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The Effect of Temperature on the Neutron Multiplication Factor for Pressurised Water Reactor Fuel Assemblies

A Temperature Analysis Benchmark

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Foreword

There is significant international interest in the effects of temperature on criticality safety evaluations. Improved access to nuclear data, notably thermal scattering data S(α,β) for hydrogen in ice, has made it possible to assess and deepen the understanding of the variation of criticality calculations associated with temperature.

Under the auspices of the Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) and of the Working Party on Nuclear Criticality Safety (WPNCS), Subgroup 3 was launched to study the impact of temperature through a wide range of codes, data libraries and methods. The group studied a pressurised water reactor (PWR) assembly in a thick water reflector at five different temperatures, ranging from ice to room temperature and up to reactor operation temperature. Ten organisations in eight countries participated, providing 34 sets of results.

With a view to launching the activity and obtaining results in a timely fashion, geometrical and material data from a previous WPNCS benchmark model were used in a new study to help examine the effect of temperature on criticality safety calculations.

The exercise was successful in bringing together a large number of institutions and employing a wide range of calculation codes and nuclear data libraries, thereby providing solid evidence for the conclusions drawn. The participants' dedication made it possible to complete the exercise in two years, providing timely support to end users.

This report contains the benchmark study and results, and was endorsed at the WPNCS Subgroup 3 meeting in July 2020.

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List of abbreviations and acronyms

CEA	Commissariat à l'énergie atomique et aux énergies alternatives (Alternative Energies and Atomic Energy Commission, France)
EMS	E Mennerdahl Systems
ENDF	Evaluated Nuclear Data File (United States)
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit (Germany)
GT	Guide tube
IRSN	Institut de Radioprotection et de Sûreté Nucléaire (Institute for Radiological Protection and Nuclear Safety, France)
JEFF	Joint Evaluated Fission and Fusion File
JENDL	Japanese Evaluated Nuclear Data Library (Japan)
LWR	Light water reactor
MCNP	Monte Carlo N-Particle Transport
MTA EK	Centre for Energy Research of the Hungarian Academy of Sciences (Hungary)
NEA	Nuclear Energy Agency
NRA	Nuclear Regulation Authority of Japan
OECD	Organisation for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory (United States)
PWR	Pressurised water reactor
RDB	Run-time Doppler Broadening
RSD	Relative standard deviation
SD	Standard deviation
SU	Single Unit
TSL	Thermal scattering law
UPM	University of Madrid (Spain)
WPNCS	Working Party on Nuclear Criticality Safety (NEA)

Executive summary

The role of temperature in criticality safety evaluations is of significant international interest since temperature affects physical parameters, such as material density or phase, as well as neutronic parameters such as reaction cross sections through the Doppler effect.

To better understand variations associated with temperature-dependent calculations for systems containing water, an inter code comparison benchmark was proposed. This benchmark is based upon a previous investigation considering the effect of an SiO_2 reflector on pressurised water reactor (PWR) fuel (NEA, 2020). A total of 30 subcases were used as a basis to assess the contribution of various parameters, primarily temperature but also boundary (reflective) conditions and burn-up.

Two main series focussed on:

- a PWR-type fuel assembly in a thick water reflector;
- an infinite array of PWR fuel assemblies.

For each series, the neutron multiplication factor was calculated at five different temperatures (233K, 253K, 293K, 333K and 588K) to assess the variation in reaction cross-section with temperature as well as the change in thermal scattering data for bound H. The effect of burn-up on these systems was also considered within the calculations, with each subcase repeated for three different values of burn-up: nul burn-up (fresh fuel), 30 GWd/t (mid-irradiation), and 45 GWd/t (typical of discharged fuels).

The spread in the results of the participants, as measured in % relative standard deviation (RSD), was low. This indicates a good agreement between the results of the participants in the majority of cases. The %RSD for calculations tends to increase away from room temperature (where there is increasing change in the physics of the system) and increases with burn-up in most, but not all, cases. The greatest %RSD is observed at 233 K.

The choice of S(α, β) data for bound H has only a small effect on the determined k_{eff} for 233K and 253K cases but the values calculated with ^{1}H bound in ice (H1_ICE) tend to be slightly higher. A criticality benchmark experiment, suitable to validate this observed trend, is yet to be performed. The key finding is that the k_{eff} determined for low-temperature calculations indicates that the choice of S(α, β) data for H has a relatively small effect on the determined k_{eff} when compared to the larger variation due to macroscopic physical effects (e.g. density).

1. Overview of the benchmark specification

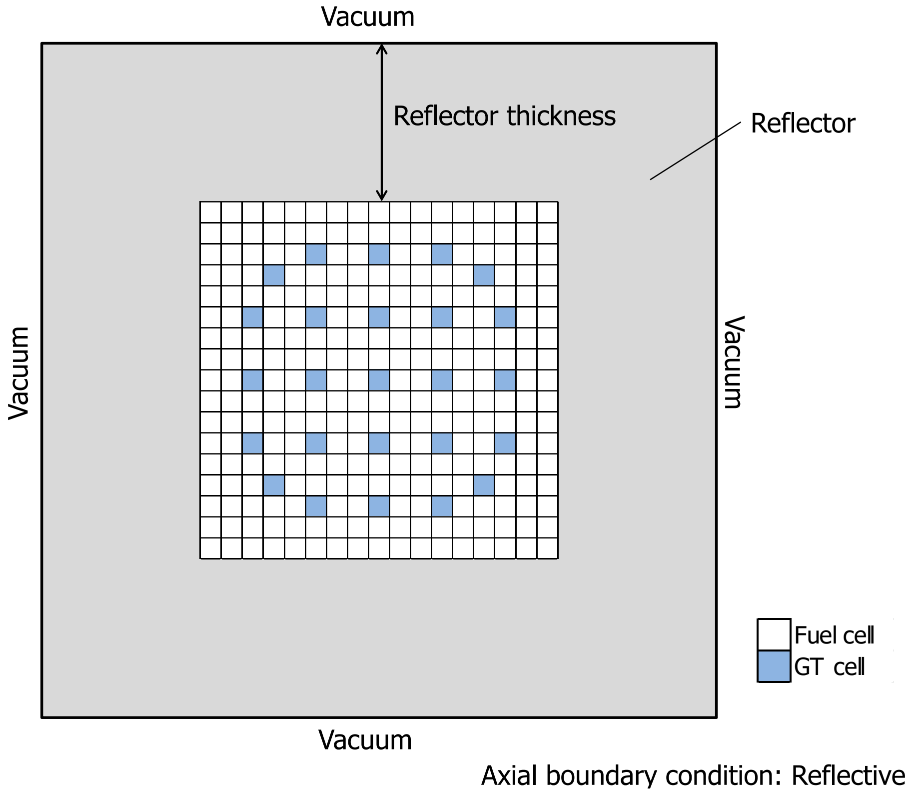
1.1. Fuel assembly geometry

A system containing a 17 × 17 type PWR fuel assembly was investigated. In the first case, the PWR assembly was held within a one-metre thick water reflector (kept consistently at room temperature [i.e. 293K] and pressure) as shown in Figure 1.1. For simplicity, this assembly was assumed to be infinite in the axial direction, hence a reflective boundary condition was applied. As a thick reflector was assumed in the radial direction, there was no requirement to assume a specific boundary condition (i.e. a vacuum).

In the second case, a radial reflective boundary condition was applied directly to the PWR fuel assembly to model an infinite repeating array of PWR fuel assemblies. For simplicity, this assembly was assumed to be infinite in the axial direction, hence a reflective boundary condition was applied.

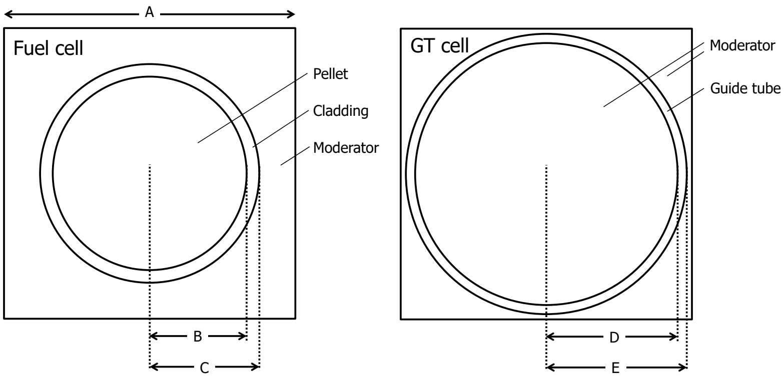
For both cases, the fuel cells and guide tube (GT) cells were modelled. The specification of the fuel rod and the guide tube is shown in Figure 1.2. The neutron multiplication factor at the temperatures of 233K, 253K, 293K, 333K and 588K should be calculated.

Figure 1.1. A schematic model for PWR benchmark problem



Source: NEA data, 2020.

Figure 1.2. Geometrical specification of fuel rod and guide tube



Source: Yamamoto, T. et al. (2002), "Benchmark problem suite for reactor physics study of LWR next generation fuels", J. Nucl. Sci. Technol., Vol. 37, No. 8, pp. 900-912.

Symbol	Subject	Value (cm)
A	Fuel rod pitch	1.265
Fuel rod		
B	Radius of pellet	0.412
C	Outer radius of cladding tube	0.476
Guide tube		
D	Inner radius of tube	0.570
E	Outer radius of tube	0.610

1.2. Moderator, cladding and reflector

The compositions of the moderator and cladding tube are shown in Table 1.1. The composition of the cladding tube was assumed to be natural zirconium rather than Zircaloy for simplicity. The grid spacer was also neglected to reduce the complexity of the model.

Table 1.1. Specification of moderator and cladding tube

	Moderator					Cladding tube
Material	Ice 1	Ice 2	Water – room temperature*	Water – elevated temperature	Water – elevated temperature and pressure	Zr-nat
Temperature (K)	233	253	293	333	588	
Density (g/cm^3)	0.9228	0.9208	0.998	0.983	0.694	6.53
	Number density (#/barn/cm)					
H_1[1]	6.17196E-02	6.15858E-02	6.67492E-02	6.57460E-02	4.64168E-02	-
^{16}O	3.08598E-02	3.07929E-02	3.33746E-02	3.28730E-02	2.32084E-02	-
Zr	-	-	-	-	-	4.3108E-02

Source: NEA data, 2020.
*Material specification for water-room temperature is to be used for the 1-m water reflector in all single unit calculations.
[1] To be modelled bound in H_2O liquid for cases with temperatures >=293K, to be modelled as bound in ice for the cases with temperatures 253K and 233K.

The composition of the 1-m water reflector in all single unit calculations, independent of the case temperature, should be that of water at room temperature as provided in Table 1.1.

1.3. Fuel composition

In this benchmark, a PWR UO_2 fuel assembly with an enrichment of 4.5 wt% ^{235}U was considered. Table 1.2 shows the nuclide number density of the fresh fuel.

Table 1.2. Nuclide number density of the fresh fuel

Number density (#/barn/cm)	
^{235}U	1.0468E-03
^{238}U	2.1935E-02
^{16}O	4.5963E-02

Source: NEA data, 2020.

Along with the fresh fuel, two used fuel cases were considered, 30 GWd/t and 45 GWd/t. The used fuel case of 45 GWd/t was selected as a representative burn-up for a typical spent PWR fuel assembly, and 30 GWd/t was considered as the intermediate case in order to understand the influence of burn-up on the trend of variation in the calculated neutron multiplication factor with temperature. For the cases considering used fuel, the concept of burn-up credit was taken into account and the fuel composition in a fuel assembly was assumed to be uniform.

The burned fuel compositions were taken directly from the previous SiO_2 reflector benchmark (NEA, 2020). These burn-up calculations were conducted with ORIGEN2.2 (Croff, 1983; Ludwig and Croff, 2002) adopting the ORLIBJ40 (Okumura et al., 2012) cross-section library. In this benchmark, 13 actinides and 15 fission products were considered within the criticality calculations.

The investigated fission product nuclides are listed in Table 1.3. These are the same nuclides selected in previous NEA Burn-up Credit Criticality Safety Benchmarks (NEA, 2020; Takano, 1994). The number densities of the used fuel compositions at burn-up values of 30 GWd/t and 45 GWd/t are specified in Table 1.4.

Table 1.3. Nuclide list for use in the criticality calculations within this benchmark

	Nuclide list
13 Actinides	^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{243}Am
15 Fission products	^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{143}Nd, ^{145}Nd, ^{153}Eu, ^{155}Gd

Source: NEA data, 2020.

Table 1.4. Number densities for 30 GWd/t and 45 GWd/t burned fuel

Burn-up	30 GWd/t	45 GWd/t
Number density (#/barn/cm)		
Actinide		
^{233}U	3.5590E-11	3.5120E-11
^{234}U	6.3908E-08	1.0024E-07
^{235}U	4.4013E-04	2.5992E-04
^{236}U	1.0735E-04	1.3269E-04
^{238}U	2.1492E-02	2.1227E-02
^{237}Np	8.5259E-06	1.4257E-05
^{238}Pu	2.2935E-06	6.2772E-06
^{239}Pu	1.3530E-04	1.4480E-04
^{240}Pu	3.9089E-05	5.6911E-05
^{241}Pu	2.5945E-05	3.9099E-05
^{242}Pu	5.9083E-06	1.5184E-05
^{241}Am	6.2531E-07	1.1751E-06
^{243}Am	8.4105E-07	3.2111E-06
Fission product		
^{95}Mo	3.4410E-05	5.2295E-05
^{99}Tc	4.1123E-05	5.8734E-05
^{101}Ru	3.8223E-05	5.6898E-05
^{103}Rh	2.1211E-05	2.9856E-05
^{109}Ag	2.6601E-06	4.8499E-06
^{133}Cs	4.3335E-05	6.0902E-05
^{147}Sm	2.3798E-06	3.8097E-06
^{149}Sm	1.1202E-07	1.0999E-07
^{150}Sm	9.4144E-06	1.4649E-05
^{151}Sm	4.8645E-07	5.6117E-07
^{152}Sm	3.5278E-07	4.5354E-06
^{143}Nd	3.1569E-05	4.1013E-05
^{145}Nd	2.4498E-05	3.4106E-05
^{153}Eu	3.3567E-06	5.6088E-06
^{155}Gd	1.9812E-09	3.7644E-09
^{16}O	4.5960E-02	4.5960E-02

Source: NEA data, 2020.

1.4. Example results table and Case IDs

Participants were requested to submit the calculated k_{eff} for each case using the example results tables set out in Tables 1.5 and 1.6. The specific IDs for each case are given below:

Table 1.5. Example results table for Single Unit (Case 1) and calculation IDs

Burn-up (GWd/t)	Temperature (K)				
	233	253	293	333	588
0	SU-T233-0	SU-T253-0	SU-T293-0	SU-T333-0	SU-T588-0
30	SU-T233-30	SU-T253-30	SU-T293-30	SU-T333-30	SU-T588-30
45	SU-T233-45	SU-T253-45	SU-T293-45	SU-T333-45	SU-T588-45

Source: NEA data, 2020.

Table 1.6. Example results table for infinite array (Case 2) and calculation IDs

Burn-up (GWd/t)	Temperature (K)				
	233	253	293	333	588
0	INF-T233-0	INF-T253-0	INF-T293-0	INF-T333-0	INF-T588-0
30	INF-T233-30	INF-T253-30	INF-T293-30	INF-T333-30	INF-T588-30
45	INF-T233-45	INF-T253-45	INF-T293-45	INF-T333-45	INF-T588-45

Source: NEA data, 2020.

Along with the completed tables above, the participants were asked to provide the following information:

- neutronics code used in study;
- nuclear data library used;
- brief description of any preparation methods used to generate the results;
- kind of bound data that was selected (i.e. ^{1}H in Ice / ^{1}H in H_2O);
- brief description of any steps taken to provide temperature correction (interpolation, nearest data point used, etc.).

2. Participants and analysis methods

Thirty-four sets of results from ten participating institutes from eight countries were received for this benchmark. The list of final participants is shown in Table 2.1, which includes the names of the participants, institutes, countries, and codes and nuclear data libraries. The countries and the institutes of the participants are summarised in Table 2.2.

The nuclear data and computer codes are summarised in Table 2.3, which shows that 18 contributions used Evaluated Nuclear Data File (ENDF) libraries (ENDF/B-VII.1 and ENDF/B-VIII.0), whereas 13 contributions used Joint Evaluated Fission and Fusion File (JEFF) libraries (JEF-2.2, JEFF-3.1.1, JEFF-3.1.2 and JEFF-3.3), and only three cases used a Japanese Evaluated Nuclear Data Library (JENDL) library (JENDL-4.0). The evaluation of nuclear data was carried out under international co-operation programmes and portions of the evaluated data among ENDF, JENDL and JEFF are shared. It can therefore prove challenging to identify the exact reason for observed differences between results adopting different libraries.

Some contributions used a number of codes, including several versions of SCALE and MCNP codes. Additionally, some contributions used computer codes such as MVP3, MONK 10B, TRIPOLI-4, MORET 5.D.1, Open MC. Continuous energy Monte Carlo codes were widely used and independent codes were developed in several institutes. This allows for comparison of the independent results. Only one contribution used a deterministic code, CASMO 5.

Table 2.4. summarises the selection of H bound data for all contributions where the participants included low-temperature calculations, i.e. those at 233K and 253K.

Table 2.1. List of participants WPNCS Subgroup 3 Benchmark

ID	Participants	Institutes	Country	Code	Nuclear Data
CEA1 CEA2 CEA3	Yi-Kang Lee Marion Tiphine Coralie Carmouze	CEA-Saclay CEA-Cadarache	France	TRIPOLI-4 TRIPOLI-4.11	JEFF-3.3 JEFF-3.3 JEFF-3.1.1
IRSN1 IRSN2 IRSN3	Nicolas Leclaire Mathieu Milin	IRSN	France	MORET 5.D.1	JEFF-3.3 JEFF-3.3[*1] JENDL-4.0[*2]
GRS1 GRS2 GRS3 GRS4 GRS5 GRS6	Fabian Sommer Matthias Behler Volker Hannstein	GRS	Germany	SCALE 6.2.2 OpenMC 0.9.0 MCNP 6.1	ENDF/B-VII.1[*3] ENDF/B-VII.1[*4] ENDF/B-VII.1 ENDF/B-VIII.0 ENDF/B-VIII.0 ENDF/B-VIII.0
MTA1 MTA2	Gabor Hordosy	MTA EK[*6]	Hungary	MCNP 6.1.1	ENDF/B-VIII.0 ENDF/B-VII
NRA1 NRA2	Shigeki Shiba Toshisha Yamamoto Tomohiro Sakai	NRA	Japan	MVP3 CASMO5	JENDL-4.0 JENDL-4.0[*5]

Table 2.1. List of participants WPNCS Subgroup 3 Benchmark (Continued)

UPM1 UPM2 UPM3 UPM4 UPM5 UPM6 UPM7 UPM8 UPM9 UPM10	Oscar Cabellos David Piedra	UPM	Spain	MCNP 6.1	ENDF/B-VII.1 ENDF/B-VIII.0 ENDF/B-VIII.0 ENDF/B-VIII.0 ENDF/B-VIII.0 JEFF 3.1.1 JEFF 3.3 JEFF 3.3 JEFF 3.3 JEFF 3.3
EMS1 EMS2 EMS3	Dennis Mennerdahl	EMS	Sweden	SCALE 6.2.3 MCNP 6.2 MCNP 6.2	ENDF/B-VII.1 ENDF/B-VIII.0 ENDF/B-VII.1
SL1	James Ryan	SL	United Kingdom	MONK 9A	JEF-2.2
WOOD1 WOOD2	David Hanlon	Wood	United Kingdom	MONK 10B MONK 11 (Dev)	JEFF-3.1.2 JEFF-3.1.2
ORNL1 ORNL2	BJ Marshall Bradley Rearden Douglas Bowen	ORNL	United States	SCALE 6.2.3	ENDF/B-VIII.0 ENDF/B-VIII.0*4

Source: NEA data, 2020.
*1. Hydrogen S(α,β)data from ENDF/B-VIII.0 was used.
*2. Hydrogen in ice S(α,β)data from JEFF-3.3 used for cases below 273 K.
*3. 56 Energy Groups.
*4. 252 Energy Groups.
*5. 19 Energy Groups.
*6. The Centre for Energy Research (EK) of the Hungarian Academy of Sciences (MTA). The calculation ID MTA was chosen for brevity.

Table 2.2. Countries and institutes

Country	Institute
France	CEA-Saclay, CEA-Cadarache and IRSN
Germany	GRS
Hungary	MTA EK
Japan	NRA
Spain	UPM
Sweden	EMS
United Kingdom	SL and Wood
United States	ORNL

Source: NEA data, 2020.

