	0.87	0.84	0.92	0.83	0.51	0.69	0.59
1463	LEU-MISC-THERM-006-002_	0.97	0.95	0.96	0.93	0.92	0.90	0.92	0.92	0.86	0.84	0.92	0.84	0.51	0.69	0.59
1464	LEU-MISC-THERM-006-003_	0.96	0.93	0.95	0.92	0.91	0.89	0.91	0.91	0.84	0.84	0.91	0.85	0.51	0.69	0.58
1465	LEU-MISC-THERM-006-004_	0.95	0.92	0.94	0.90	0.89	0.88	0.89	0.89	0.83	0.84	0.91	0.85	0.52	0.68	0.57
1466	LEU-MISC-THERM-006-005_	0.93	0.89	0.92	0.88	0.86	0.86	0.87	0.87	0.81	0.84	0.90	0.85	0.52	0.68	0.57
1467	LEU-MISC-THERM-006-006_	0.98	0.97	0.97	0.95	0.94	0.90	0.93	0.92	0.86	0.82	0.90	0.81	0.49	0.69	0.59
1468	LEU-MISC-THERM-006-007_	0.97	0.96	0.97	0.94	0.93	0.89	0.92	0.92	0.86	0.82	0.91	0.82	0.49	0.68	0.59
1469	LEU-MISC-THERM-006-008_	0.96	0.94	0.96	0.92	0.91	0.89	0.91	0.91	0.84	0.83	0.91	0.84	0.50	0.69	0.58
1470	LEU-MISC-THERM-006-009_	0.95	0.93	0.95	0.91	0.90	0.88	0.90	0.90	0.83	0.83	0.91	0.84	0.51	0.68	0.58