Table 2.3. Nuclear data and computer codes applied to the benchmark calculations

Nuclear data	Computer code (Participant ID in Table 2.1)	No. of results
ENDF/B-VII.1	MCNP 6.1 (UPM) MCNP 6.1.1 (MTA) MCNP 6.2 (EMS) SCALE 6.2.2 (GRS) SCALE 6.2.3 (EMS)	7
ENDF/B-VIII.0	MCNP 6.1 (GRS/UPM) MCNP 6.1.1 (MTA) MCNP 6.2 (EMS) OpenMC (GRS) SCALE 6.2.2 (GRS) SCALE 6.2.3 (ORNL)	11
JEF-2.2	MONK 9A (SL)	1
JEFF-3.1.1	MCNP 6.1 (UPM) TRIPOLI-4.11 (CEA)	2
JEFF-3.1.2	MONK 10B (WOOD) MONK 11-Dev (WOOD)	2
JEFF-3.3	MCNP 6.1 (UPM) MORET 5.D.1 (IRSN) TRIPOLI-4 (CEA) TRIPOLI-4.11 (CEA)	8
JENDL-4.0	MVP3 (NRA) CASMO5 (NRA) MORET 5.D.1 (IRSN)	3

Source: NEA data, 2020.

Table 2.4. Selection of bound H data in low-temperature calculations (i.e. 233K and 253K)

^{1}H in H_2O	^{1}H in ICE
EMS1	CEA1
GRS1	CEA2
GRS2	EMS2
GRS3	GRS4
NRA1	GRS5
NRA2	GRS6
	IRSN1
	IRSN2
	IRSN3
	MTA1
	ORNL1
	ORNL2
	UPM2
	UPM3
	UPM4
	UPM5
	UPM6
	UPM7
	UPM8
	UPM9
	UPM10
	WOOD1
	WOOD2

Source: NEA data, 2020.

3. Results

Out of the 34 contributions to this study, 28 were complete (they reported the k_{eff} of all 30 cases) and 6 were partial. In general, partial results were provided where the code and nuclear data library combinations were unable to calculate the k_{eff} for the low-temperature cases (233K and 253K).

The typical standard deviation on individual participant results was < 0.0005. This is very small compared with the calculated value of k_{eff}. Comparison of the mean k_{eff} for each case demonstrates that the peak k_{eff} for both single unit and infinite cases were associated with the 293K calculations, where the water density is the greatest among the cases considered in this benchmark. The determined k_{eff} for each case decreases as burn-up increases.

Before providing an in-depth consideration of individual cases, it is relevant to first understand the distribution of the reported results. This was done by considering the average neutron multiplication factor from the data provided by the participants for each case and the spread of the results around this mean. The spread is measured by the %RSD. This is calculated using the standard deviation (SD) and the average as follows:

$$Ave. = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$SD = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - Ave.)^2}$$

$$RSD(\%) = \frac{SD}{Ave.}\times 100$$

Figures A.1 to A.40 show the raw results received from each participant. Figure A.41 shows the variation in the relative standard deviation as a percentage (%RSD) across all results for each case as the temperature is increased. Based on Figure A.41, general observations can be drawn.

- The smallest %RSD is obtained at 293K (room temperature). As the temperature deviates from this well-defined reference, the %RSD of associated calculations increases.
- As expected, the associated %RSD of cases tends most often to increase with the burn-up of the system, where the fission product nuclear cross-sections become increasingly important. However, this is not always the case (see for example 588-INF cases).
- The greatest overall %RSD is associated with calculations at 233K. This is probably due to the high variability in the methods used to represent low temperature in the calculations. For example, some participants used bound data for liquid H_2O, others for H in ice, and some participants (e.g. IRSN3) used one nuclear data library with bound data from another library.
- Single unit calculations are associated with the largest %RSD.

The summary graphs in Appendix A show that, in general, there is good agreement between participants' results at each temperature for both single unit and infinite cases. This is supported by the calculated values of %RSD of <0.3% in all cases (see Table A.12).

The variation in k_{eff} for each case between different nuclear data libraries was examined. Figures A.42 and A.44 show this variation. Figures A.43 and A.45 show the %RSD for results using each data library. From these graphs the following observations have been made:

For infinite cases:

- The RSD for results using each data library is small (<0.3 %) across all data libraries and all temperatures. The largest values of RSD are associated most often with calculations using JENDL-4.0 or otherwise ENDF/B-VII.1.
- At temperatures of 233K and 253K, the range in average k_{eff} for each library is small (~0.005 in k_{eff}) (see Figure A.42).
- At temperatures of 293K, 333K and 588K, the range in the average result for the infinite cases increases to ~0.01 in k_{eff}.
- The lowest average results for infinite cases consistently come from results using ENDF/B-VIII.0 (see Figure A.42) for zero burn-up. For example, at 588K, there is a Δk of ~0.005 between the average results for the ENDF-BVIII.0 and JEFF3.3 libraries at zero burn-up[1]. At other burn-ups, the data library giving the lowest average result varies between temperature cases.

For single unit cases:

- The RSD for results using each data library is small (<0.25 %) at 293K (see Figure A.45).
- All data libraries other than JENDL-4.0 (see Figure A.45) have an RSD <0.25 % at all other temperatures for all burn-ups. JENDL-4.0 has an RSD up to 0.45% away from 293K. The %RSD in the JENDL-4.0 calculations tends to increase with burn-up.
- At all temperatures, the range in average k_{eff} for each library is small (~0.005 in k_{eff}) (see Figure A.44).
- The highest average result for these cases consistently comes from calculations using JEFF-3.3.

The results were also examined to determine the effect of using S(α,β) data for H bound in ice (H1_ICE) rather than H bound in water (H1_H_2O) for the 233K and 253K cases. Table A.15 shows these results. The difference in mean result for each case between results using H1_H_2O and H1_ICE is at most ~0.005 in $k_{eff.}$ This shows that, on average, for the cases modelled the effect of changing bound H data is very small, particularly when compared to the substantially larger variation due to macroscopic physical effects (e.g. density, changes in which give a variation of approximately 2 000 pcm for single unit cases between 233K and 293K). However, there is an indication that H1_ICE gives slightly higher values of k_{eff} with this trend increasing slightly as the temperature is reduced. It should be noted that these are calculated results and not comparisons to critical experiment models. The higher reactivity predictions from H1_ICE may lead to more conservative physical limits, but it is unknown if they are a more accurate representation of real systems.

Tables A.17 and A.18 show the variation in k_{eff} by nuclear data library where more than one code has been used for the same case. This comparison demonstrates that, typically,

1. Work by UPM indicates that a large contribution to the difference between these two libraries may be the result of differences in the ^{235}U fission cross-section data.

there is very small variation in the average k_{eff} determined using different codes when the nuclear data library selection is kept constant. The results for individual codes for each case are very close to the mean for each data library. The typical difference between average results for each code and the overall average for codes using this data library is <0.001. This is comparable to the typical statistical uncertainty in the calculations. This suggests that the selection of nuclear data library has a much larger effect on the determined k_{eff} than the choice of code.

4. Conclusion

The spread in the participants' results as measured in %RSD is low. This indicates a good agreement between participant results in the majority of cases. The %RSD for calculations tends to increase away from room temperature (as the physics of the system changes) and increases with burn-up in most cases. The greatest %RSD is observed at 233K, the lowest temperature studied here.

The choice of S(α, β) data for bound H has only a small effect on the determined k_{eff} for 233K and 253K cases but there is a trend that the values calculated with H bound in ice (H1_ICE) are slightly higher, with the difference being slightly greater at 233K than 253K. While this may lead to more conservative physical limits, it is not necessarily more accurate. Critical experiments using ice would be required to perform an assessment of the accuracy of this trend as indicated by calculations.

It is apparent from the results that the limited spread in k_{eff} for low-temperature calculations indicates that the choice of S(α, β) data for H has a relatively small effect on the determined k_{eff} when compared to the larger variation due to macroscopic physical effects (e.g. density). For the cases in this benchmark, a calculation at room temperature would be a conservative way of representing the systems at 233K and 253K, where water could be present as ice.

Finally, when the same nuclear data library is used by different codes for the same case, the difference in average k_{eff} obtained by each code is very small. The greatest difference between codes using the same data library is in the three cases using JENDL-4.0.

References

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Appendix A. Calculation results of the participants

Table A.1. Participant results for T233-SU cases

Case ID: T233-SU	Burn-up (GWd/te)		
Participant	**0**	**30**	**45**
CEA1	0.90786	0.75742	0.68961
CEA2	0.90839	0.75784	0.68977
EMS1	0.90269	0.75079	0.68579
EMS2	0.90368	0.75235	0.68704
GRS1	0.90326	0.75363	0.68708
GRS2	0.90188	0.75197	0.68527
GRS3	0.90237	0.75289	0.68580
GRS4	0.90259	0.75389	0.68565
GRS5	0.90463	0.75502	0.68791
GRS6	0.90348	0.75406	0.68688
IRSN1	0.90815	0.75746	0.68974
IRSN2	0.90728	0.75695	0.68913
IRSN3	0.90603	0.75610	0.68887
MTA1	0.90362	0.75444	0.68738
ORNL1	0.90435	0.75504	0.68770
ORNL2	0.90407	0.75424	0.68689
NRA1	0.90167	0.75131	0.68290
NRA2	0.90317	0.75281	0.68585
UPM2	0.90389	0.75440	0.68702
UPM3	0.90400	0.75457	0.68710
UPM4	0.90376	0.75427	0.68689
UPM5	0.90377	0.75427	0.68706
UPM7	0.90798	0.75704	0.68933
UPM8	0.90797	0.75712	0.68960
UPM9	0.90774	0.75693	0.68934
UPM10	0.90768	0.75708	0.68940
WOOD1	0.90317	0.75193	0.68515
WOOD2	0.90445	0.75270	0.68476
Mean	0.90477	0.75459	0.68732
RSD (%)	0.24%	0.27%	0.26%

Source: NEA data, 2020.

Table A.2. Participant results for T233-INF cases

Case ID: T233-INF	Burn-up (GWd/te)		
Participant ID	**0**	**30**	**45**
CEA1	1.48186	1.22699	1.11791
CEA2	1.48192	1.22685	1.11831
EMS1	1.48114	1.22011	1.11594
EMS2	1.47884	1.22228	1.11810
GRS1	1.47830	1.22144	1.11312
GRS2	1.47849	1.22096	1.11304
GRS3	1.48071	1.22434	1.11645
GRS4	1.47788	1.22515	1.11670
GRS5	1.48075	1.22800	1.11985
GRS6	1.47932	1.22650	1.11866
IRSN1	1.48227	1.22671	1.11797
IRSN2	1.48187	1.22663	1.11785
IRSN3	1.48513	1.22830	1.11931
MTA1	1.48146	1.22799	1.11944
ORNL1	1.48062	1.22816	1.12040
ORNL2	1.47761	1.22516	1.11753
NRA1	1.48208	1.22396	1.11586
NRA2	1.48122	1.22163	1.11315
UPM2	1.47950	1.22660	1.11841
UPM3	1.47969	1.22678	1.11853
UPM4	1.47951	1.22643	1.11824
UPM5	1.47928	1.22644	1.11815
UPM7	1.48156	1.22611	1.11729
UPM8	1.48171	1.22612	1.11748
UPM9	1.48146	1.22593	1.11725
UPM10	1.48142	1.22595	1.11709
WOOD1	1.48401	1.22470	1.11409
WOOD2	1.48339	1.22540	1.11464
Mean	1.48082	1.22542	1.11717
RSD (%)	0.12%	0.18%	0.18%

Source: NEA data, 2020.

Table A.3. Participant results for T253-SU cases

Case ID: T253-SU	Burn-up (GWd/te)		
Participant ID	**0**	**30**	**45**
CEA1	0.90675	0.75567	0.68832
CEA2	0.90662	0.75574	0.68845
EMS1	0.90197	0.75001	0.68509
EMS2	0.90231	0.75079	0.68560
GRS1	0.90282	0.75258	0.68474
GRS2	0.90139	0.75150	0.68423
GRS3	0.90301	0.75160	0.68492
GRS4	0.90138	0.75223	0.68542
GRS5	0.90216	0.75260	0.68587
GRS6	0.90150	0.75257	0.68558
IRSN1	0.90657	0.75543	0.68851
IRSN2	0.90547	0.75520	0.68745
IRSN3	0.90425	0.75450	0.68737
MTA1	0.90294	0.75257	0.68542
ORNL1	0.90265	0.75334	0.68619
ORNL2	0.90200	0.75239	0.68548
NRA1	0.90095	0.75071	0.68235
NRA2	0.90246	0.75219	0.68529
UPM2	0.90218	0.75251	0.68549
UPM3	0.90242	0.75264	0.68564
UPM4	0.90182	0.75247	0.68555
UPM5	0.90204	0.75240	0.68544
UPM7	0.90622	0.75528	0.68785
UPM8	0.90654	0.75555	0.68804
UPM9	0.90610	0.75532	0.68778
UPM10	0.90601	0.75535	0.68774
WOOD1	0.90237	0.75100	0.68323
WOOD2	0.90274	0.75054	0.68342
Mean	0.90342	0.75302	0.68594
RSD (%)	0.22%	0.24%	0.24%

Source: NEA data, 2020.

Table A.4. Participant results for T253-INF cases

Case ID: T253-INF	Burn-up (GWd/te)		
Participant ID	**0**	**30**	**45**
CEA1	1.48081	1.22539	1.11709
CEA2	1.48123	1.22559	1.11694
EMS1	1.48088	1.21977	1.11578
EMS2	1.47852	1.22157	1.11759
GRS1	1.47872	1.22125	1.11425
GRS2	1.47802	1.22116	1.11335
GRS3	1.48104	1.22416	1.11569
GRS4	1.47868	1.22466	1.11789
GRS5	1.47871	1.22550	1.11780
GRS6	1.47818	1.22527	1.11766
IRSN1	1.48087	1.22537	1.11738
IRSN2	1.48114	1.22511	1.11744
IRSN3	1.48449	1.22770	1.11863
MTA1	1.47882	1.22569	1.11852
ORNL1	1.47952	1.22691	1.11899
ORNL2	1.47645	1.22367	1.11621
NRA1	1.48178	1.22390	1.11549
NRA2	1.48099	1.22134	1.11287
UPM2	1.47846	1.22525	1.11743
UPM3	1.47867	1.22538	1.11748
UPM4	1.47829	1.22506	1.11721
UPM5	1.47834	1.22502	1.11711
UPM7	1.48081	1.22473	1.11637
UPM8	1.48105	1.22496	1.11653
UPM9	1.48066	1.22458	1.11632
UPM10	1.48060	1.22469	1.11617
WOOD1	1.48286	1.22269	1.11358
WOOD2	1.48246	1.22358	1.11411
Mean	1.48004	1.22428	1.11650
RSD (%)	0.12%	0.15%	0.14%

Source: NEA data, 2020.

Table A.5. Participant results for T293-SU cases

Case ID: T293-SU	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	0.93071	0.77561	0.70675
CEA2	0.93056	0.77577	0.70653
CEA3	0.92834	0.77314	0.70383
EMS1	0.92890	0.77306	0.70599
EMS2	0.92891	0.77313	0.70590
EMS3	0.92874	0.77297	0.70578
GRS1	0.92889	0.77487	0.70636
GRS2	0.92809	0.77448	0.70592
GRS3	0.92938	0.77473	0.70552
GRS4	0.92917	0.77599	0.70600
GRS5	0.92872	0.77474	0.70571
GRS6	0.92914	0.77523	0.70590
IRSN1	0.92993	0.77544	0.70667
IRSN2	0.93228	0.77698	0.70742
IRSN3	0.92795	0.77417	0.70516
MTA1	0.92893	0.77477	0.70586
MTA2	0.92936	0.77455	0.70451
ORNL1	0.92856	0.77496	0.70591
ORNL2	0.92922	0.77511	0.70579
NRA1	0.92845	0.77423	0.70311
NRA2	0.92929	0.77515	0.70613
SL	0.92850	0.77210	0.70290
UPM1	0.92883	0.77482	0.70595
UPM2	0.92873	0.77510	0.70586
UPM3	0.92898	0.77508	0.70586
UPM4	0.92868	0.77499	0.70578
UPM5	0.92876	0.77494	0.70607
UPM6	0.92810	0.77250	0.70320
UPM7	0.93002	0.77507	0.70609
UPM8	0.93012	0.77508	0.70611
UPM9	0.93005	0.77503	0.70601
UPM10	0.93000	0.77493	0.70594
WOOD1	0.92760	0.77190	0.70310
WOOD2	0.92744	0.77213	0.70334
Mean	0.92910	0.77449	0.70550
RSD (%)	0.10%	0.15%	0.16%

Source: NEA data, 2020.

Table A.6. Participant results for T293-INF cases

Case ID: T293-INF	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	1.48681	1.23204	1.12441
CEA2	1.48734	1.23261	1.12461
CEA3	1.48926	1.23114	1.12195
EMS1	1.48903	1.23018	1.12550
EMS2	1.48439	1.22895	1.12470
EMS3	1.48906	1.22992	1.12497
GRS1	1.48698	1.23134	1.12349
GRS2	1.48659	1.23174	1.12336
GRS3	1.48917	1.23423	1.12507
GRS4	1.48481	1.23305	1.12561
GRS5	1.48432	1.23251	1.12476
GRS6	1.48445	1.23293	1.12466
IRSN1	1.48749	1.23300	1.12470
IRSN2	1.48644	1.23235	1.12403
IRSN3	1.49005	1.23381	1.12559
MTA1	1.48417	1.23248	1.12462
MTA2	1.48929	1.23161	1.12203
ORNL1	1.48453	1.23319	1.12510
ORNL2	1.48299	1.23192	1.12386
NRA1	1.49011	1.23400	1.12537
NRA2	1.48923	1.23168	1.12269
SL	1.49260	1.23150	1.12290
UPM1	1.48909	1.23386	1.12516
UPM2	1.48463	1.23296	1.12468
UPM3	1.48465	1.23302	1.12498
UPM4	1.48437	1.23283	1.12475
UPM5	1.48445	1.23294	1.12481
UPM6	1.48818	1.23022	1.12095
UPM7	1.48665	1.23168	1.12365
UPM8	1.48656	1.23175	1.12372
UPM9	1.48646	1.23165	1.12364
UPM10	1.48656	1.23152	1.12356
WOOD1	1.48835	1.23145	1.12193
WOOD2	1.48892	1.23079	1.12190
Mean	1.48700	1.23208	1.12405
RSD (%)	0.15%	0.10%	0.11%

Source: NEA data, 2020.

Table A.7. Participant results for T333-SU cases

Case ID: T333-SU	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	0.92311	0.76903	0.70087
CEA2	0.92347	0.76914	0.70130
CEA3	0.92157	0.76716	0.69864
EMS1	0.92134	0.76621	0.70077
EMS2	0.92108	0.76643	0.70032
GRS1	0.92157	0.76809	0.70084
GRS2	0.92098	0.76789	0.70023
GRS3	0.92210	0.76736	0.70016
GRS4	0.92152	0.76874	0.69959
GRS5	0.92136	0.76838	0.70039
GRS6	0.92172	0.76878	0.70077
IRSN1	0.92337	0.76892	0.70093
IRSN2	0.92535	0.77077	0.70198
IRSN3	0.91969	0.76699	0.69912
MTA1	0.92218	0.76885	0.70077
MTA2	0.92185	0.76710	0.69885
ORNL1	0.92115	0.76828	0.70033
ORNL2	0.92156	0.76847	0.70046
NRA1	0.92062	0.76727	0.69767
NRA2	0.92328	0.76985	0.70129
SL	0.92000	0.76560	0.69810
UPM1	0.92161	0.76847	0.70045
UPM2	0.92136	0.76834	0.70036
UPM3	0.92168	0.76875	0.70073
UPM4	0.92160	0.76880	0.70060
UPM5	0.92163	0.76860	0.70035
UPM6	0.92081	0.76607	0.69775
UPM7	0.92302	0.76868	0.70053
UPM8	0.92304	0.76863	0.70055
UPM9	0.92302	0.76853	0.70039
UPM10	0.92298	0.76850	0.70044
WOOD1	0.92007	0.76572	0.69645
WOOD2	0.92008	0.76539	0.69727
Mean	0.92181	0.76799	0.69998
RSD	0.13%	0.16%	0.18%

Source: NEA data, 2020.