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1471	LEU-MISC-THERM-006-010_E	0.94	0.91	0.93	0.89	0.88	0.86	0.88	0.88	0.82	0.83	0.90	0.84	0.51	0.68	0.57
1472	LEU-SOL-THERM-001-001_E	0.91	0.92	0.90	0.93	0.94	0.90	0.93	0.90	0.89	0.79	0.88	0.78	0.47	0.64	0.54
1473	LEU-SOL-THERM-002-001_E	0.80	0.76	0.79	0.77	0.78	0.81	0.80	0.77	0.75	0.77	0.81	0.75	0.46	0.55	0.43
1474	LEU-SOL-THERM-002-002_E	0.83	0.81	0.82	0.82	0.82	0.83	0.83	0.80	0.79	0.77	0.82	0.75	0.45	0.57	0.45
1475	LEU-SOL-THERM-002-003_E	0.82	0.79	0.81	0.80	0.81	0.83	0.82	0.79	0.78	0.77	0.82	0.75	0.45	0.56	0.44
1476	LEU-SOL-THERM-003-001_E	0.82	0.84	0.81	0.84	0.86	0.82	0.85	0.81	0.82	0.71	0.79	0.71	0.38	0.52	0.44
1477	LEU-SOL-THERM-003-002_E	0.81	0.82	0.80	0.82	0.84	0.81	0.84	0.79	0.81	0.72	0.79	0.71	0.39	0.52	0.43
1478	LEU-SOL-THERM-003-003_E	0.81	0.81	0.80	0.82	0.84	0.81	0.83	0.79	0.80	0.73	0.79	0.72	0.39	0.52	0.43
1479	LEU-SOL-THERM-003-004_E	0.81	0.81	0.80	0.82	0.83	0.81	0.83	0.79	0.80	0.73	0.79	0.72	0.40	0.52	0.43
1480	LEU-SOL-THERM-003-005_E	0.76	0.73	0.76	0.74	0.75	0.78	0.77	0.74	0.74	0.74	0.78	0.73	0.42	0.51	0.40
1481	LEU-SOL-THERM-003-006_E	0.75	0.71	0.75	0.73	0.74	0.77	0.76	0.73	0.72	0.74	0.78	0.72	0.42	0.51	0.39
1482	LEU-SOL-THERM-003-007_E	0.75	0.70	0.74	0.72	0.72	0.77	0.75	0.72	0.71	0.74	0.77	0.72	0.42	0.50	0.39
1483	LEU-SOL-THERM-003-008_E	0.69	0.61	0.68	0.64	0.64	0.72	0.68	0.66	0.64	0.74	0.74	0.71	0.43	0.48	0.35
1484	LEU-SOL-THERM-003-009_E	0.69	0.61	0.68	0.63	0.63	0.72	0.67	0.65	0.63	0.73	0.73	0.71	0.43	0.48	0.35
1485	LEU-SOL-THERM-004-001_E	0.82	0.83	0.82	0.84	0.86	0.83	0.86	0.82	0.83	0.74	0.81	0.73	0.40	0.54	0.44
1486	LEU-SOL-THERM-004-002_E	0.81	0.82	0.81	0.83	0.85	0.83	0.85	0.81	0.82	0.74	0.81	0.73	0.41	0.54	0.44
1487	LEU-SOL-THERM-004-003_E	0.81	0.80	0.80	0.82	0.83	0.82	0.84	0.80	0.81	0.75	0.81	0.73	0.41	0.53	0.43
1488	LEU-SOL-THERM-004-004_E	0.80	0.79	0.79	0.80	0.81	0.82	0.82	0.79	0.80	0.75	0.80	0.74	0.42	0.53	0.42
1489	LEU-SOL-THERM-004-005_E	0.79	0.77	0.78	0.79	0.80	0.81	0.81	0.78	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1490	LEU-SOL-THERM-004-006_E	0.78	0.76	0.78	0.77	0.78	0.80	0.80	0.77	0.77	0.75	0.80	0.74	0.42	0.53	0.41
1491	LEU-SOL-THERM-004-007_E	0.77	0.74	0.77	0.76	0.77	0.80	0.79	0.76	0.76	0.76	0.79	0.74	0.43	0.52	0.41
1492	LEU-SOL-THERM-005-001_E	0.78	0.71	0.77	0.73	0.73	0.80	0.77	0.75	0.73	0.79	0.80	0.76	0.48	0.55	0.41
1493	LEU-SOL-THERM-005-002_E	0.77	0.70	0.76	0.72	0.72	0.80	0.76	0.74	0.72	0.79	0.80	0.77	0.48	0.55	0.41
1494	LEU-SOL-THERM-005-003_E	0.75	0.66	0.74	0.68	0.67	0.78	0.73	0.71	0.68	0.79	0.79	0.77	0.50	0.55	0.39
1495	LEU-SOL-THERM-006-001_E	0.84	0.87	0.84	0.89	0.91	0.86	0.90	0.86	0.88	0.75	0.83	0.74	0.41	0.56	0.47
1496	LEU-SOL-THERM-006-002_E	0.85	0.86	0.84	0.88	0.90	0.86	0.90	0.86	0.87	0.76	0.84	0.75	0.42	0.56	0.47
1497	LEU-SOL-THERM-006-003_E	0.85	0.86	0.85	0.87	0.89	0.87	0.89	0.86	0.87	0.77	0.84	0.77	0.43	0.57	0.47
1498	LEU-SOL-THERM-006-004_E	0.85	0.86	0.85	0.87	0.89	0.87	0.89	0.86	0.87	0.78	0.85	0.77	0.44	0.57	0.47
1499	LEU-SOL-THERM-006-005_E	0.85	0.84	0.85	0.85	0.87	0.87	0.88	0.85	0.85	0.80	0.86	0.79	0.46	0.58	0.47
1500	LEU-SOL-THERM-007-001_E	0.82	0.84	0.82	0.85	0.87	0.82	0.85	0.81	0.83	0.72	0.80	0.71	0.39	0.53	0.44
1501	LEU-SOL-THERM-007-002_E	0.81	0.83	0.81	0.83	0.85	0.82	0.84	0.80	0.82	0.72	0.80	0.71	0.39	0.53	0.44
1502	LEU-SOL-THERM-007-003_E	0.81	0.81	0.80	0.82	0.84	0.81	0.83	0.79	0.80	0.73	0.80	0.72	0.40	0.53	0.43
1503	LEU-SOL-THERM-007-004_E	0.80	0.80	0.80	0.81	0.82	0.81	0.82	0.78	0.79	0.74	0.80	0.72	0.40	0.52	0.42
1504	LEU-SOL-THERM-007-005_E	0.79	0.78	0.79	0.79	0.81	0.80	0.81	0.77	0.78	0.74	0.79	0.73	0.41	0.52	0.42
1505	LEU-SOL-THERM-008-001_E	0.79	0.77	0.79	0.78	0.80	0.81	0.81	0.77	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1506	LEU-SOL-THERM-008-002_E	0.79	0.77	0.78	0.78	0.79	0.81	0.81	0.77	0.78	0.76	0.80	0.74	0.42	0.53	0.42
1507	LEU-SOL-THERM-008-003_E	0.79	0.77	0.78	0.78	0.79	0.81	0.81	0.78	0.78	0.76	0.80	0.74	0.43	0.53	0.42
1508	LEU-SOL-THERM-008-004_E	0.79	0.76	0.78	0.78	0.79	0.81	0.81	0.77	0.78	0.76	0.80	0.74	0.43	0.53	0.42
1509	LEU-SOL-THERM-009-001_E	0.79	0.77	0.79	0.78	0.80	0.81	0.81	0.77	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1510	LEU-SOL-THERM-009-002_E	0.79	0.77	0.79	0.79	0.80	0.81	0.81	0.77	0.78	0.75	0.80	0.73	0.42	0.53	0.42
1511	LEU-SOL-THERM-009-003_E	0.79	0.77	0.79	0.79	0.80	0.81	0.81	0.77	0.78	0.75	0.80	0.73	0.42	0.53	0.42
1512	LEU-SOL-THERM-010-001_E	0.79	0.77	0.79	0.79	0.80	0.81	0.81	0.78	0.78	0.75	0.80	0.73	0.42	0.53	0.42

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1513	LEU-SOL-THERM-010-002_E	0.79	0.77	0.78	0.79	0.80	0.81	0.81	0.78	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1514	LEU-SOL-THERM-010-003_E	0.79	0.77	0.78	0.79	0.80	0.81	0.81	0.78	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1515	LEU-SOL-THERM-010-004_E	0.79	0.77	0.78	0.79	0.80	0.81	0.81	0.78	0.78	0.75	0.80	0.74	0.42	0.53	0.42
1516	LEU-SOL-THERM-011-001_E	0.83	0.80	0.82	0.82	0.82	0.84	0.84	0.81	0.80	0.79	0.83	0.77	0.46	0.57	0.45
1517	LEU-SOL-THERM-011-002_E	0.82	0.79	0.81	0.80	0.81	0.84	0.83	0.80	0.79	0.79	0.83	0.77	0.46	0.57	0.44
1518	LEU-SOL-THERM-011-003_E	0.81	0.77	0.80	0.78	0.79	0.83	0.81	0.78	0.77	0.79	0.82	0.77	0.47	0.56	0.43
1519	LEU-SOL-THERM-011-004_E	0.79	0.74	0.78	0.76	0.77	0.81	0.80	0.77	0.76	0.79	0.81	0.76	0.47	0.55	0.42
1520	LEU-SOL-THERM-011-005_E	0.78	0.73	0.77	0.75	0.75	0.81	0.78	0.75	0.74	0.78	0.81	0.76	0.47	0.55	0.41
1521	LEU-SOL-THERM-011-006_E	0.77	0.71	0.76	0.73	0.73	0.79	0.76	0.74	0.72	0.78	0.80	0.76	0.47	0.54	0.41
1522	LEU-SOL-THERM-011-007_E	0.76	0.69	0.75	0.71	0.71	0.79	0.75	0.73	0.71	0.78	0.79	0.76	0.47	0.54	0.40
1523	LEU-SOL-THERM-011-008_E	0.83	0.81	0.83	0.82	0.83	0.84	0.84	0.81	0.80	0.77	0.83	0.76	0.45	0.57	0.45
1524	LEU-SOL-THERM-011-009_E	0.83	0.80	0.82	0.81	0.82	0.83	0.83	0.80	0.79	0.78	0.82	0.76	0.45	0.56	0.44
1525	LEU-SOL-THERM-011-010_E	0.81	0.78	0.80	0.79	0.80	0.82	0.82	0.79	0.77	0.78	0.82	0.76	0.46	0.56	0.43
1526	LEU-SOL-THERM-011-011_E	0.80	0.75	0.79	0.77	0.77	0.81	0.80	0.77	0.75	0.78	0.81	0.76	0.46	0.55	0.42
1527	LEU-SOL-THERM-011-012_E	0.79	0.74	0.78	0.75	0.75	0.80	0.78	0.76	0.74	0.78	0.81	0.76	0.46	0.55	0.42
1528	LEU-SOL-THERM-011-013_E	0.77	0.71	0.77	0.73	0.73	0.79	0.77	0.74	0.72	0.78	0.80	0.75	0.46	0.54	0.41
1529	LEU-SOL-THERM-016-001_E	0.84	0.88	0.84	0.90	0.92	0.86	0.90	0.86	0.88	0.74	0.83	0.73	0.40	0.56	0.47
1530	LEU-SOL-THERM-016-002_E	0.84	0.87	0.84	0.89	0.91	0.86	0.90	0.86	0.88	0.74	0.83	0.74	0.40	0.56	0.47
1531	LEU-SOL-THERM-016-003_E	0.83	0.85	0.83	0.88	0.89	0.86	0.89	0.85	0.87	0.75	0.83	0.74	0.41	0.55	0.46
1532	LEU-SOL-THERM-016-004_E	0.83	0.85	0.83	0.87	0.89	0.85	0.88	0.84	0.86	0.76	0.83	0.75	0.42	0.55	0.46
1533	LEU-SOL-THERM-016-005_E	0.83	0.84	0.82	0.86	0.88	0.85	0.88	0.84	0.86	0.76	0.83	0.75	0.42	0.55	0.45
1534	LEU-SOL-THERM-016-006_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.85	0.76	0.83	0.75	0.42	0.55	0.45
1535	LEU-SOL-THERM-016-007_E	0.82	0.82	0.81	0.84	0.86	0.85	0.87	0.83	0.84	0.77	0.83	0.76	0.43	0.55	0.44
1536	LEU-SOL-THERM-017-001_E	0.84	0.88	0.84	0.89	0.91	0.85	0.89	0.85	0.87	0.73	0.82	0.72	0.39	0.55	0.47
1537	LEU-SOL-THERM-017-002_E	0.84	0.87	0.83	0.89	0.91	0.84	0.89	0.85	0.87	0.72	0.81	0.72	0.39	0.55	0.46
1538	LEU-SOL-THERM-017-003_E	0.83	0.86	0.83	0.87	0.89	0.84	0.88	0.84	0.86	0.73	0.81	0.73	0.39	0.54	0.45
1539	LEU-SOL-THERM-017-004_E	0.83	0.85	0.82	0.86	0.88	0.84	0.88	0.83	0.85	0.74	0.82	0.73	0.40	0.54	0.45
1540	LEU-SOL-THERM-017-005_E	0.82	0.84	0.82	0.86	0.87	0.84	0.87	0.83	0.84	0.75	0.82	0.74	0.41	0.54	0.45
1541	LEU-SOL-THERM-017-006_E	0.82	0.83	0.82	0.85	0.87	0.84	0.87	0.83	0.84	0.75	0.82	0.74	0.41	0.54	0.44
1542	LEU-SOL-THERM-018-001_E	0.82	0.82	0.82	0.84	0.86	0.85	0.87	0.83	0.84	0.77	0.83	0.76	0.43	0.55	0.45
1543	LEU-SOL-THERM-018-002_E	0.82	0.83	0.82	0.85	0.86	0.84	0.86	0.82	0.84	0.76	0.82	0.75	0.42	0.55	0.44
1544	LEU-SOL-THERM-018-003_E	0.82	0.83	0.82	0.85	0.86	0.84	0.87	0.83	0.84	0.76	0.83	0.75	0.42	0.55	0.44
1545	LEU-SOL-THERM-018-004_E	0.82	0.83	0.82	0.85	0.86	0.85	0.87	0.83	0.84	0.76	0.83	0.75	0.42	0.55	0.45
1546	LEU-SOL-THERM-018-005_E	0.82	0.83	0.82	0.85	0.86	0.85	0.87	0.83	0.84	0.77	0.83	0.76	0.43	0.55	0.45
1547	LEU-SOL-THERM-018-006_E	0.82	0.82	0.82	0.85	0.86	0.85	0.87	0.83	0.84	0.77	0.83	0.76	0.43	0.55	0.45
1548	LEU-SOL-THERM-019-001_E	0.82	0.83	0.82	0.85	0.87	0.84	0.87	0.83	0.84	0.75	0.82	0.74	0.41	0.55	0.45
1549	LEU-SOL-THERM-019-002_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.84	0.76	0.83	0.75	0.42	0.55	0.45
1550	LEU-SOL-THERM-019-003_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.85	0.76	0.83	0.75	0.42	0.55	0.45
1551	LEU-SOL-THERM-019-004_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.85	0.76	0.83	0.75	0.42	0.55	0.45
1552	LEU-SOL-THERM-019-005_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.85	0.76	0.83	0.75	0.42	0.55	0.45
1553	LEU-SOL-THERM-019-006_E	0.82	0.83	0.82	0.85	0.87	0.85	0.87	0.83	0.85	0.76	0.83	0.75	0.42	0.55	0.45
1554	LEU-SOL-THERM-020-001_E	0.80	0.78	0.79	0.80	0.81	0.82	0.82	0.79	0.79	0.75	0.81	0.74	0.42	0.53	0.42