Table A.8. Participant results for T333-INF cases

Case ID: T333-INF	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	1.48404	1.22866	1.12177
CEA2	1.48440	1.22895	1.12153
CEA3	1.48588	1.22769	1.11949
EMS1	1.48590	1.22641	1.12286
EMS2	1.48087	1.22464	1.12161
GRS1	1.48284	1.22695	1.12029
GRS2	1.48234	1.22731	1.11979
GRS3	1.48560	1.23016	1.12274
GRS4	1.48229	1.22957	1.12294
GRS5	1.48159	1.22940	1.12264
GRS6	1.48065	1.22905	1.12079
IRSN1	1.48448	1.22870	1.12124
IRSN2	1.48402	1.22794	1.12117
IRSN3	1.48724	1.22995	1.12358
MTA1	1.48317	1.23047	1.12379
MTA2	1.48662	1.22835	1.11975
ORNL1	1.48151	1.22976	1.12268
ORNL2	1.48000	1.22844	1.12165
NRA1	1.48685	1.23024	1.12273
NRA2	1.48593	1.22785	1.12018
SL	1.49110	1.22860	1.11960
UPM1	1.48592	1.22985	1.12225
UPM2	1.48145	1.22932	1.12240
UPM3	1.48153	1.22930	1.12221
UPM4	1.48138	1.22920	1.12206
UPM5	1.48139	1.22931	1.12210
UPM6	1.48511	1.22641	1.11809
UPM7	1.48352	1.22792	1.12059
UPM8	1.48377	1.22787	1.12071
UPM9	1.48368	1.22772	1.12054
UPM10	1.48360	1.22782	1.12072
WOOD1	1.48521	1.22675	1.11803
WOOD2	1.48573	1.22700	1.11884
Mean	1.48393	1.22841	1.12125
RSD	0.16%	0.11%	0.13%

Source: NEA data, 2020.

Table A.9. Participant results for T588-SU cases

Case ID: T588-SU	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	0.79554	0.66149	0.60667
CEA2	0.79631	0.66172	0.60667
CEA3	0.79303	0.65980	0.60477
EMS1	0.79255	0.65966	0.60699
EMS2	0.79286	0.65975	0.60733
GRS1	0.79401	0.66277	0.60899
GRS2	0.79206	0.66149	0.60728
GRS3	0.79245	0.66113	0.60723
GRS4	0.79316	0.66133	0.60789
GRS5	0.79317	0.66147	0.60694
GRS6	0.79348	0.66189	0.60769
IRSN1	0.79575	0.66158	0.60659
IRSN2	0.79818	0.66339	0.60817
IRSN3	0.79095	0.66007	0.60590
MTA1	0.79318	0.66142	0.60727
MTA2	0.79361	0.66091	0.60546
ORNL1	0.79325	0.66181	0.60758
ORNL2	0.79443	0.66246	0.60797
NRA1	0.79139	0.65964	0.60470
NRA2	0.79406	0.66249	0.60814
SL	0.79410	0.65990	0.60400
UPM1	0.79316	0.66112	0.60649
UPM2	0.79350	0.66185	0.60740
UPM3	0.79425	0.66213	0.60731
UPM4	0.79418	0.66203	0.60732
UPM5	0.79407	0.66206	0.60731
UPM6	0.79228	0.65906	0.60412
UPM7	0.79545	0.66118	0.60604
UPM8	0.79575	0.66135	0.60623
UPM9	0.79542	0.66112	0.60609
UPM10	0.79558	0.66111	0.60604
WOOD1	0.79114	0.65803	0.60399
WOOD2	0.79158	0.65862	0.60382
Mean	0.79375	0.66109	0.60656
RSD (%)	0.20%	0.18%	0.22%

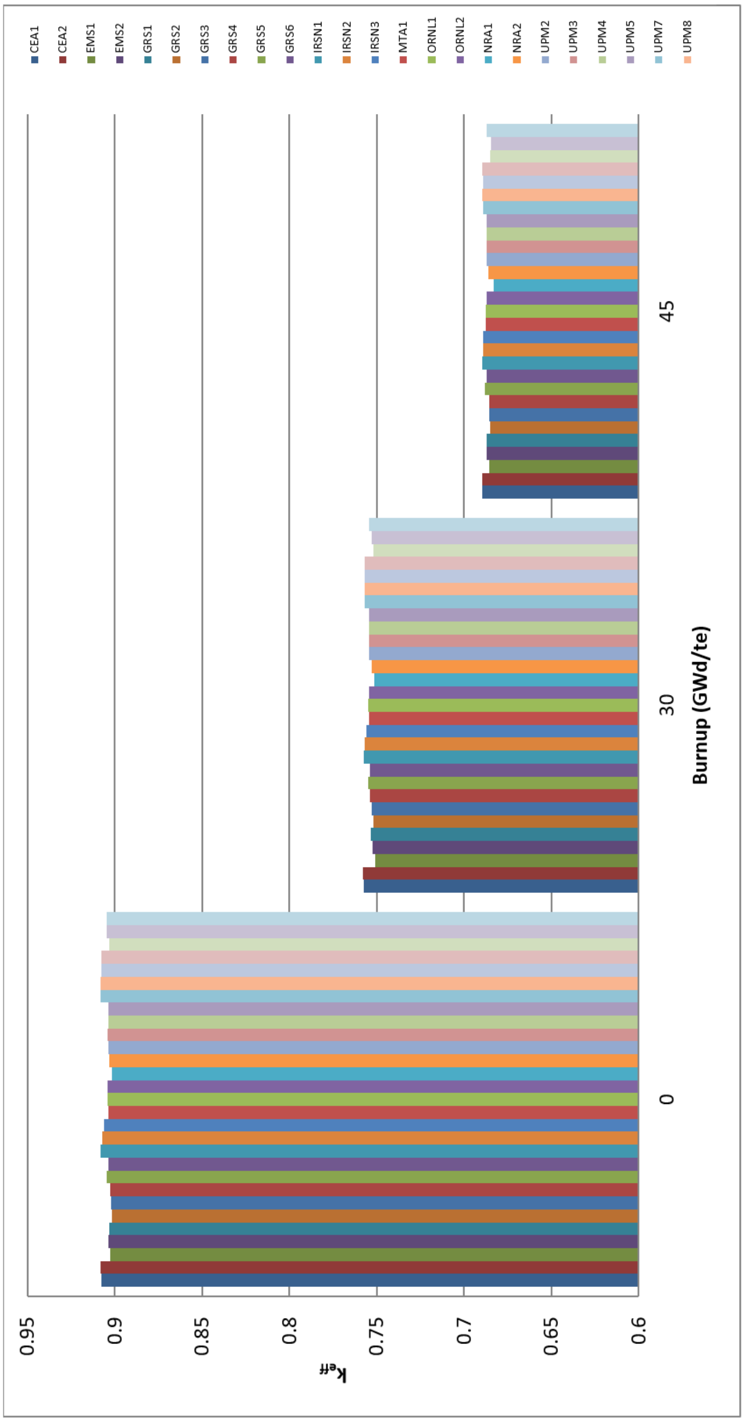
Source: NEA data, 2020.

Table A.10. Participant results for T588-INF cases

Case ID: T588-INF	Burn-up (GWd/te)		
Participant ID	0	30	45
CEA1	1.42326	1.16034	1.06305
CEA2	1.42361	1.16043	1.06276
CEA3	1.42329	1.15957	1.06155
EMS1	1.42275	1.15739	1.06465
EMS2	1.41787	1.15598	1.06419
GRS1	1.42219	1.15935	1.06230
GRS2	1.41985	1.15985	1.06292
GRS3	1.42232	1.16216	1.06541
GRS4	1.41940	1.16209	1.06621
GRS5	1.41814	1.16061	1.06421
GRS6	1.41839	1.16122	1.06462
IRSN1	1.42360	1.16043	1.06249
IRSN2	1.42285	1.15940	1.06136
IRSN3	1.42384	1.16171	1.06485
MTA1	1.41781	1.15995	1.06312
MTA2	1.42265	1.15866	1.06103
ORNL1	1.41825	1.16122	1.06474
ORNL2	1.41759	1.16075	1.06419
NRA1	1.42436	1.16237	1.06521
NRA2	1.42206	1.15882	1.06136
SL	1.42990	1.16170	1.06360
UPM1	1.42272	1.16093	1.06329
UPM2	1.41813	1.16057	1.06409
UPM3	1.41836	1.16063	1.06373
UPM4	1.41824	1.16063	1.06358
UPM5	1.41839	1.16060	1.06367
UPM6	1.42179	1.15785	1.05970
UPM7	1.42277	1.15922	1.06144
UPM8	1.42282	1.15936	1.06162
UPM9	1.42286	1.15932	1.06157
UPM10	1.42284	1.15917	1.06145
WOOD1	1.42252	1.15887	1.06055
WOOD2	1.42287	1.15890	1.06139
Mean	1.42146	1.16000	1.06303
RSD (%)	0.19%	0.12%	0.15%

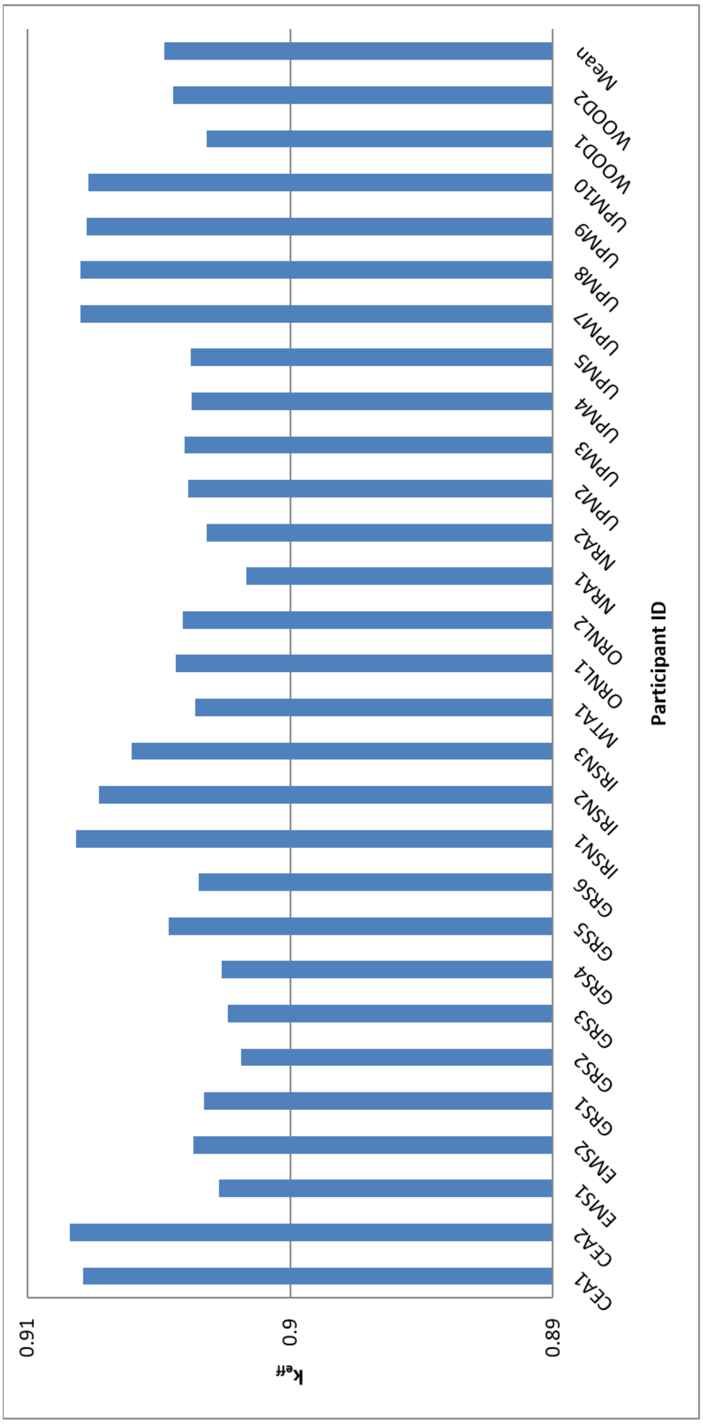
Source: NEA data, 2020.

Figure A.1. Summary graph of results for T233-SU cases



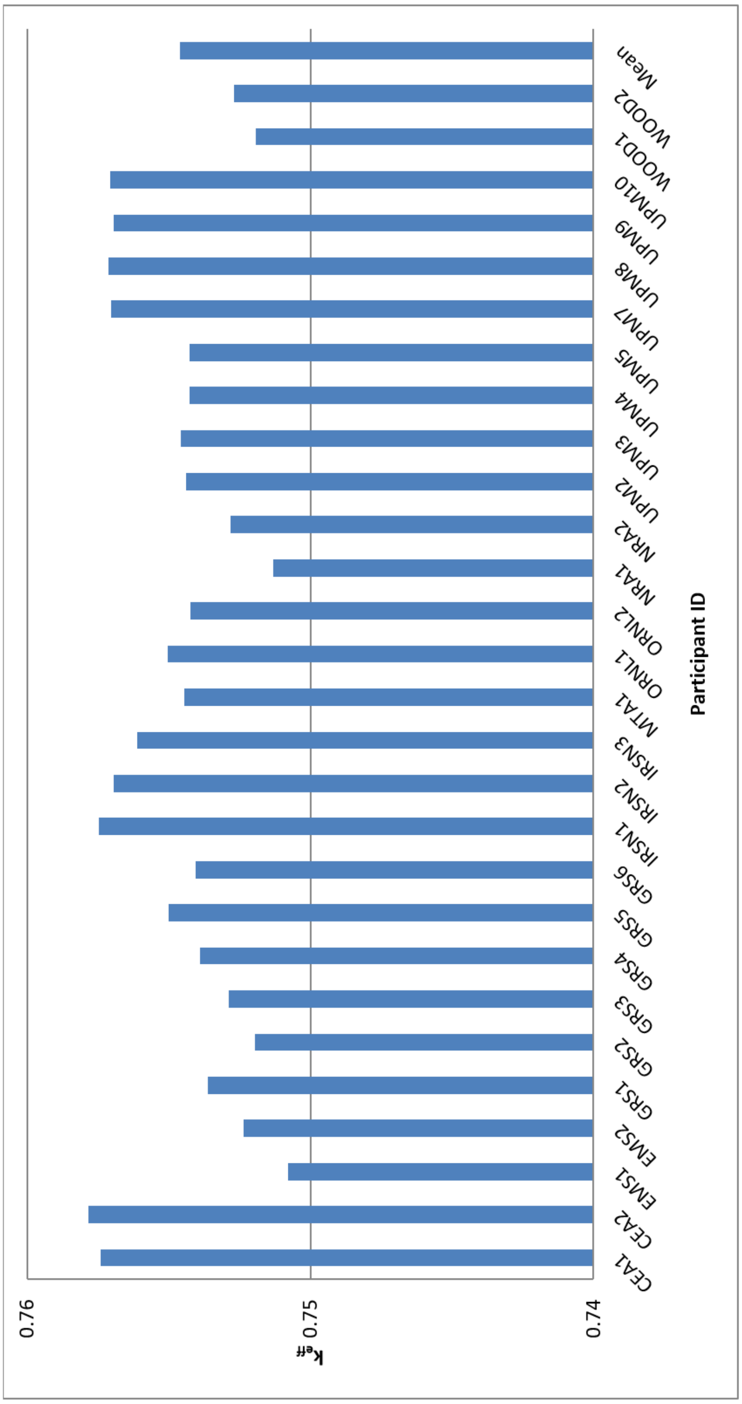
Source: NEA data, 2020.

Figure A.2. Participant results for case T233-SU-0



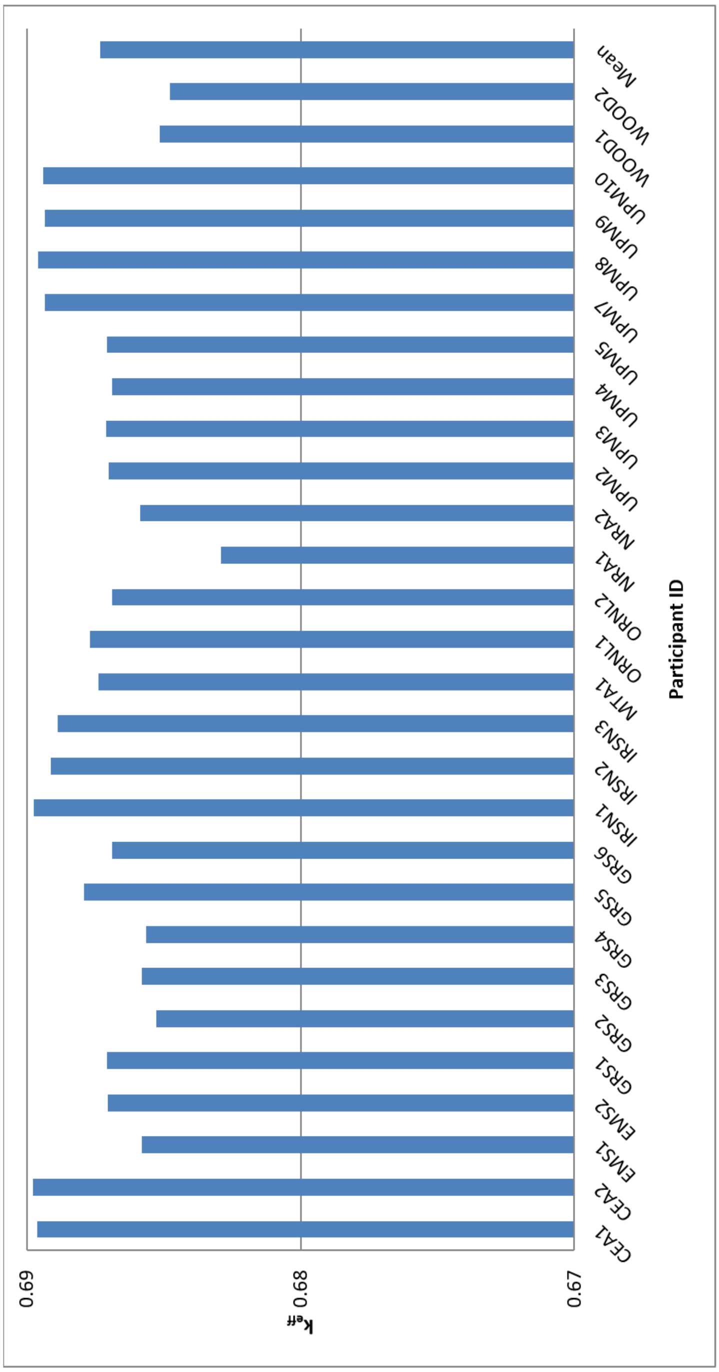
Source: NEA data, 2020.

Figure A.3. Participant results for case T233-SU-30



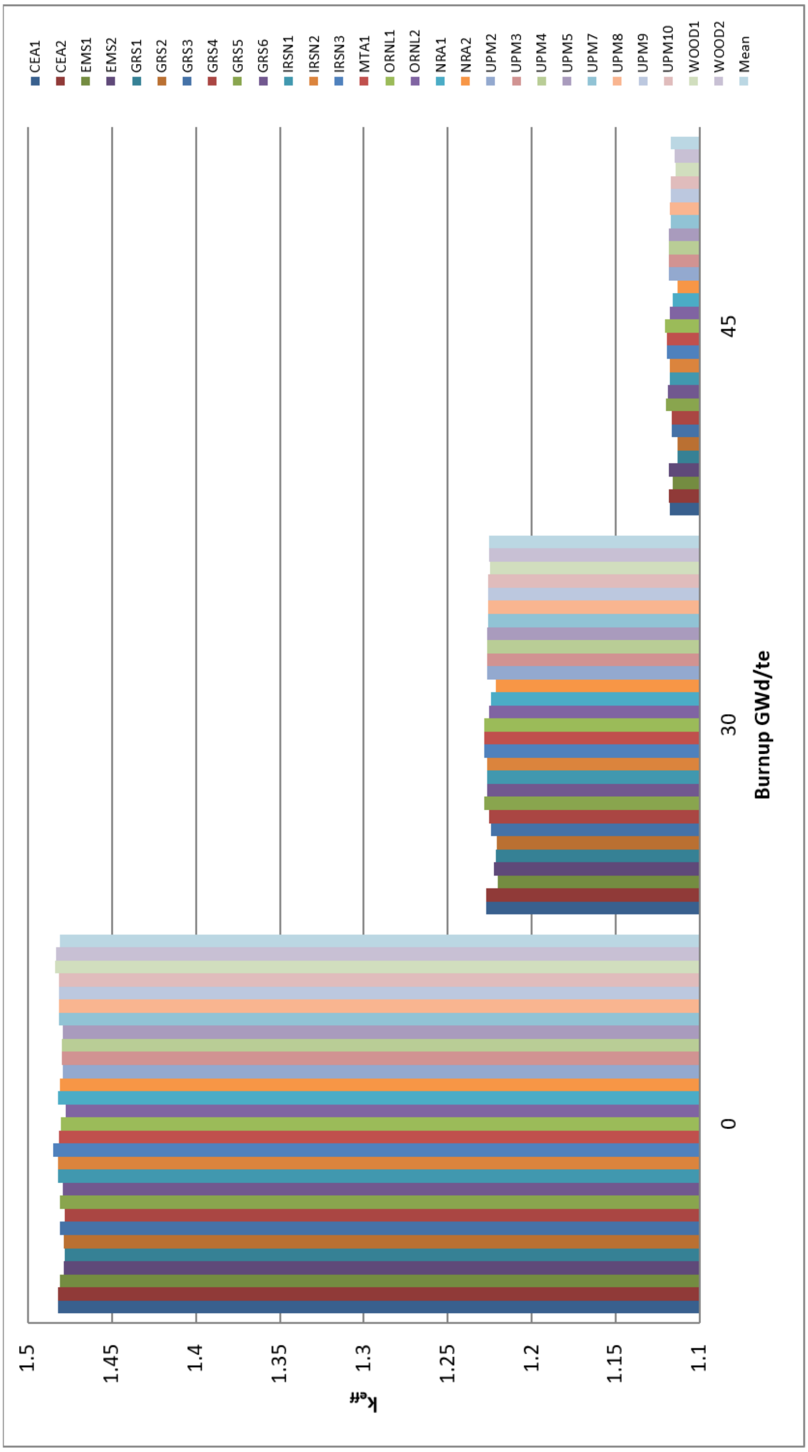
Source: NEA data, 2020.