Case	Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1555	LEU-SOL-THERM-020-002_E	0.78	0.75	0.78	0.77	0.79	0.80	0.80	0.77	0.77	0.76	0.80	0.74	0.42	0.52	0.41
1556	LEU-SOL-THERM-020-003_E	0.76	0.72	0.75	0.74	0.75	0.78	0.77	0.74	0.74	0.75	0.78	0.73	0.43	0.51	0.40
1557	LEU-SOL-THERM-020-004_E	0.74	0.69	0.73	0.71	0.71	0.77	0.74	0.72	0.71	0.75	0.77	0.73	0.43	0.51	0.38
1558	LEU-SOL-THERM-022-001_E	0.82	0.82	0.82	0.84	0.86	0.84	0.86	0.82	0.84	0.76	0.83	0.75	0.42	0.55	0.44
1559	LEU-SOL-THERM-022-002_E	0.82	0.82	0.82	0.84	0.86	0.84	0.86	0.82	0.83	0.76	0.83	0.75	0.42	0.55	0.44
1560	LEU-SOL-THERM-022-003_E	0.82	0.82	0.82	0.84	0.86	0.84	0.86	0.82	0.83	0.76	0.83	0.75	0.42	0.55	0.44
1561	LEU-SOL-THERM-022-004_E	0.82	0.82	0.82	0.84	0.86	0.84	0.86	0.82	0.83	0.76	0.83	0.75	0.42	0.55	0.44
1562	LEU-SOL-THERM-023-001_E	0.82	0.80	0.81	0.83	0.84	0.85	0.86	0.82	0.83	0.79	0.84	0.77	0.44	0.56	0.44
1563	LEU-SOL-THERM-023-002_E	0.82	0.81	0.82	0.83	0.85	0.85	0.86	0.82	0.83	0.78	0.84	0.77	0.44	0.55	0.44
1564	LEU-SOL-THERM-023-003_E	0.82	0.81	0.82	0.83	0.85	0.84	0.86	0.82	0.83	0.78	0.83	0.76	0.43	0.55	0.44
1565	LEU-SOL-THERM-023-004_E	0.82	0.81	0.81	0.83	0.84	0.84	0.85	0.82	0.83	0.78	0.83	0.76	0.43	0.55	0.44
1566	LEU-SOL-THERM-023-005_E	0.82	0.81	0.81	0.83	0.84	0.84	0.85	0.81	0.82	0.77	0.83	0.76	0.43	0.55	0.44
1567	LEU-SOL-THERM-023-006_E	0.82	0.81	0.81	0.83	0.85	0.83	0.85	0.81	0.82	0.76	0.82	0.75	0.42	0.54	0.44
1568	LEU-SOL-THERM-023-007_E	0.82	0.82	0.81	0.83	0.85	0.83	0.85	0.81	0.82	0.76	0.82	0.75	0.41	0.54	0.44
1569	LEU-SOL-THERM-023-008_E	0.82	0.82	0.81	0.83	0.85	0.83	0.85	0.81	0.82	0.76	0.82	0.75	0.41	0.54	0.44
1570	LEU-SOL-THERM-023-009_E	0.82	0.82	0.81	0.84	0.85	0.83	0.85	0.81	0.82	0.75	0.82	0.74	0.41	0.54	0.44
1571	LEU-SOL-THERM-024-001_E	0.82	0.81	0.82	0.83	0.84	0.85	0.86	0.82	0.83	0.79	0.84	0.77	0.44	0.56	0.44
1572	LEU-SOL-THERM-024-002_E	0.82	0.81	0.82	0.83	0.84	0.85	0.86	0.82	0.83	0.78	0.84	0.77	0.44	0.55	0.44
1573	LEU-SOL-THERM-024-003_E	0.82	0.81	0.82	0.83	0.85	0.84	0.86	0.82	0.83	0.77	0.83	0.76	0.43	0.55	0.44
1574	LEU-SOL-THERM-024-004_E	0.82	0.82	0.82	0.84	0.85	0.84	0.86	0.82	0.83	0.76	0.83	0.75	0.42	0.55	0.44
1575	LEU-SOL-THERM-024-005_E	0.82	0.82	0.82	0.84	0.85	0.84	0.86	0.82	0.83	0.76	0.82	0.75	0.42	0.54	0.44
1576	LEU-SOL-THERM-024-006_E	0.82	0.82	0.82	0.84	0.85	0.84	0.86	0.82	0.83	0.76	0.83	0.75	0.42	0.54	0.44
1577	LEU-SOL-THERM-024-007_E	0.82	0.82	0.82	0.84	0.85	0.84	0.86	0.82	0.83	0.76	0.82	0.75	0.42	0.54	0.44
1578	LEU-SOL-THERM-025-001_E	0.82	0.80	0.81	0.83	0.84	0.85	0.85	0.82	0.83	0.78	0.84	0.77	0.44	0.55	0.44
1579	LEU-SOL-THERM-025-002_E	0.82	0.81	0.81	0.83	0.84	0.84	0.85	0.82	0.83	0.78	0.83	0.77	0.44	0.55	0.44
1580	LEU-SOL-THERM-025-003_E	0.82	0.81	0.81	0.83	0.84	0.84	0.85	0.82	0.83	0.78	0.83	0.76	0.43	0.55	0.44
1581	LEU-SOL-THERM-025-004_E	0.82	0.81	0.81	0.83	0.85	0.84	0.85	0.82	0.83	0.77	0.83	0.76	0.43	0.55	0.44
1582	LEU-SOL-THERM-025-005_E	0.82	0.81	0.81	0.83	0.85	0.84	0.85	0.81	0.83	0.77	0.83	0.75	0.42	0.54	0.44
1583	LEU-SOL-THERM-025-006_E	0.82	0.82	0.82	0.83	0.85	0.84	0.85	0.82	0.83	0.77	0.83	0.75	0.42	0.54	0.44
1584	LEU-SOL-THERM-025-007_E	0.82	0.82	0.82	0.83	0.85	0.84	0.85	0.82	0.83	0.76	0.83	0.75	0.42	0.54	0.44

APPENDIX B. TN-B1 WATER MODELING EFFECT ON BENCHMARK EXPERIMENT c_k

The 6.7 wt.% ^{235}U , 13 Gd rods/assembly, $6 \times 1 \times 6$ HAC array model was assessed by using two different modeling approaches for water in the package. The intent of this study was to determine whether subdividing the different water regions by using different material numbers rather than by using one material number for multiple regions has an impact on c_k and the identification of applicable experiments.

The first approach is documented in Section 5.4, which uses material 7 for water in the entire fuel lattice (Gd and non-Gd rods), in the space between poly blocks and fuel, and in the reflector. The second approach uses different material numbers for Gd rod lattice water, non-Gd rod lattice water, water in spaces, and the water reflector. Both cases have essentially the same forward and adjoint k_{eff} and forward EALF within the uncertainty of the cases.

Base case: T3D_HAC_6-7wt_13Gd_6x6, 658 experiments with $c_k \geq 0.9$

Alternate case: T3D_HAC_6-7wt_13Gd_6x6_Hrefl, 646 experiments with $c_k \geq 0.9$

There is a shift of 12 benchmarks identified as “similar.” In each case, the change in c_k is small and involves a case with c_k very close to 0.9. The statistics in Table B-1 characterize the change in c_k of the 1,584 benchmarks. The change is very small.

Table B-1. Statistics that characterize the change in c_k of the 1,584 benchmarks (6 x 1 x 6 array).

Statistic	Change in c_k
Median base c_k	0.8902
Max diff.	0.0014
Median diff.	0.0004
Avg. diff.	0.0003
Std. dev. diff.	0.0003

The same comparison process was used with the 8 wt.% ^{235}U , 24 Gd rods/assembly, $10 \times 1 \times 10$ HAC array model. As with the 6.7 wt.% model, both cases have essentially the same forward and adjoint k_{eff} and forward EALF within the uncertainty of the cases.

Base case: T3D_HAC_8wt_24Gd_10x10a, 132 experiments with $c_k \geq 0.9$

Alternate case: T3D_HAC_8wt_24Gd_10x10_Hrefl, 126 experiments with $c_k \geq 0.9$

There is a shift of nine benchmarks identified as “similar.” In each case, the change in c_k is small—although larger than the 6.7 wt.% changes—and involves a case with c_k very close to 0.9. The statistics below characterize the change in c_k of the 1584 benchmarks. The change is small, confirming that the details of water modeling in the TN-B1 are relatively unimportant to the desired result.

Table B-2. Statistics that characterize the change in c_k of the 1,584 benchmarks (10 x 1 x 10 array).

Statistic	Change in c_k
Median base c_k	0.8107
Max diff.	0.0028
Median diff.	0.0012
Avg. diff.	0.0010
Std. dev. diff.	0.0010

APPENDIX C. TN-B1 ARRAY SIZE MODELING EFFECT ON BENCHMARK EXPERIMENT c_k

The 5 wt.% ^{235}U , 13 Gd rods/assembly, $10 \times 1 \times 10$ HAC array model was assessed by using two additional modeling approaches for TSUNAMI. The intent of this study was to determine whether using a single package—either with reflective boundary conditions or with a 30cm water reflector—changes the identification of applicable benchmark experiments by using c_k .

At first glance, these systems might appear similar. The same enrichment, same fuel form, and some moderators are in use in all three systems. The physical size of the systems differ, and these differences drive differences in reactivity, neutron spectrum, and some sensitivities. Several sensitivities are provided in Table C-1, as well as the system k_{eff} and the EALF value. SDF file names are provided in Table C-2. The large differences in k_{eff} reflect the differences in physical size and the leakage of neutrons from the system. Similarly, the spectrum of neutrons in the system softens as the system gets larger neutrons are resident in the system for longer. This longer lifetime allows more scattering and greater thermalization of some of the neutrons.