Figure A.4. Participant results for case T233-SU-45



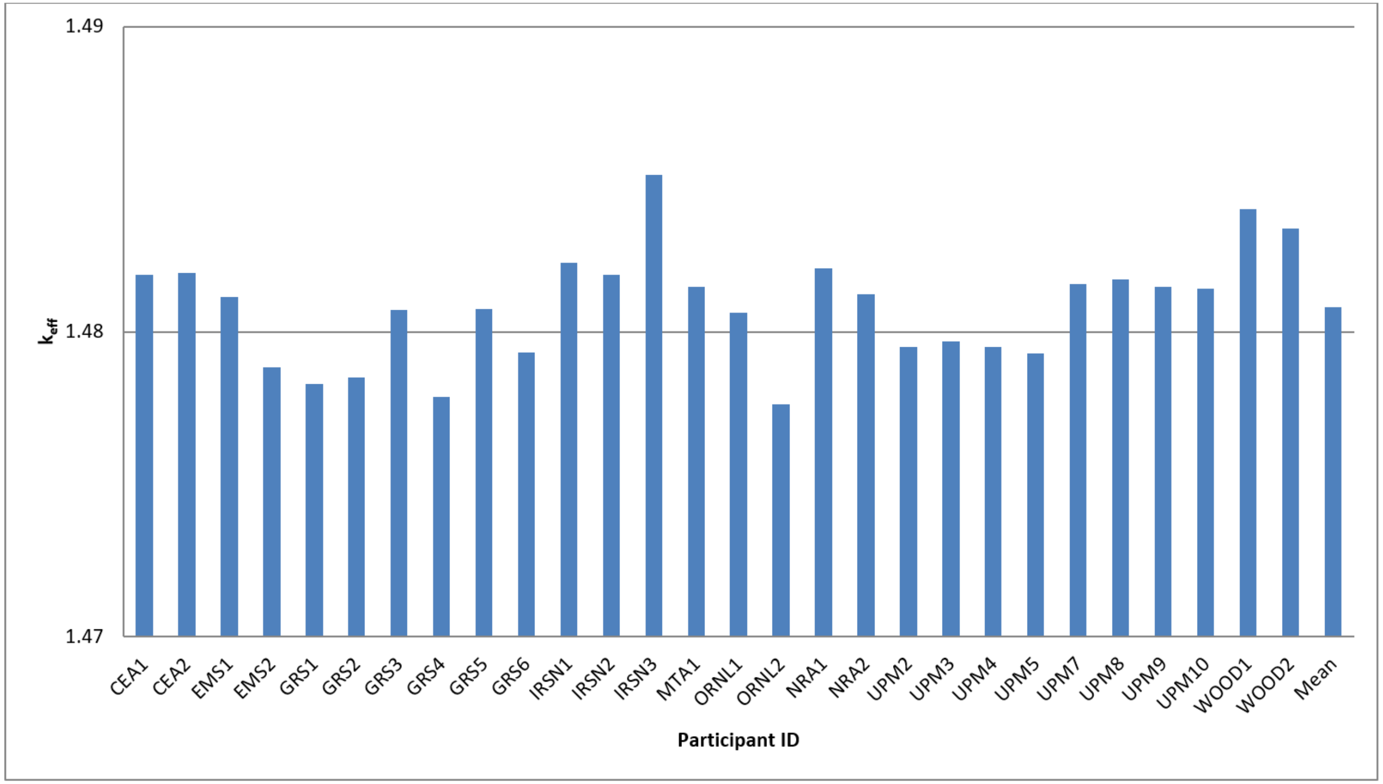
Source: NEA data, 2020.

Figure A.5. Summary graph of results for T233-INF cases



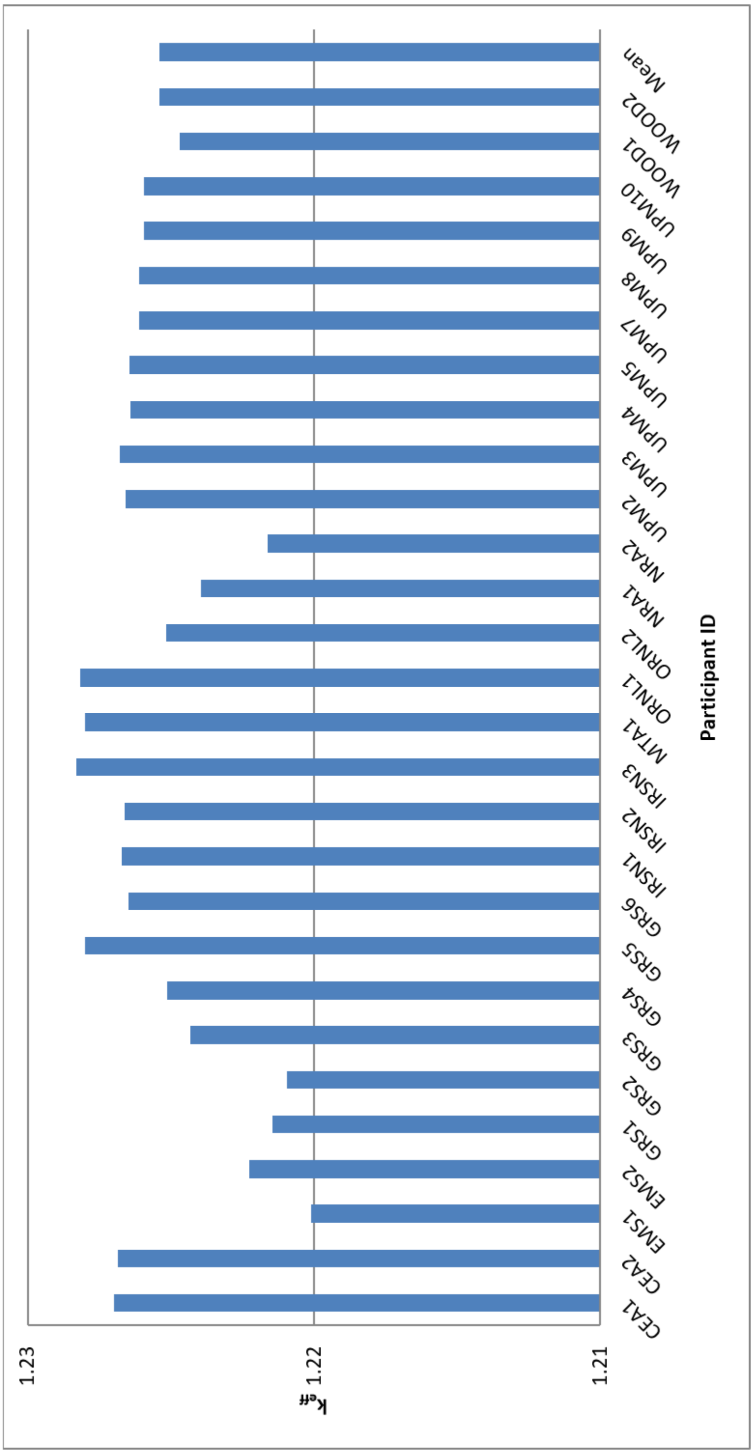
Source: NEA data, 2020.

Figure A.6. Participant results for case T233-INF-0



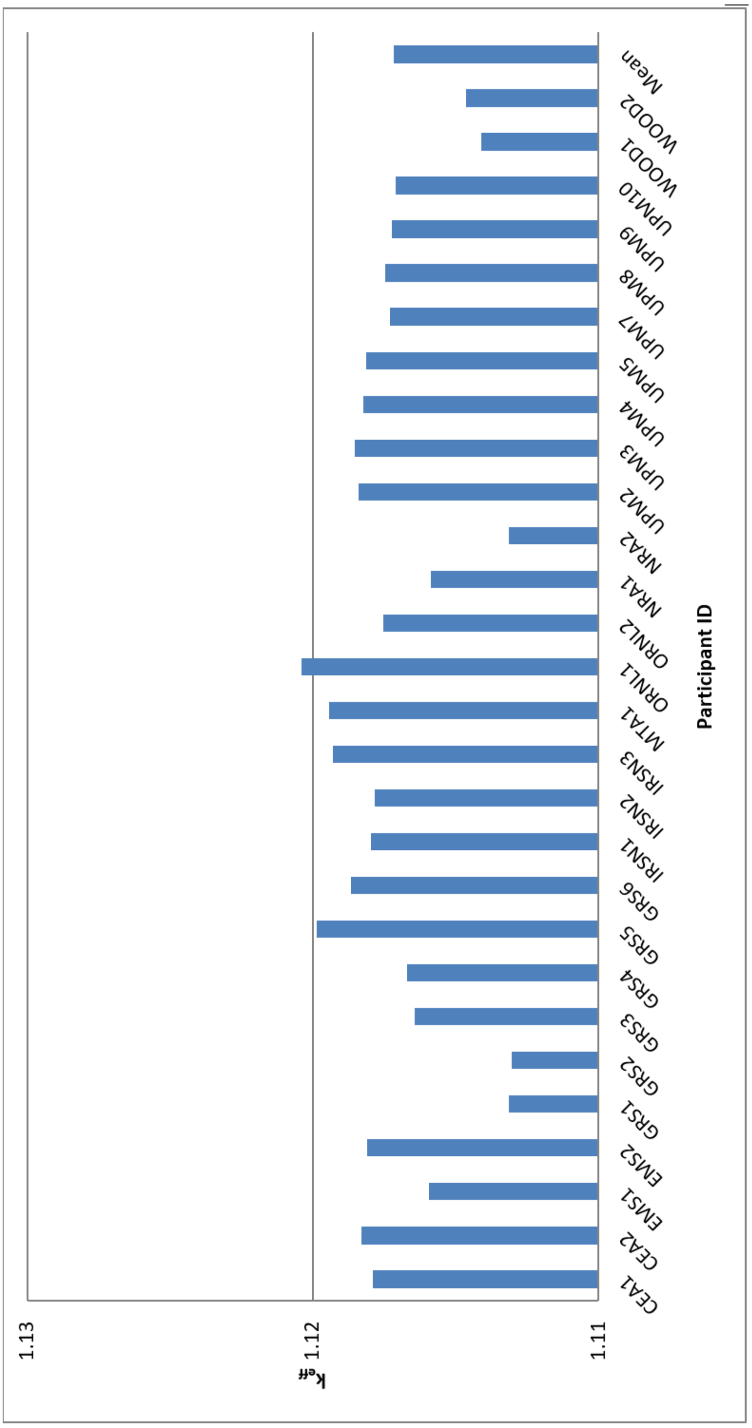
Source: NEA data, 2020.

Figure A.7. Participant results for case T233-INF-30



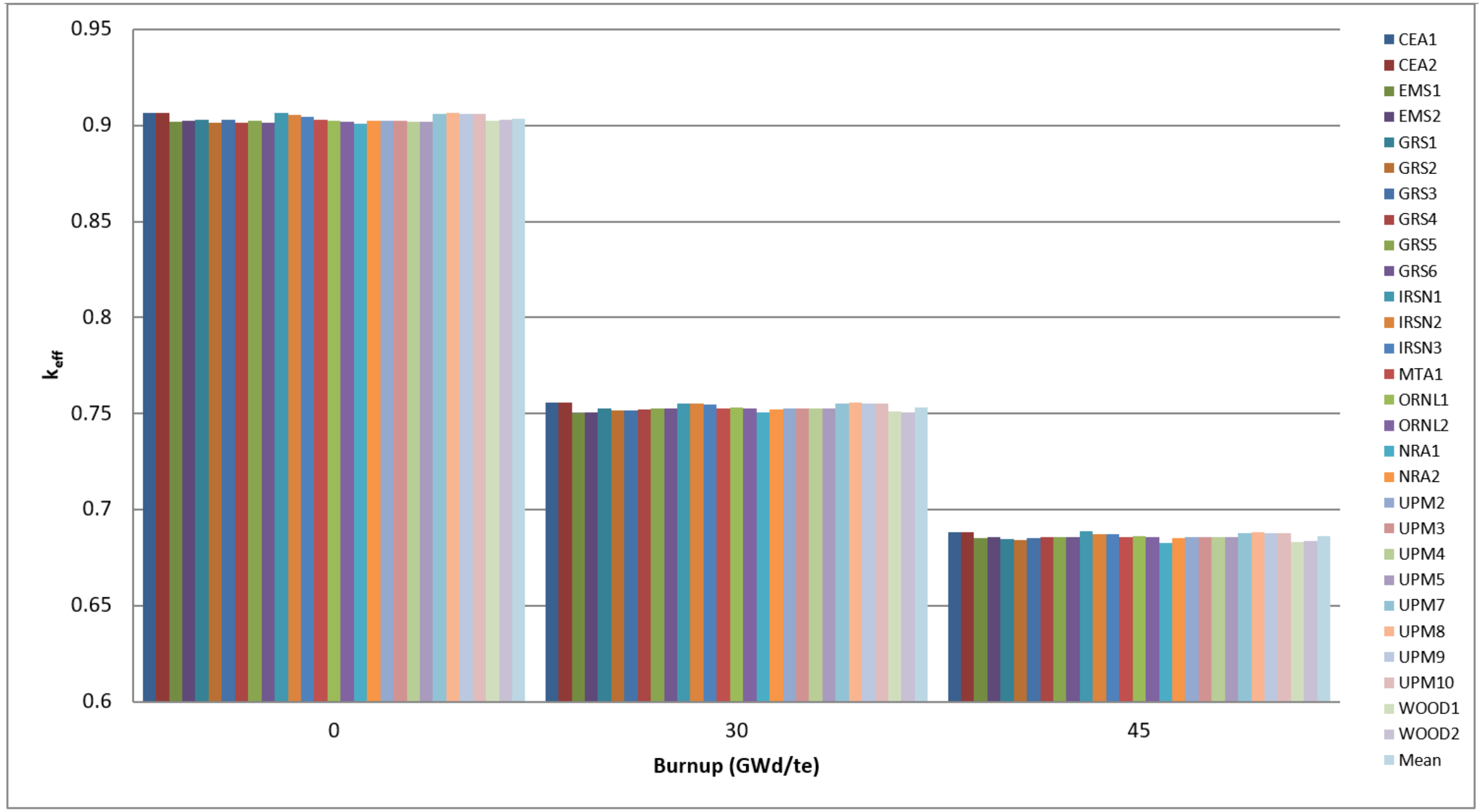
Source: NEA data, 2020.

Figure A.8. Participant results for case T233-INF-45



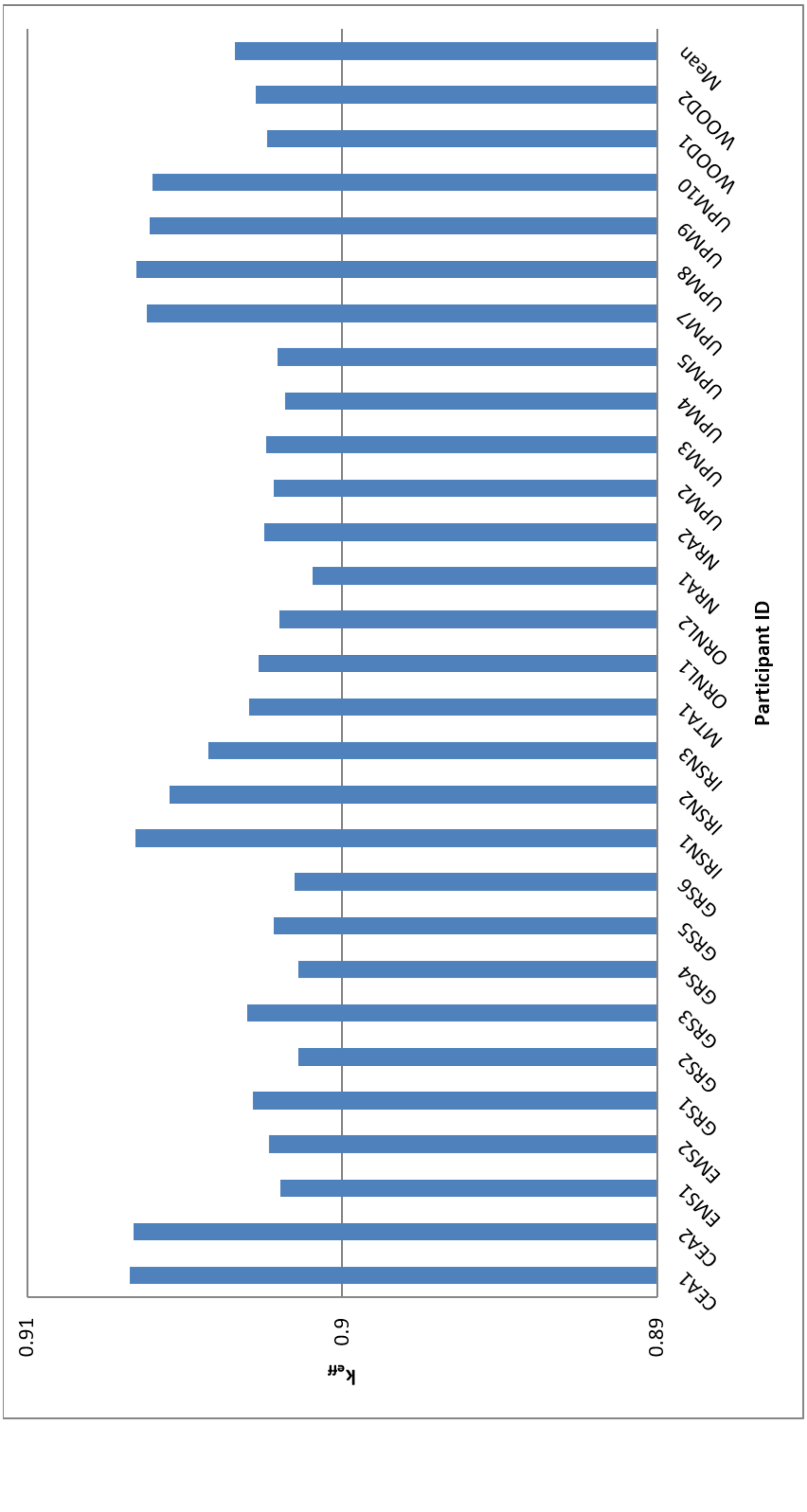
Source: NEA data, 2020.