Table C-1. Key Sensitivities Among the Three Models Considered

5 wt.% TN-B1 sensitivities			
Nuclide	Single package	100 array	Inf. array
$^1\text{H}(\text{H}_2\text{O})$	0.391	0.109	0.03
^{235}U	0.215	0.221	0.217
$^1\text{H}(\text{poly})$	0.148	0.054	0.033
^{16}O	0.046	0.015	0.004
^{238}U	-0.017	-0.073	-0.085
k_{eff}	0.627	0.938	1.045
EALF	0.333	0.248	0.233

Table C-2. SDF File Names

Single package	T3D_HAC_5wt_13Gd_sgl.sdf
100 array	T3D_HAC_5wt_13Gd_10x10.sdf
Inf. array	T3D_HAC_5wt_13Gd_inf.sdf

The integral total ^{235}U sensitivity is largely invariant to system size in this scenario, although other sensitivities change significantly. The ^{235}U total sensitivity is shown in Figure C-1, which shows greater sensitivity at high energies and lower sensitivity at thermal energies for the single package model. This is consistent with the higher EALF value reported in Table C-1.

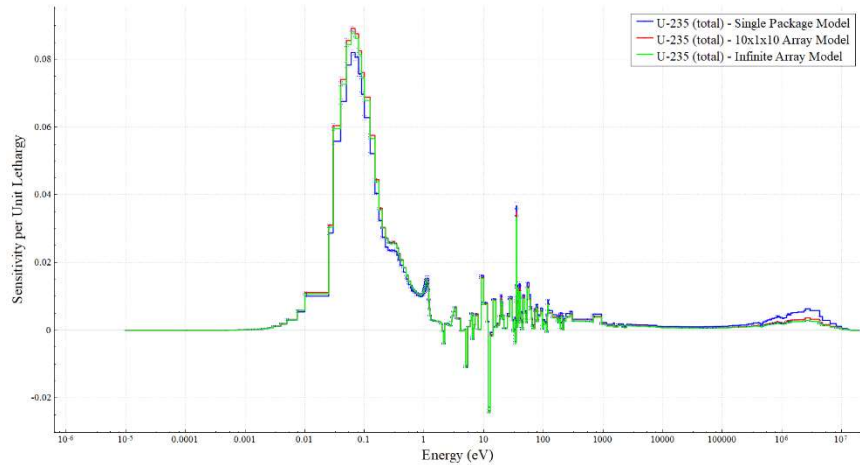


Figure C-1. Total ^{235}U sensitivity profiles for the three models.

All three moderating species— $^1\text{H}(\text{H}_2\text{O})$, $^1\text{H}(\text{poly})$, and ^{16}O —have significantly higher sensitivity in the single package model. The profiles are shown in Figure C-2. The model is fairly small, and many neutrons will leak from the system if they are not scattered first. Hence, collisions with light nuclei that lead to large energy losses on average are very important in the small system. In the larger models, these nuclei are less important because the neutron has a much lower, or zero, leakage probability. Eventually, the neutrons will reach thermal energy, although slowing down also increases the probability of parasitic absorption.

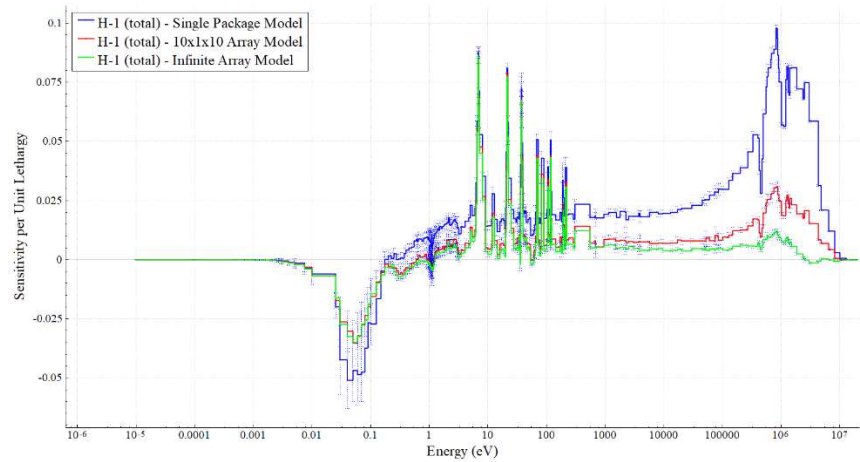


Figure C-2. Total ^1H sensitivity profiles for the three models.

The longer neutron lifetimes in the larger model also increase the magnitude of the ^{238}U sensitivity; more neutrons are absorbed by ^{238}U since there are no longer any neutrons leaking. The sensitivity profiles are shown in Figure C-3. The softening of the spectrum with the additional neutron scatter also reduces the fast fission contribution from ^{238}U , as clearly shown in Figure C-3.

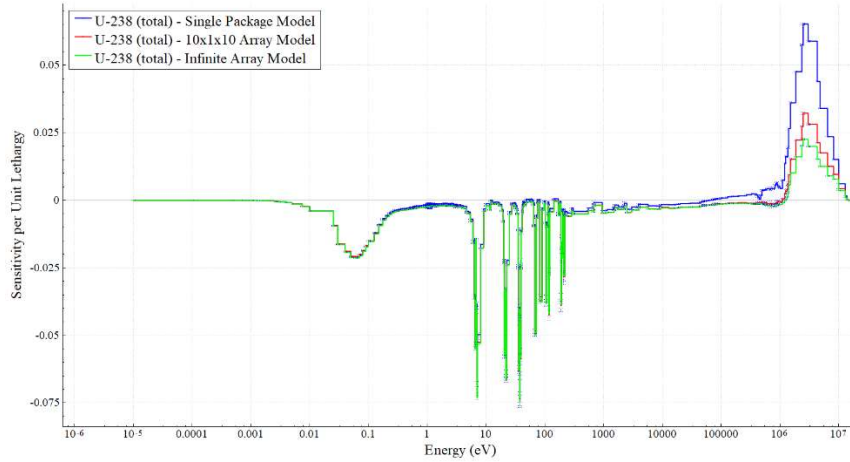


Figure C-3. Total ^{238}U sensitivity profiles for the three models.

The remaining question is how the differences in sensitivities will impact similarity assessments with available benchmark experiments. The results of the comparisons for these three models against the suite of 1,584 critical experiments are summarized in Table C-3 and shown in Figures C-4 through C-6. The figures illustrate that the pattern of c_k values is similar, but the values drop approximately uniformly from the single package to the finite array to the infinite array models. The finite array model also shows less spread in c_k values, especially for the LCT experiments, than either the single package or infinite array models.

Table C-3. Summary of similarity assessments for the 1,584 critical experiment suite.

	Single package	100 array	Inf. array
Median c_k	0.866	0.823	0.646
IEU	0	0	0
LEU	47	0	0
LCT	518	167	12
LMT	5	0	0
LST	1	0	0

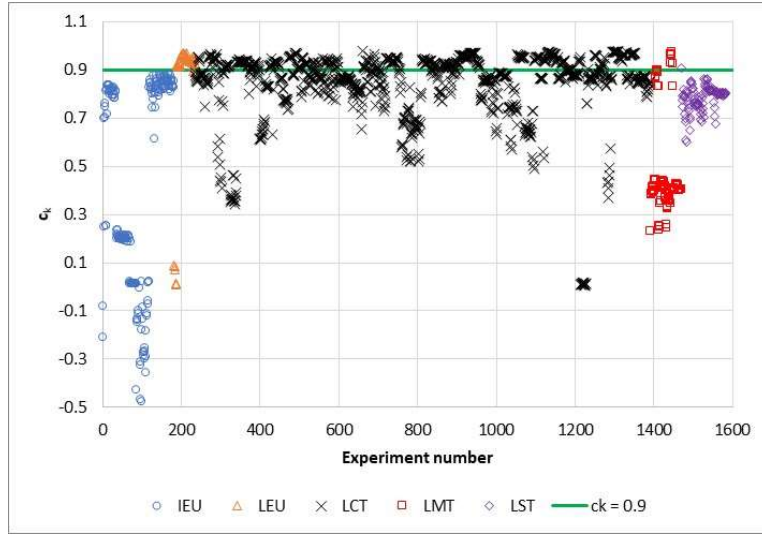


Figure C-4. c_k values for single package model.

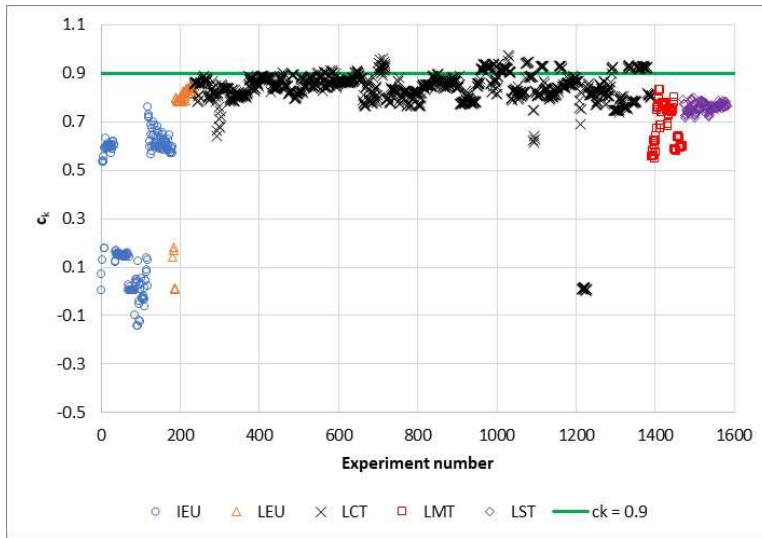


Figure C-5. c_k values for $10 \times 1 \times 10$ package array.

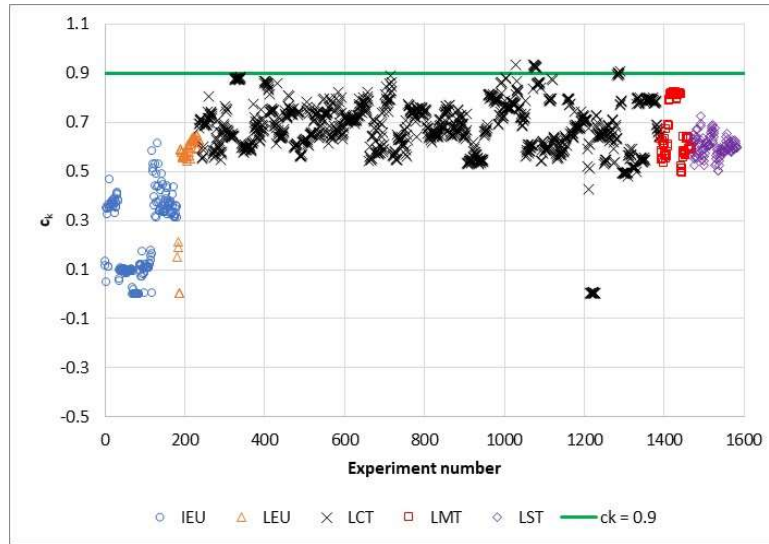


Figure C-6. c_k values for infinite package array.