Figure A.9. Summary graph of results for T253-SU cases



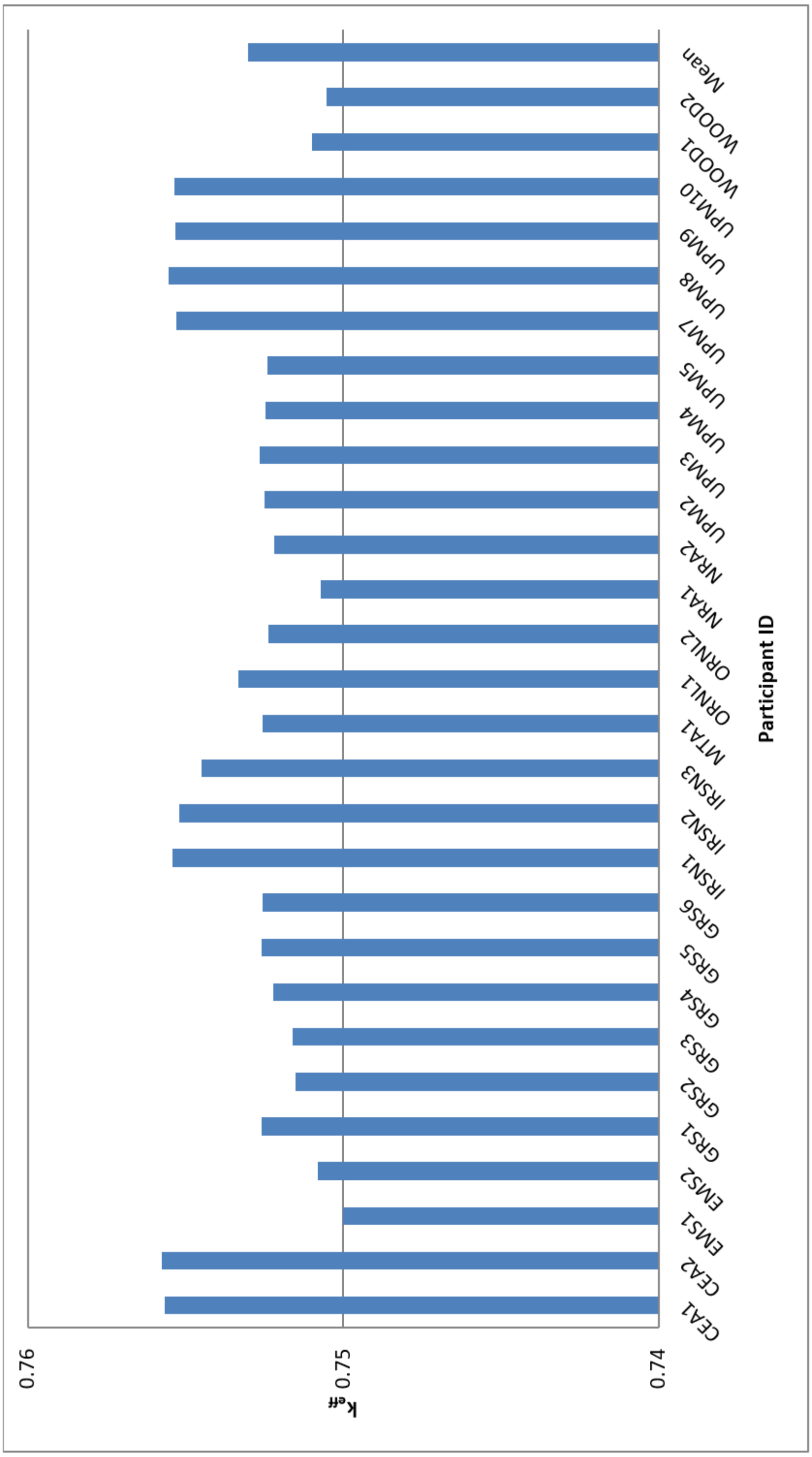
Source: NEA data, 2020.

Figure A.10. Participant results for case T253-SU-0



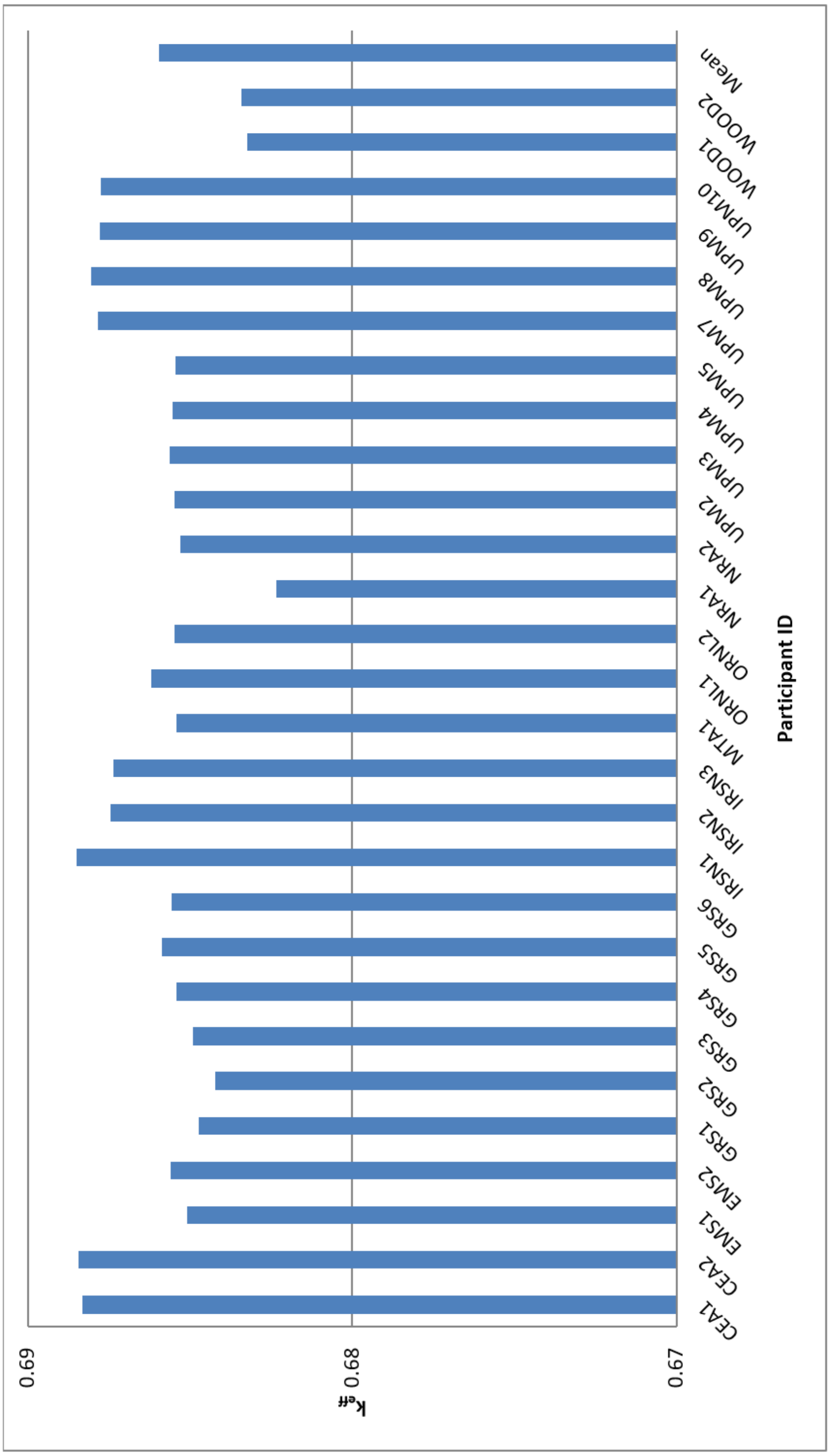
Source: NEA data, 2020.

Figure A.11. Participant results for case T253-SU-30



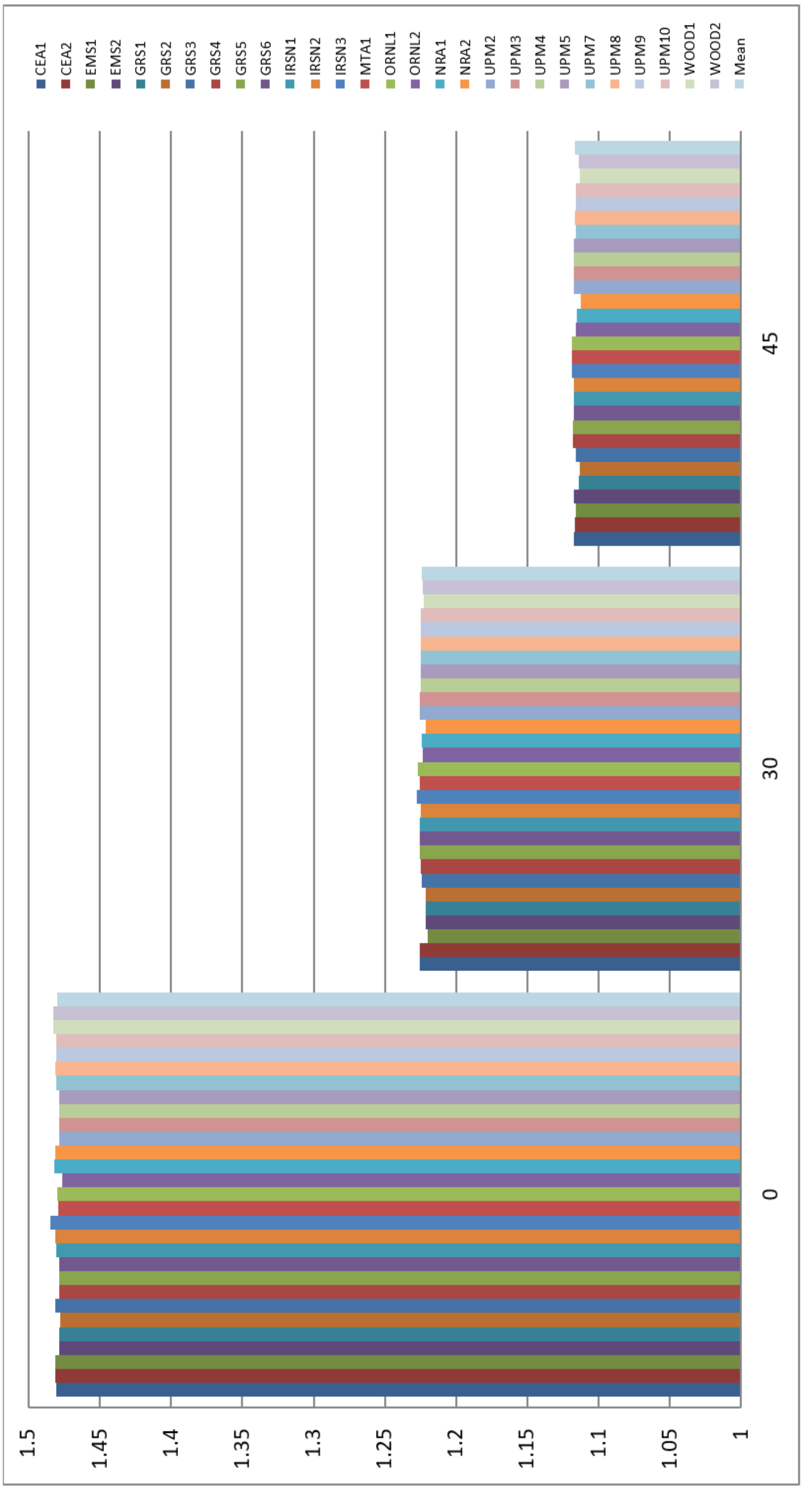
Source: NEA data, 2020.

Figure A.12. Participant results for case T253-SU-45



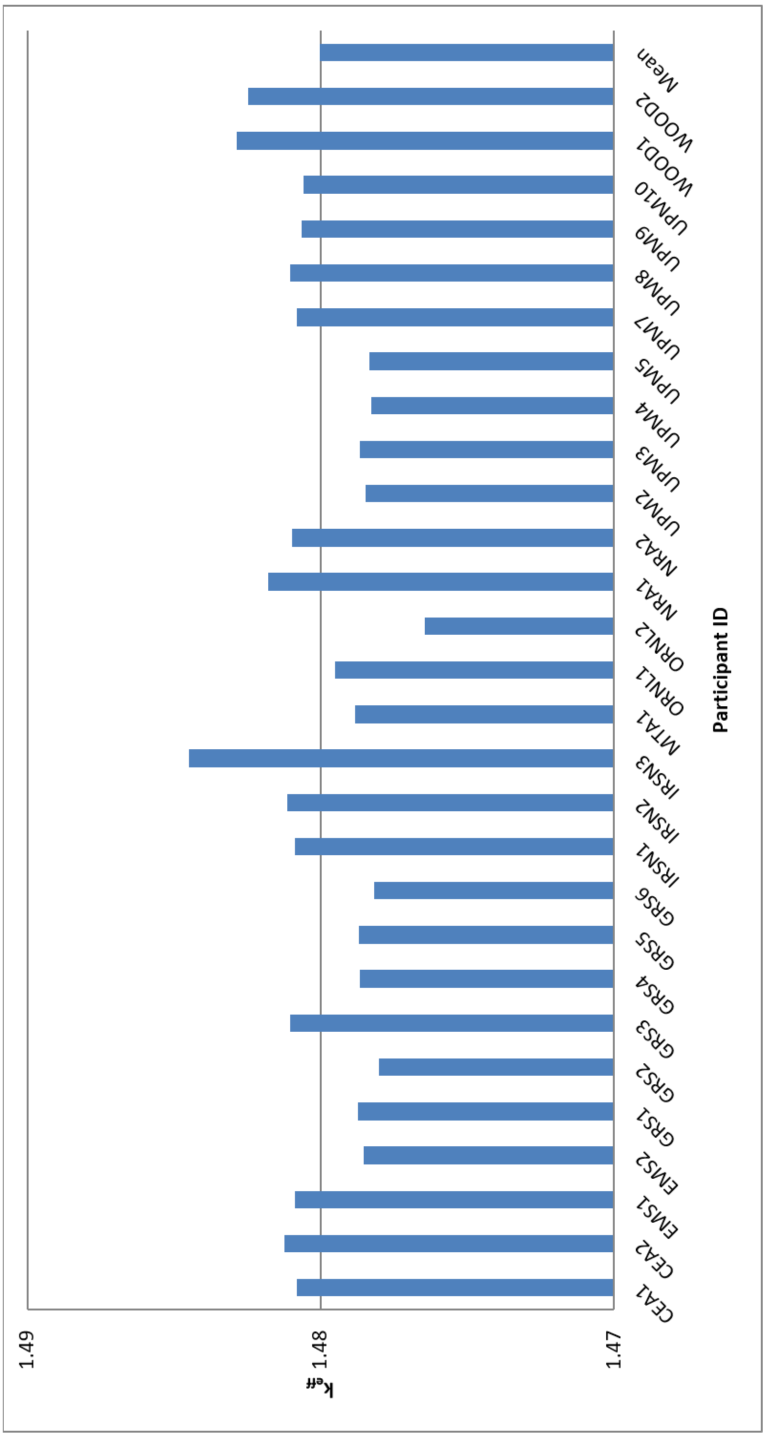
Source: NEA data, 2020.

Figure A.13. Summary graph of results for T253-INF cases



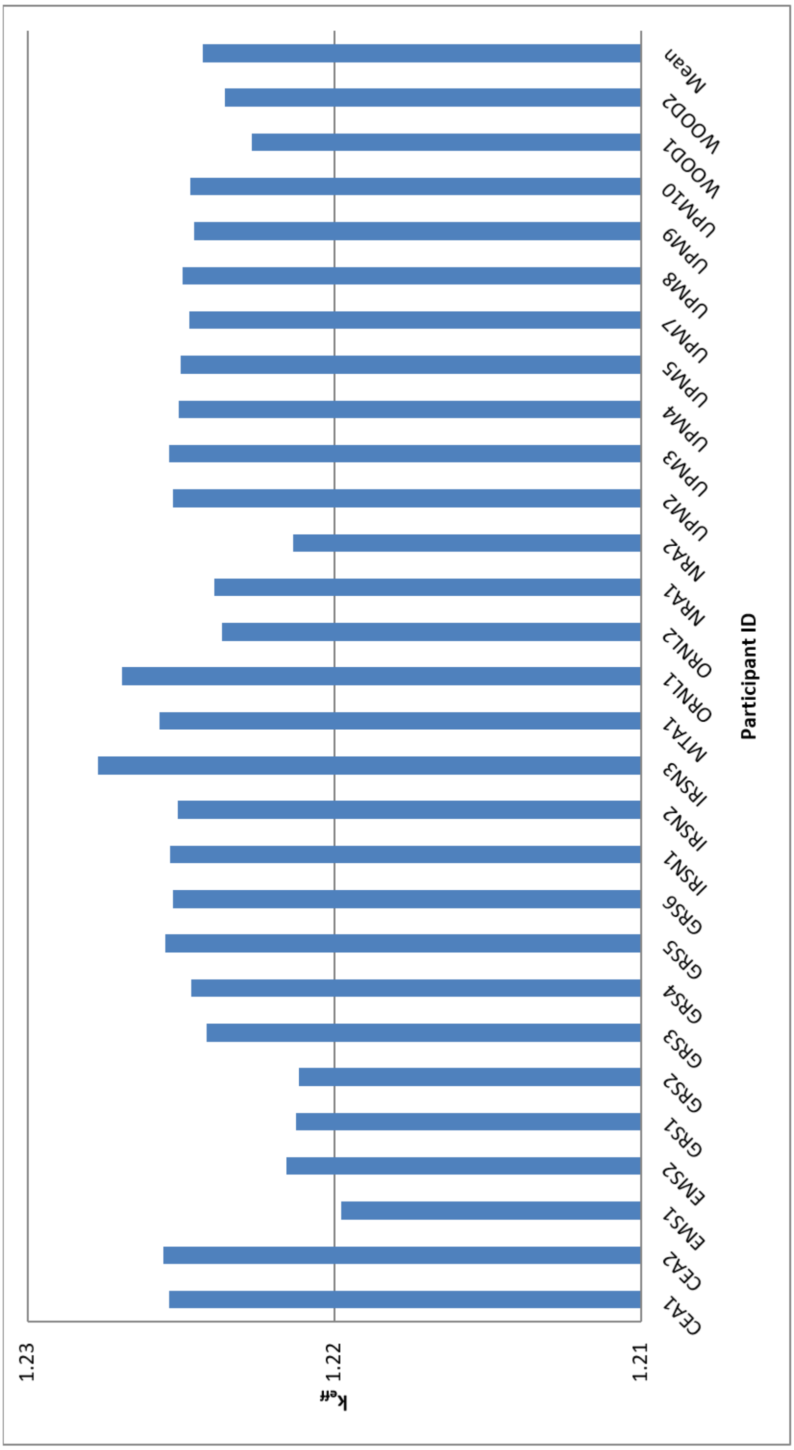
Source: NEA data, 2020.

Figure A.14. Participant results for case T253-INF-0



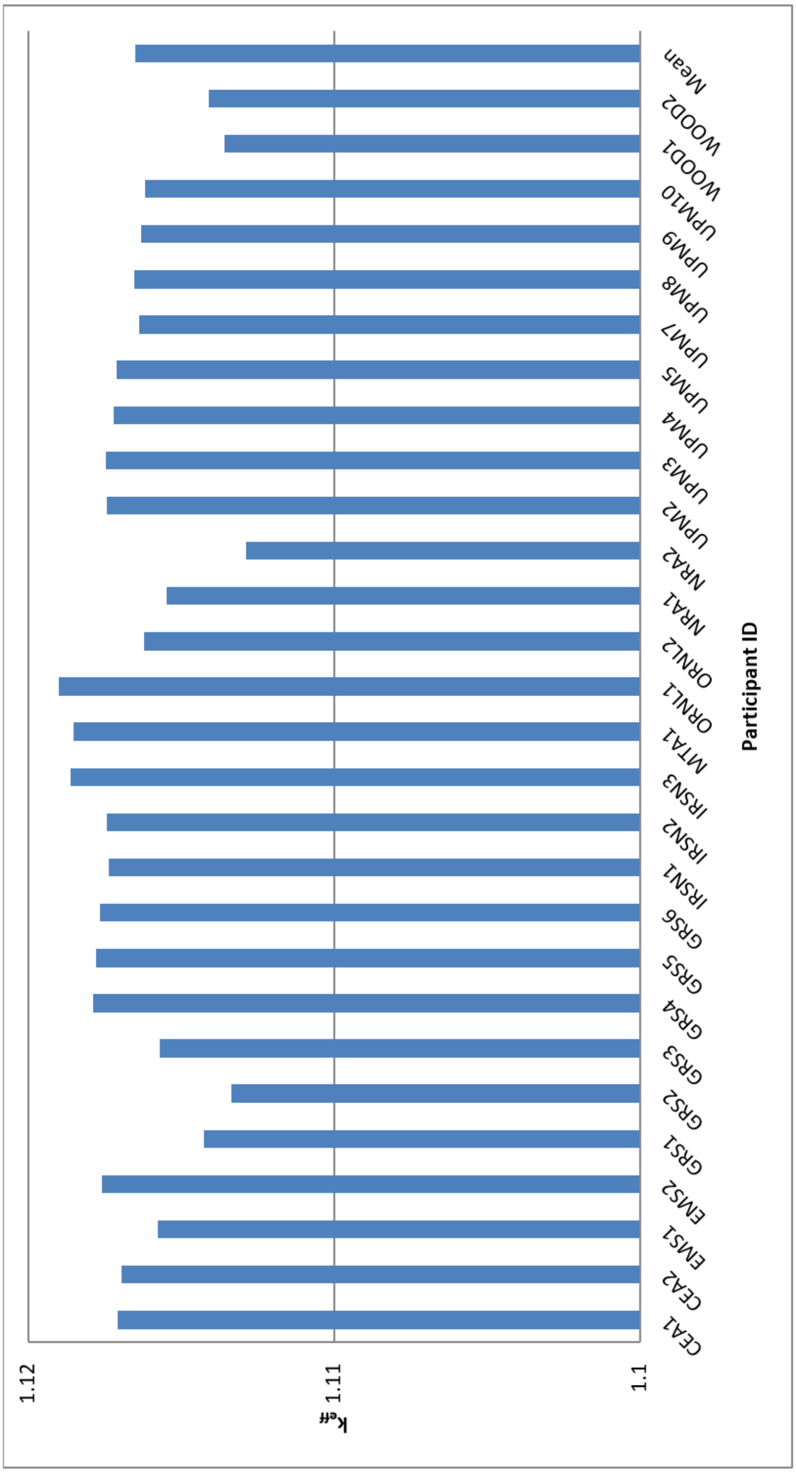
Source: NEA data, 2020.

Figure A.15. Participant results for case T253-INF-30



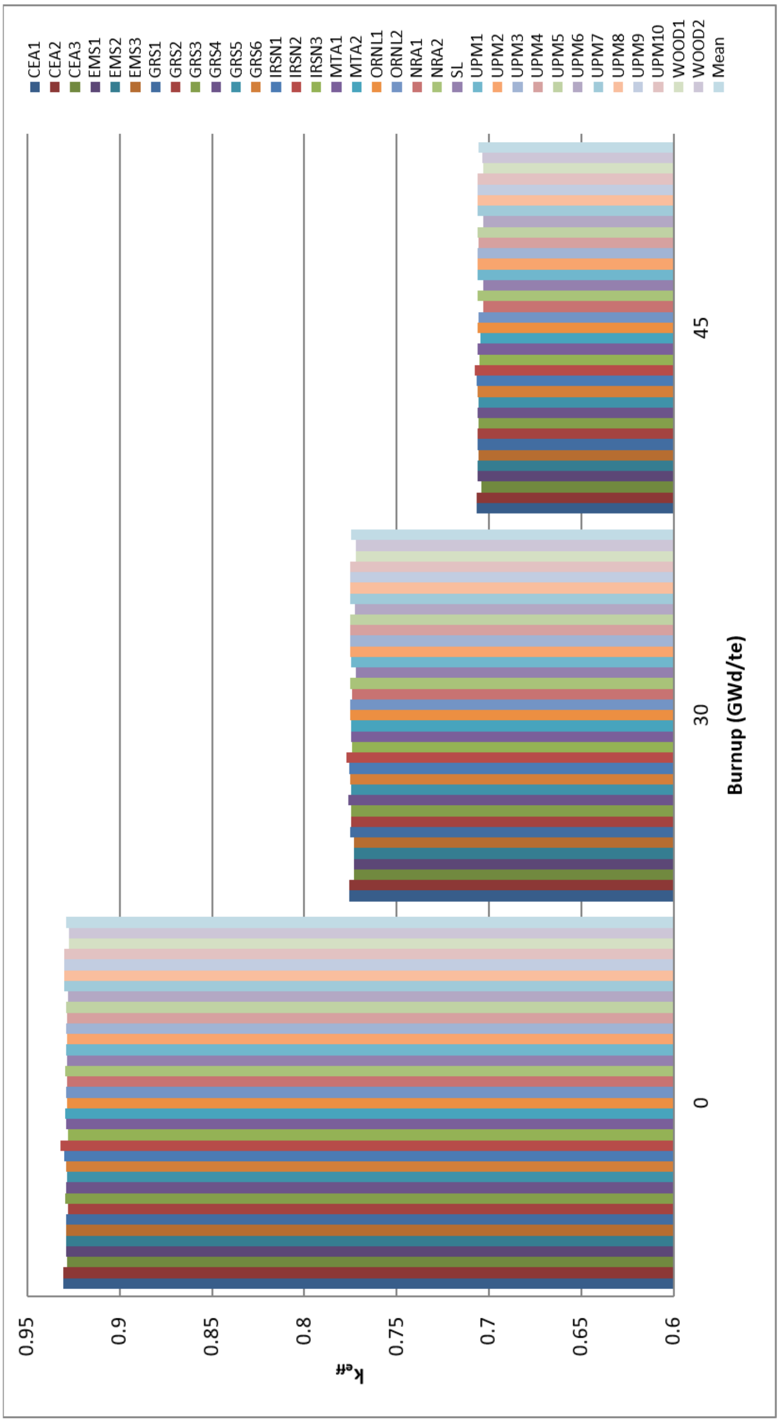
Source: NEA data, 2020.

Figure A.16. Participant results for case T253-INF-45



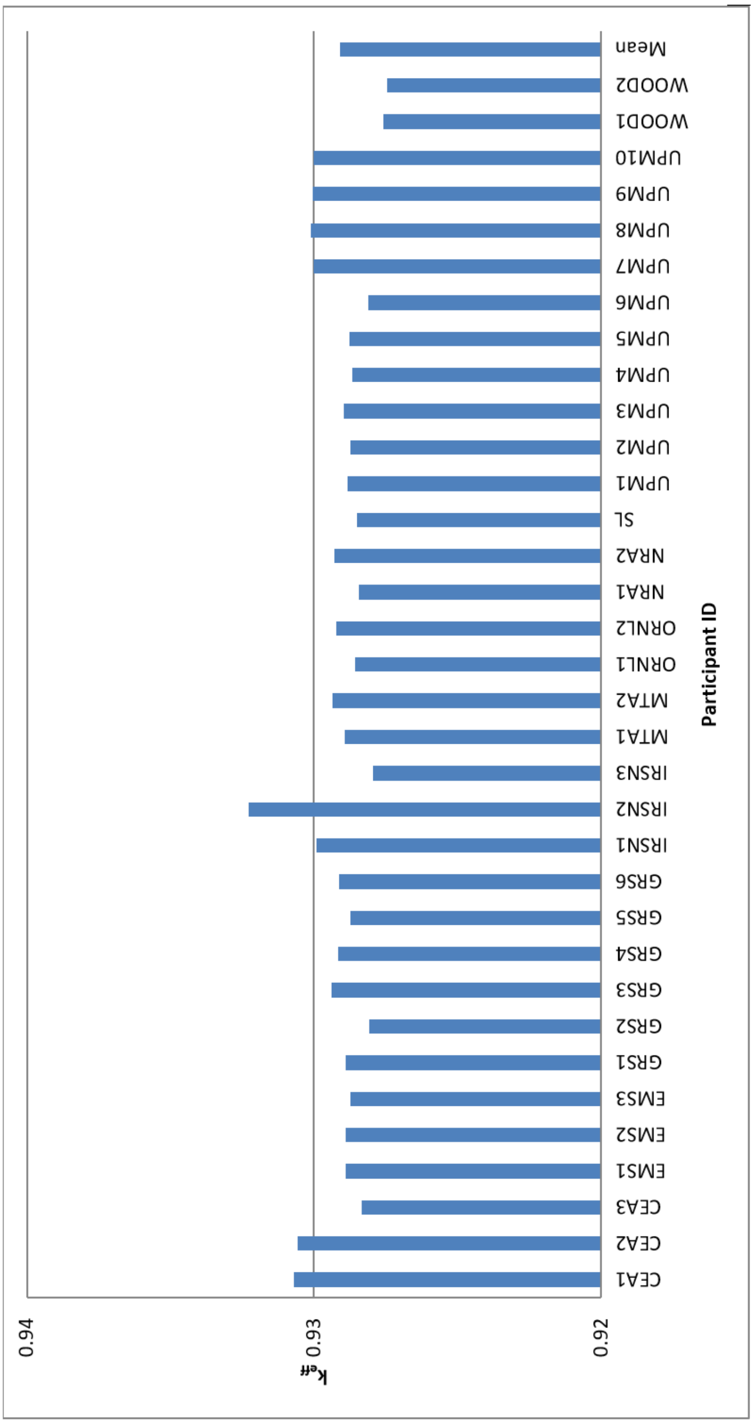
Source: NEA data, 2020.

Figure A.17. Summary graph of results for T293-SU cases



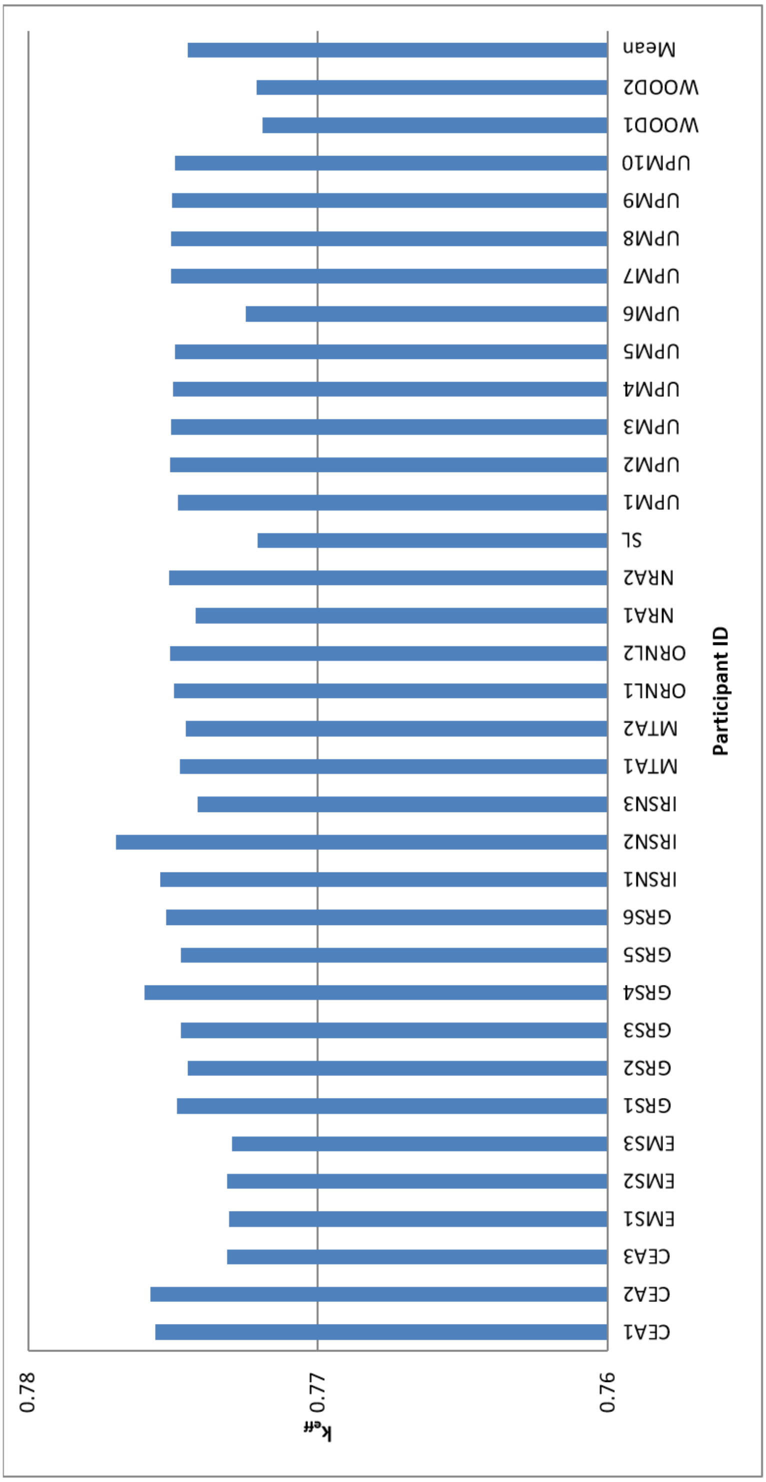
Source: NEA data, 2020.

Figure A.18. Participant results for case T293-SU-0



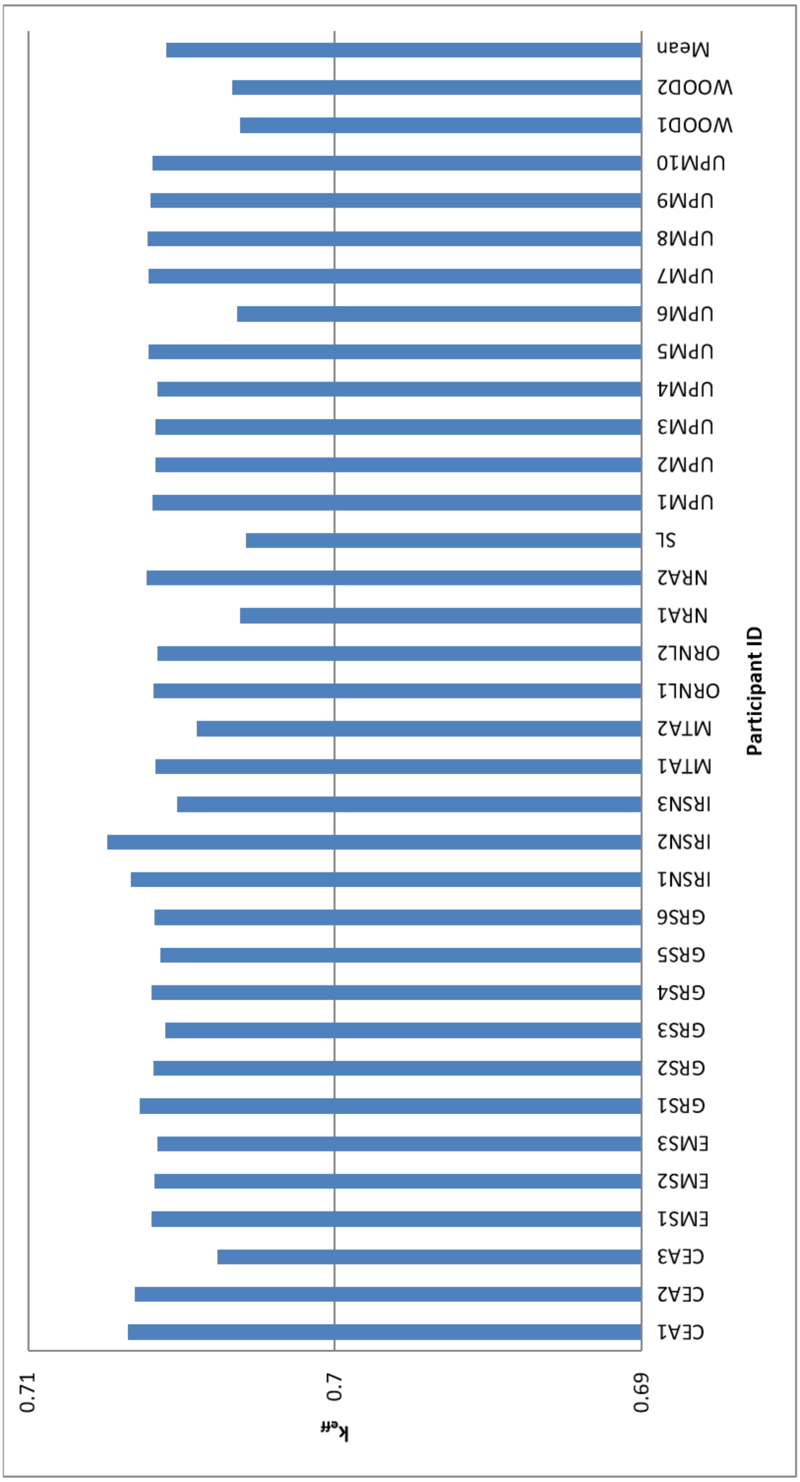
Source: NEA data, 2020.

Figure A.19. Participant results for case T293-SU-30



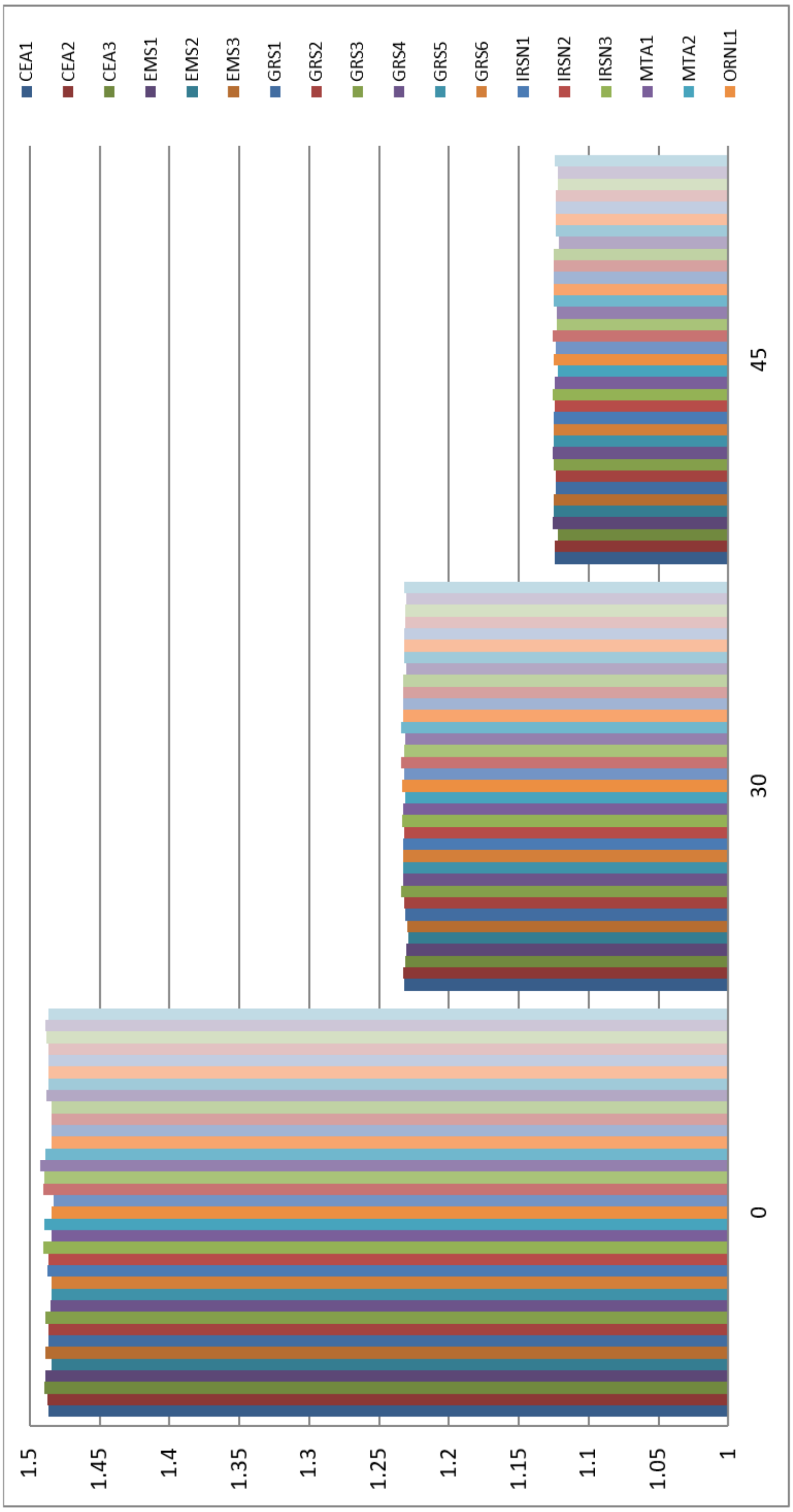
Source: NEA data, 2020.

Figure A.20. Participant results for case T293-SU-45



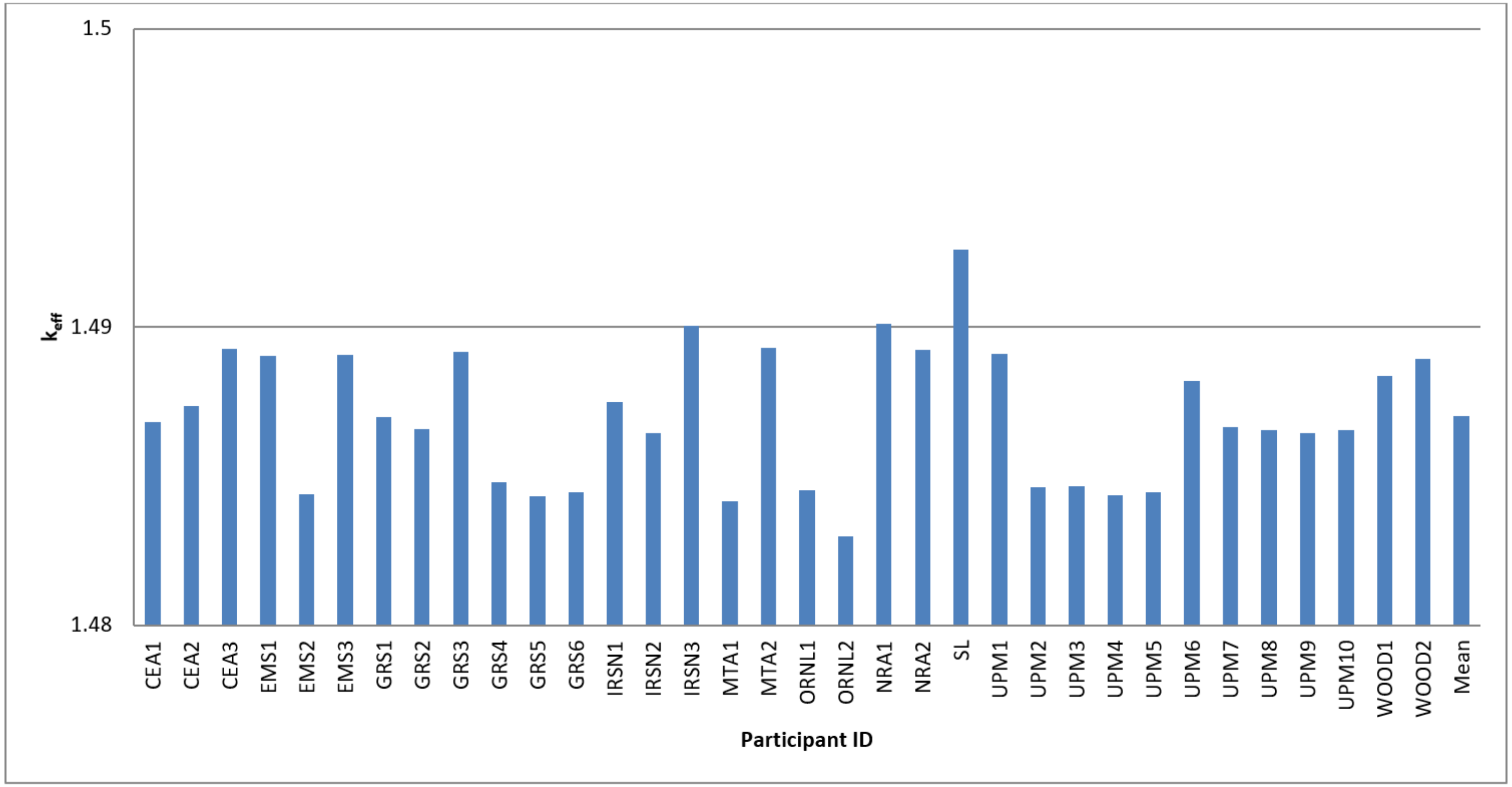
Source: NEA data, 2020.