The integral parameter c_k correlates the impact of nuclear data on k_{eff} between systems, so an examination of the nuclear data-induced uncertainty and its top contributors for each system can help explain the differences observed in c_k values. The total nuclear data-induced uncertainty for each application model and the top 10 contributors are shown in Table C-4. There are dramatic differences in the overall cross section uncertainty; the single package model uncertainty is more than 70% higher than the two array models. It is also clear that although the list of reactions contributing to the single package and infinite array models are quite different, the finite array model has a blend of the reactions that are prominent in the other two models. Therefore, both single unit models might predict applicable benchmarks for the HAC model, but the two models would do so for very different reasons. Neither model is likely to be a highly reliable indicator of benchmark applicability for the finite array model used in the safety basis analysis for this package.

Table C-4. Nuclear data-induced uncertainty for the three models.

Total Uncertainty	Single package		100 array		Inf. array	
	0.924% Δk		0.536% Δk		0.518% Δk	
	Reaction	Unc (% Δk)	Reaction	Unc (% Δk)	Reaction	Unc (% Δk)
Contributor #1	^{235}U X	0.587	^{235}U $\bar{\nu}$	0.353	^{235}U $\bar{\nu}$	0.355
Contributor #2	^{238}U inel.	0.486	^{56}Fe (n, γ)	0.182	^{56}Fe (n, γ)	0.207
Contributor #3	^{235}U $\bar{\nu}$	0.345	^{238}U (n, γ)	0.164	^{238}U (n, γ)	0.166
Contributor #4	^{16}O elastic	0.204	^{235}U (n, γ)	0.159	^{235}U (n, γ)	0.161
Contributor #5	^{238}U inel./el.	-0.187	^{235}U fis/(n, γ)	0.119	^{235}U fis/(n, γ)	0.119
Contributor #6	^{238}U (n, γ)	0.162	^{235}U X	0.115	^{235}U fission	0.113
Contributor #7	^{235}U (n, γ)	0.158	^{238}U inel.	0.114	^1H (n, γ)	0.079
Contributor #8	^1H elastic	0.148	^{235}U fission	0.114	^{238}U $\bar{\nu}$	0.051
Contributor #9	^{235}U fis/(n, γ)	0.115	^1H (n, γ)	0.082	^{157}Gd (n, γ)	0.044
Contributor #10	^{235}U fission	0.108	^{56}Fe elastic	0.058	^{235}U X	0.041

APPENDIX D. COMPUTER INPUT AND OUTPUT FILES

Section 2

Spreadsheets:

Modeling, tables, and plots: Traveller_TM_cases.xlsx

Direct perturbation vs. TSUNAMI sensitivity: DP_Trav_asbly_5wt.xlsx,
DP_Trav_asbly_8wt_IFBA.xlsx, DP_Trav_asbly_8wt_single_axial2, DP_Trav_RP_5wt.xlsx,
DP_Trav_RP_5wt.xlsx

Computer input and output:

Excel spreadsheets and computer input and output for Traveller calculations are included in .zip file Traveller.zip.

Section 3

Spreadsheets (pellet and powder models):

Modeling, tables, and plots: CHT-OP-TU_model_data.xlsx

Direct perturbation vs. TSUNAMI sensitivity: DP_CHTOPTU_5wt_48_rev3.xlsx,
DP_CHTOPTU_8wt_18_rev3_7-5in_rev3.xlsx, DP_CHTOPTU_18_6-9wt_7-5pel_rev3a.xlsx,
DP_CHTOPTU_48_16-5wt_7-5pel_rev3.xlsx

Computer input and output:

Excel spreadsheets and computer input and output for CHT-OP-TU calculations are included in .zip file CHT-OP-TU.zip. Some 8 wt.% $3 \times 3 \times 2$ files are misnamed with 48 indicating 48 packages rather than the correct number of 18 packages.

Section 5

Spreadsheets:

Modeling, tables, and plots: TN-B1_data.xlsx

Direct perturbation vs. TSUNAMI sensitivity: DP_HAC_5wt_13Gd_10x10.xlsx, DP_HAC_6-7wt_13Gd_6x6.xlsx, DP_HAC_8wt_24Gd_10x10a.xlsx

Computer input and output:

Excel spreadsheets and computer input and output for TN-B1 calculations are included in .zip file TN-B1.zip.

Section 6

Spreadsheets:

Modeling, tables, and plots: UF6_sampler_data.xlsx, DN30_TSUNAMI_results.xlsx

Direct perturbation vs. TSUNAMI sensitivity: DP_DN30_5wt_inf.xlsx, DP_DN30_6-7wt_3x2.xlsx,
DP_DN30_12-5wt_sgl.xlsx

Computer input and output:

Excel spreadsheets and computer input and output for TN-B1 calculations are included in .zip file DN30.zip.

Appendices

Spreadsheets: Combined_front_end_TSUNAMI_results_rev1, TN-B1_AppendixC.xlsx