Figure A.21. Summary graph of results for T293-INF cases



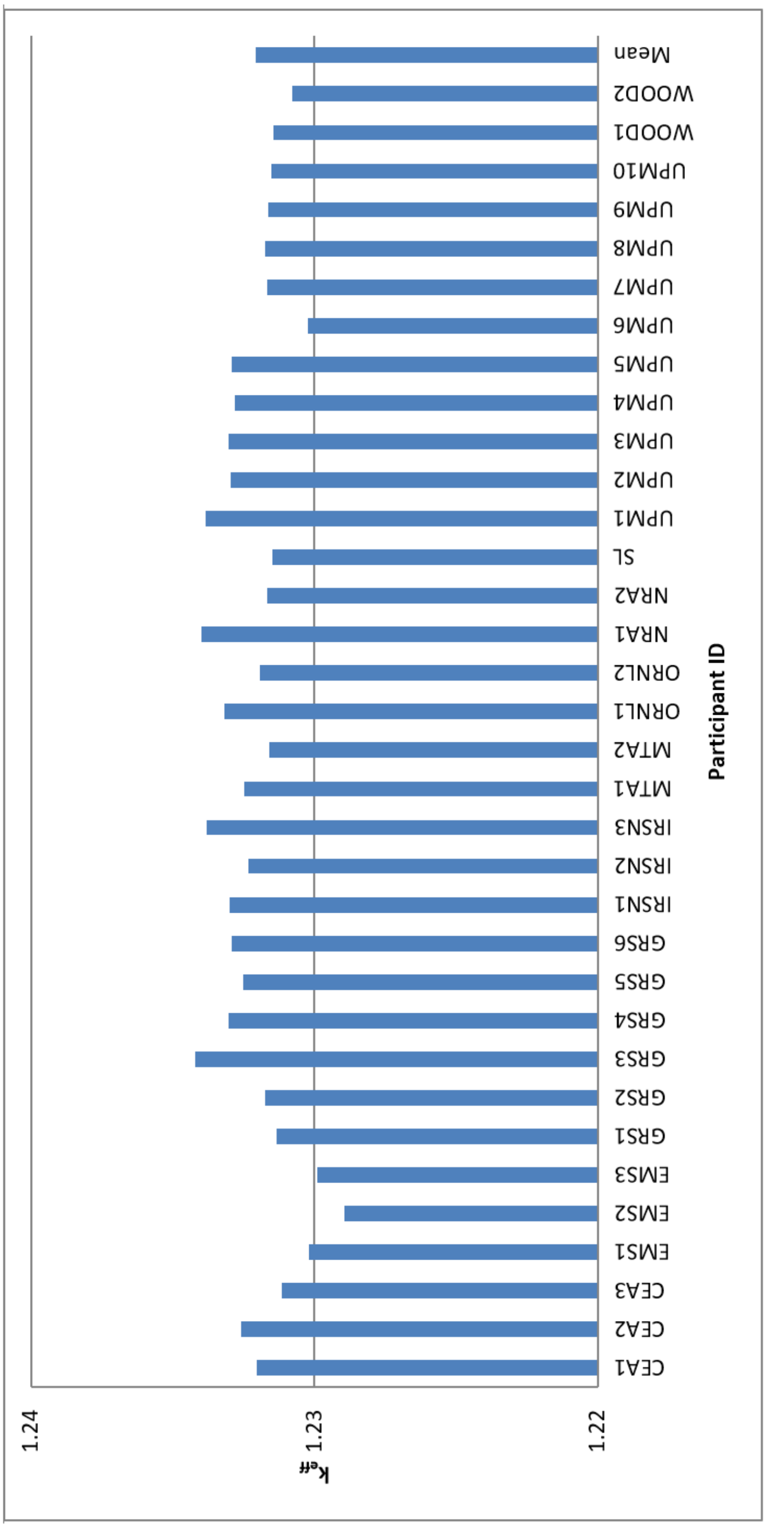
Source: NEA data, 2020.

Figure A.22. Participant results for case T293-INF-0



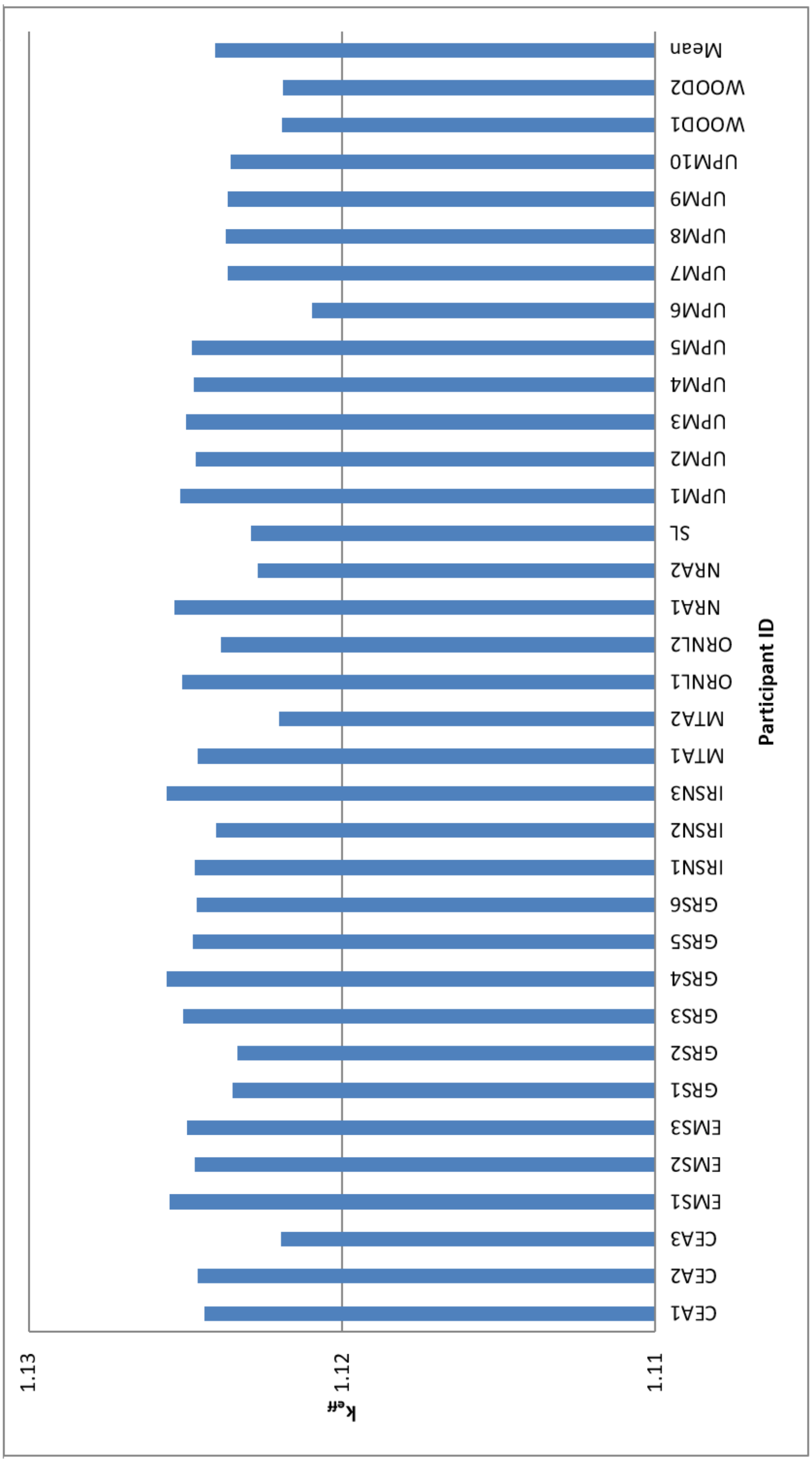
Source: NEA data, 2020.

Figure A.23. Participant results for case T293-INF-30



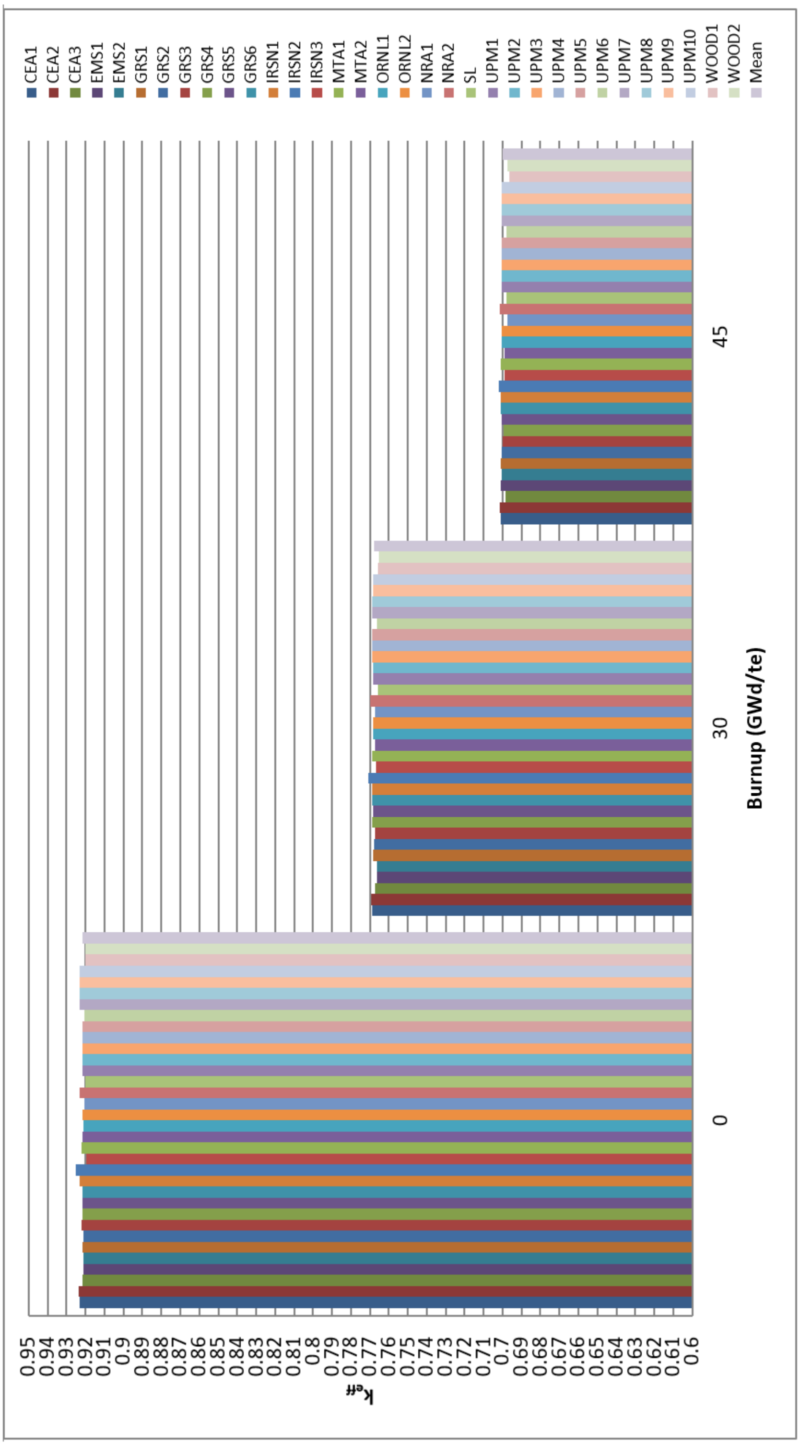
Source: NEA data, 2020.

Figure A.24. Participant results for case T293-INF-45



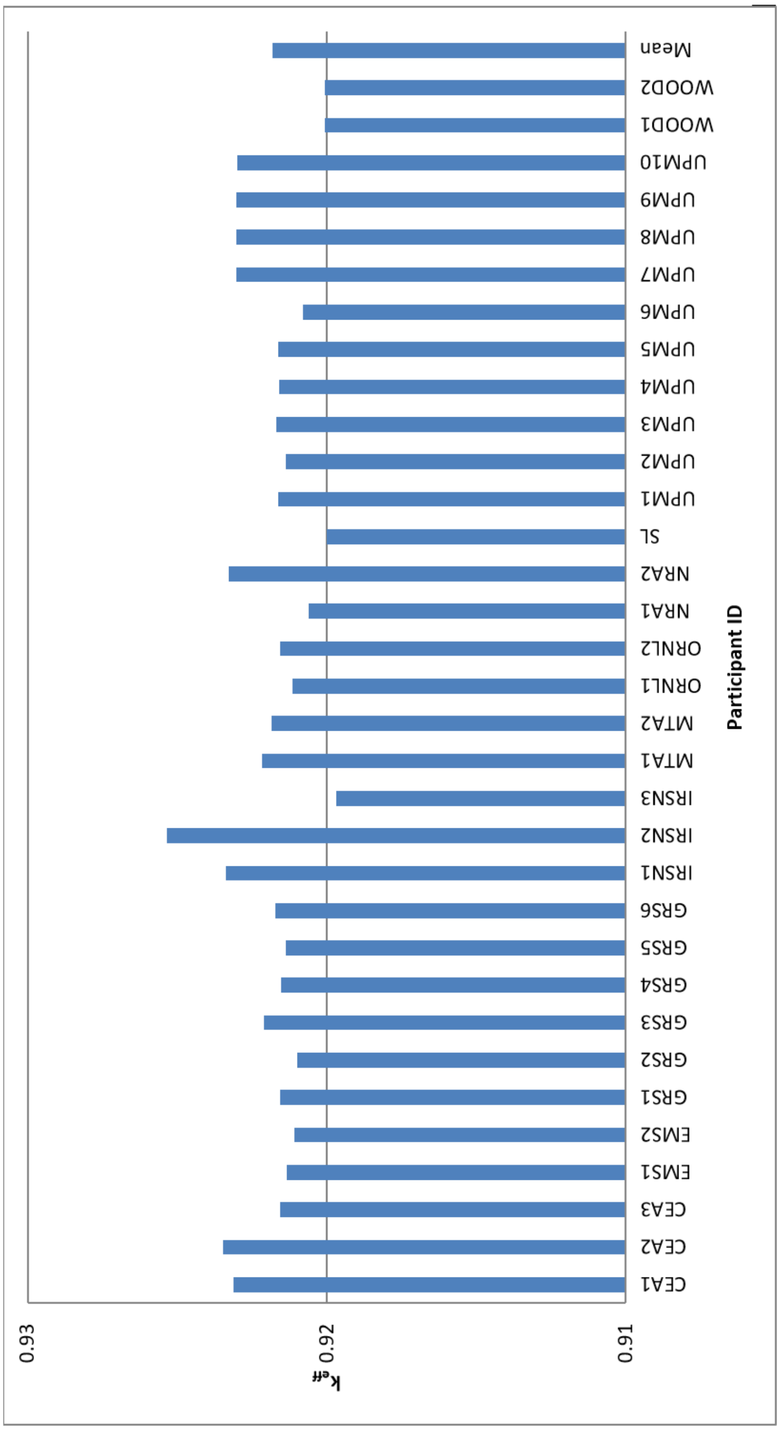
Source: NEA data, 2020.

Figure A.25. Summary graph of results for T333-SU cases



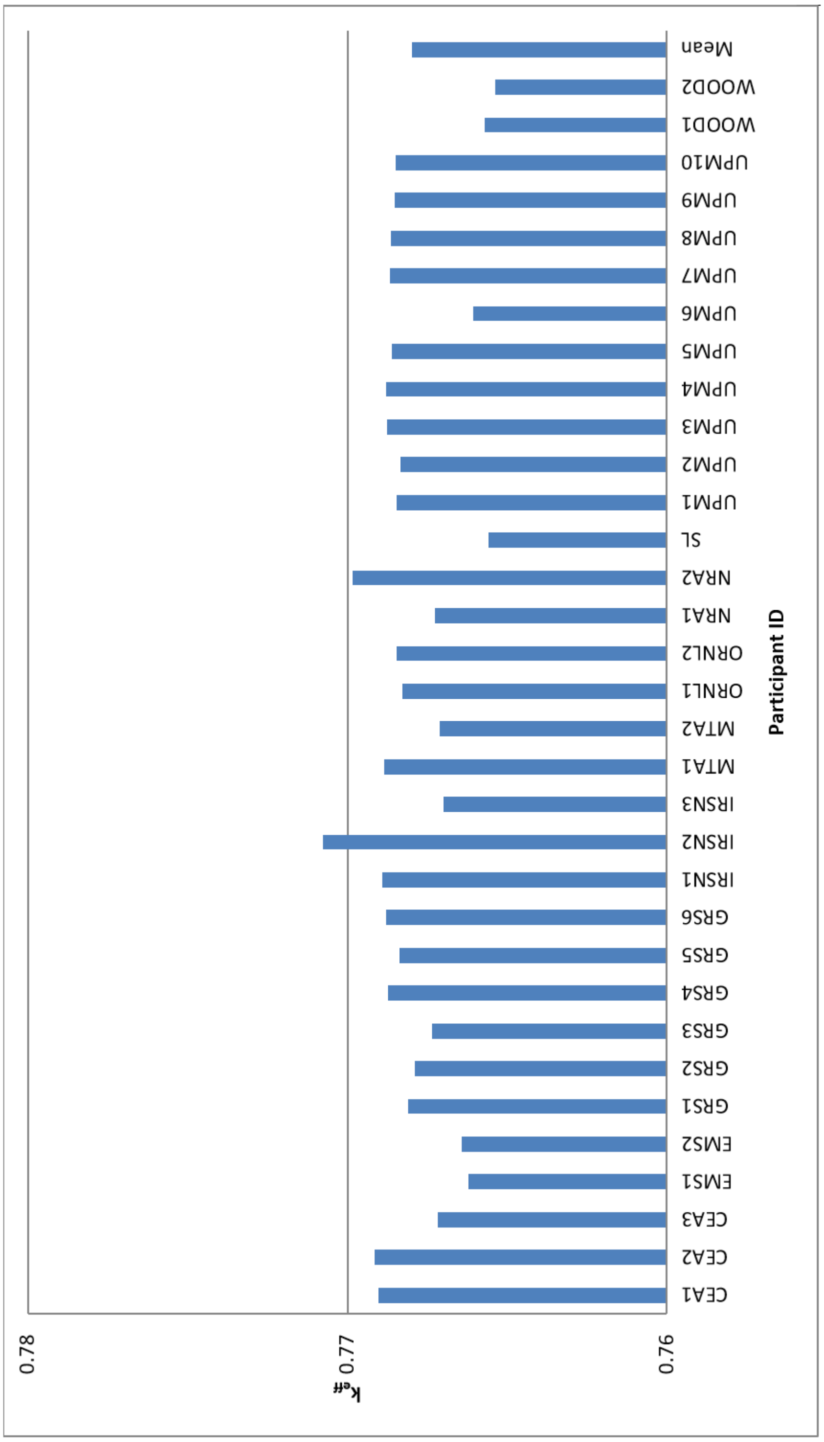
Source: NEA data, 2020.

Figure A.26. Participant results for case T333-SU-0



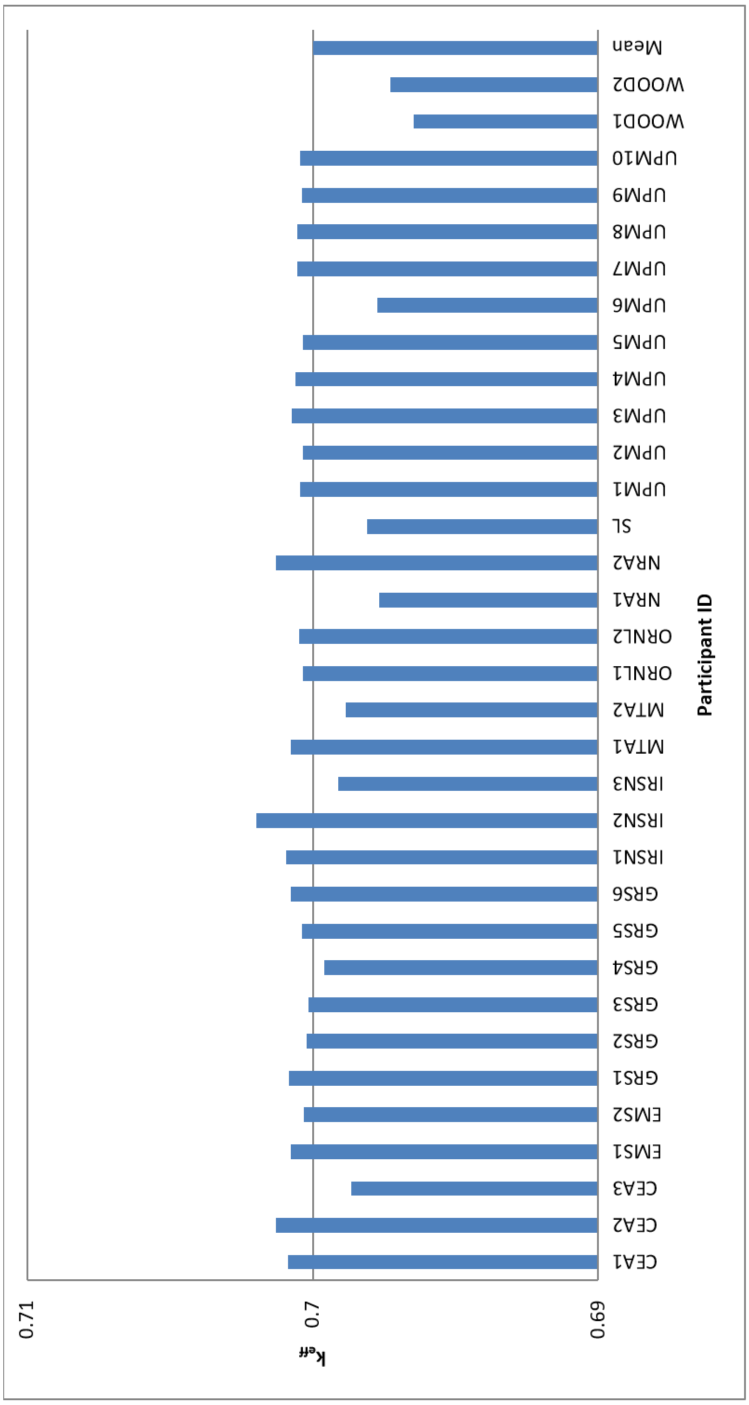
Source: NEA data, 2020.

Figure A.27. Participant results for case T333-SU-30



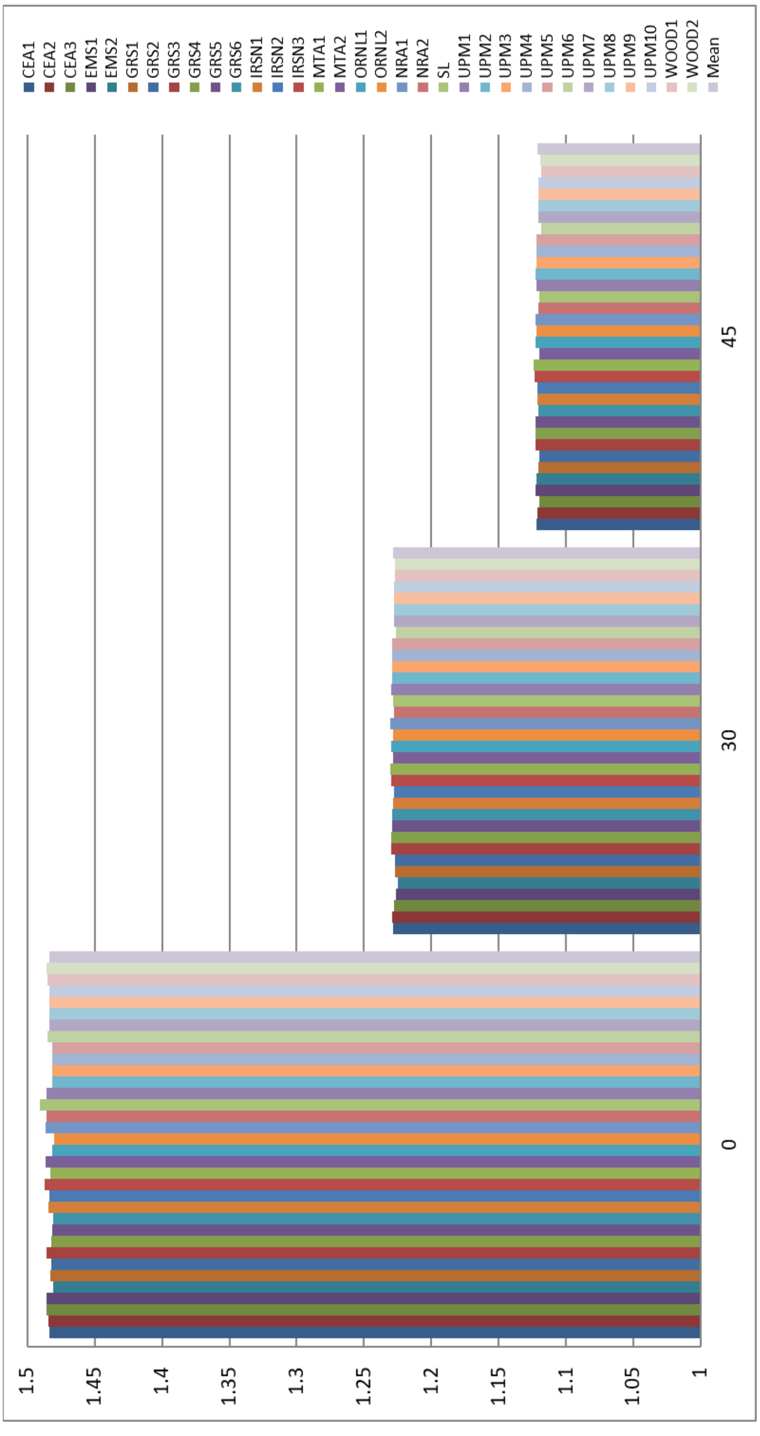
Source: NEA data, 2020.

Figure A.28. Participant results for case T333-SU-45



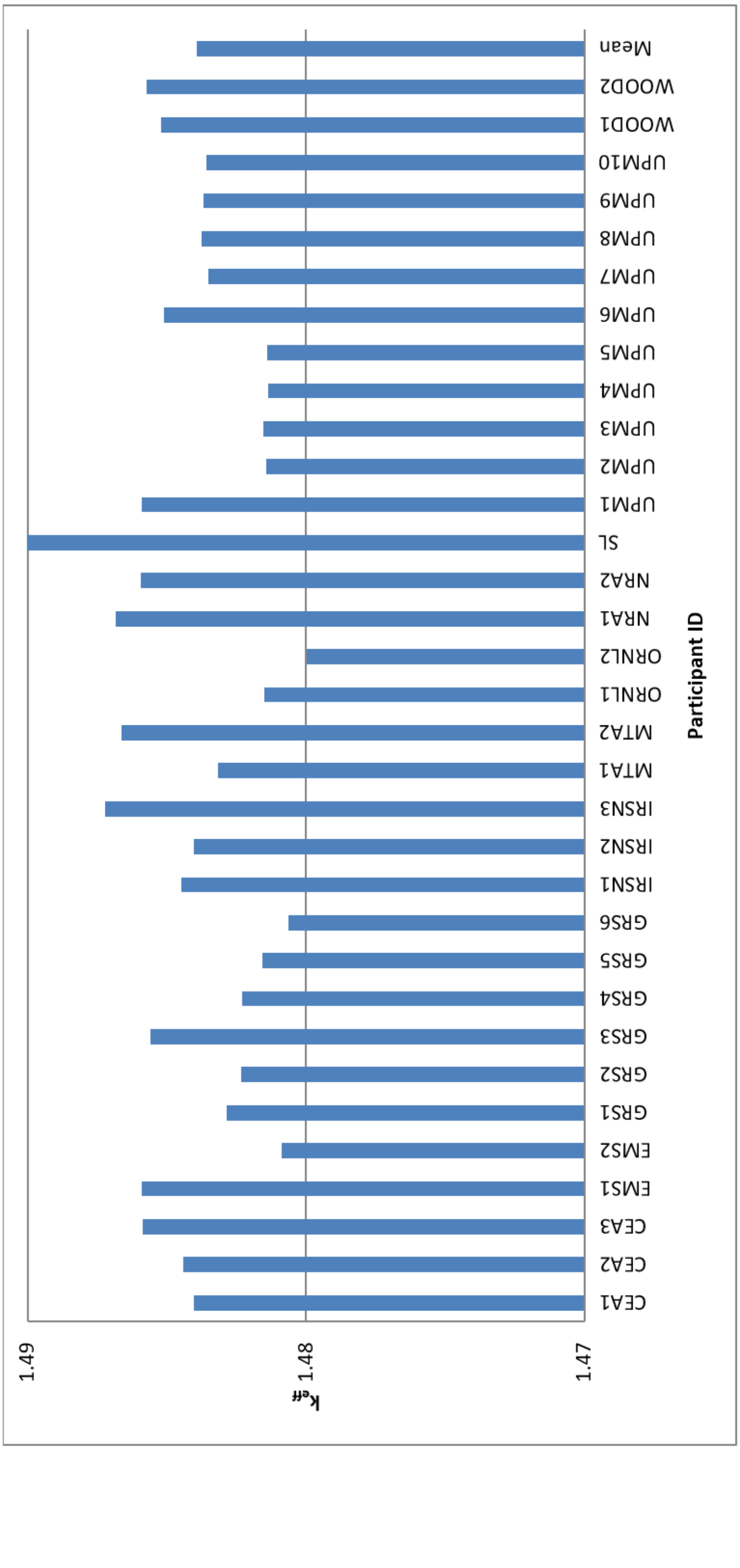
Source: NEA data, 2020.

Figure A.29. Summary graph of results for T333-INF cases



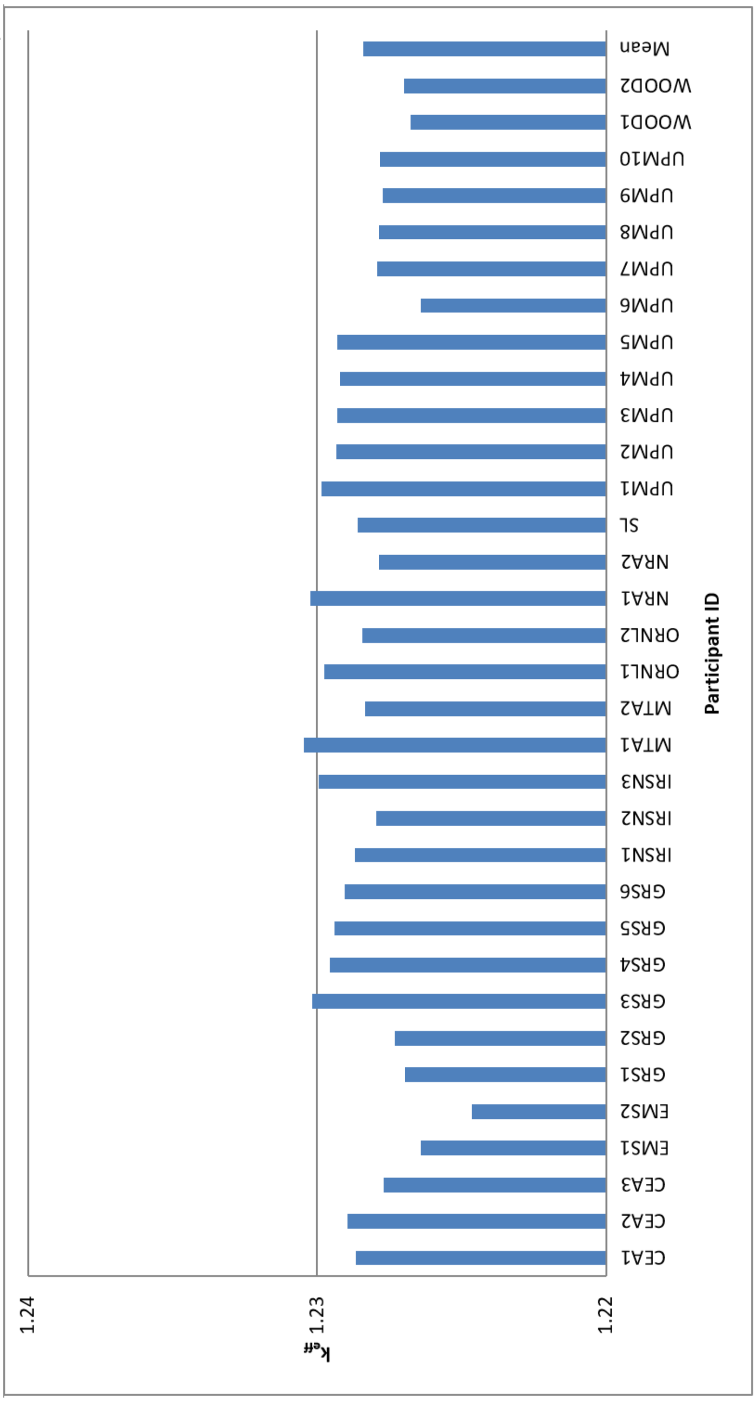
Source: NEA data, 2020.

Figure A.30. Participant results for case T333-INF-0



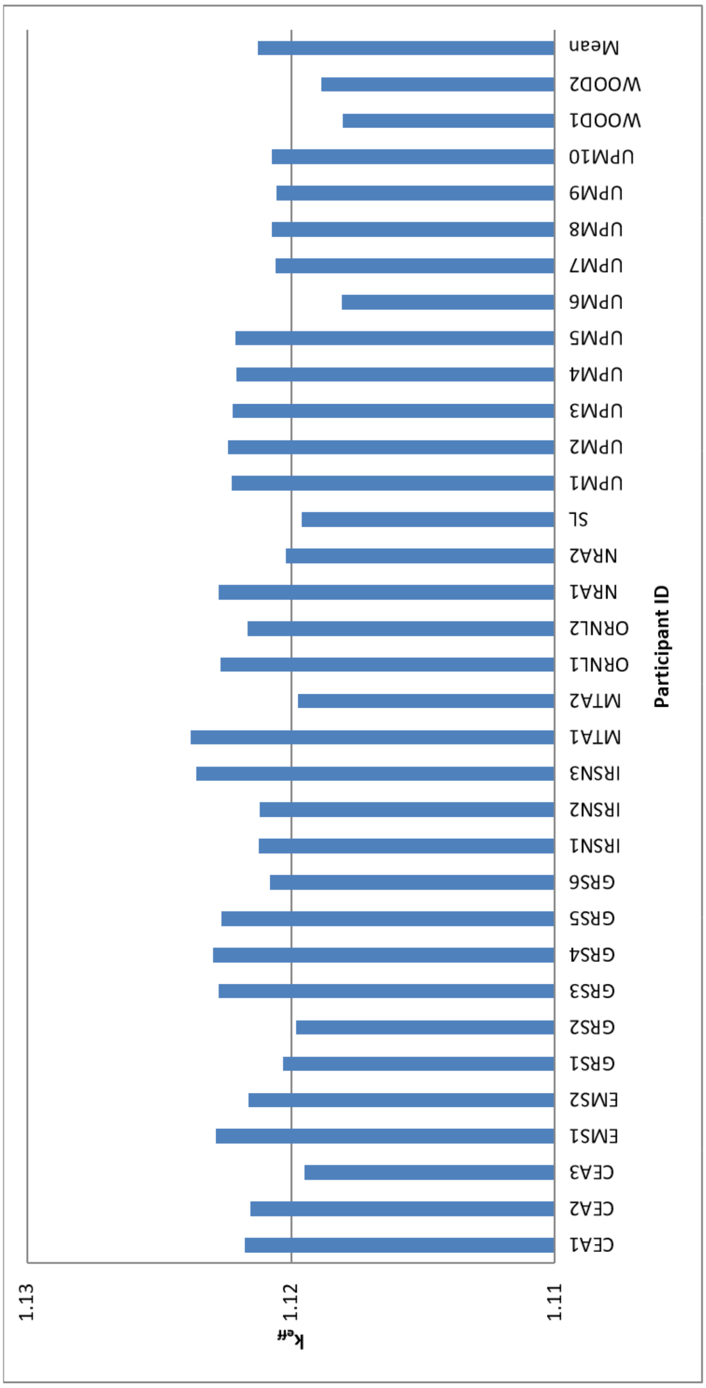
Source: NEA data, 2020.

Figure A.31. Participant results for case T333-INF-30



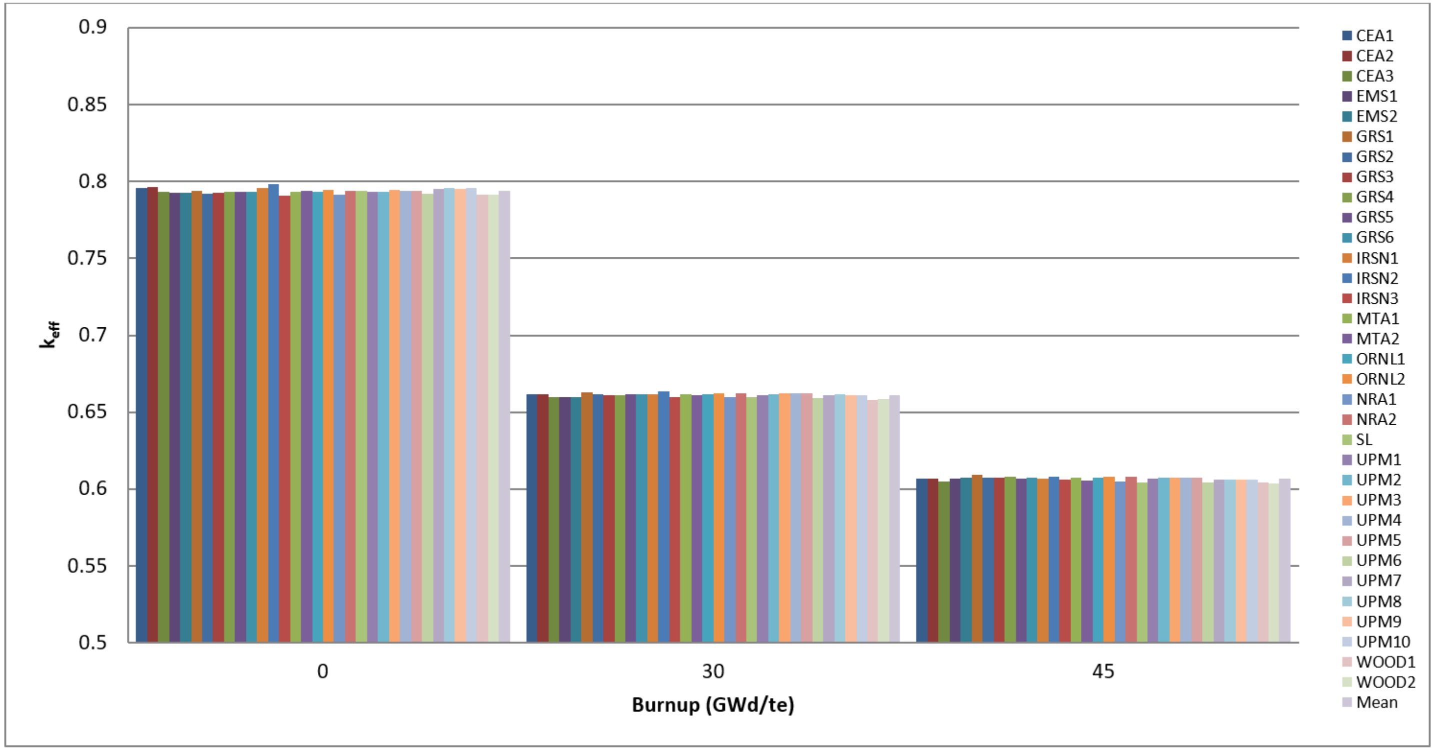
Source: NEA data, 2020.

Figure A.32. Participant results for case T333-INF-45



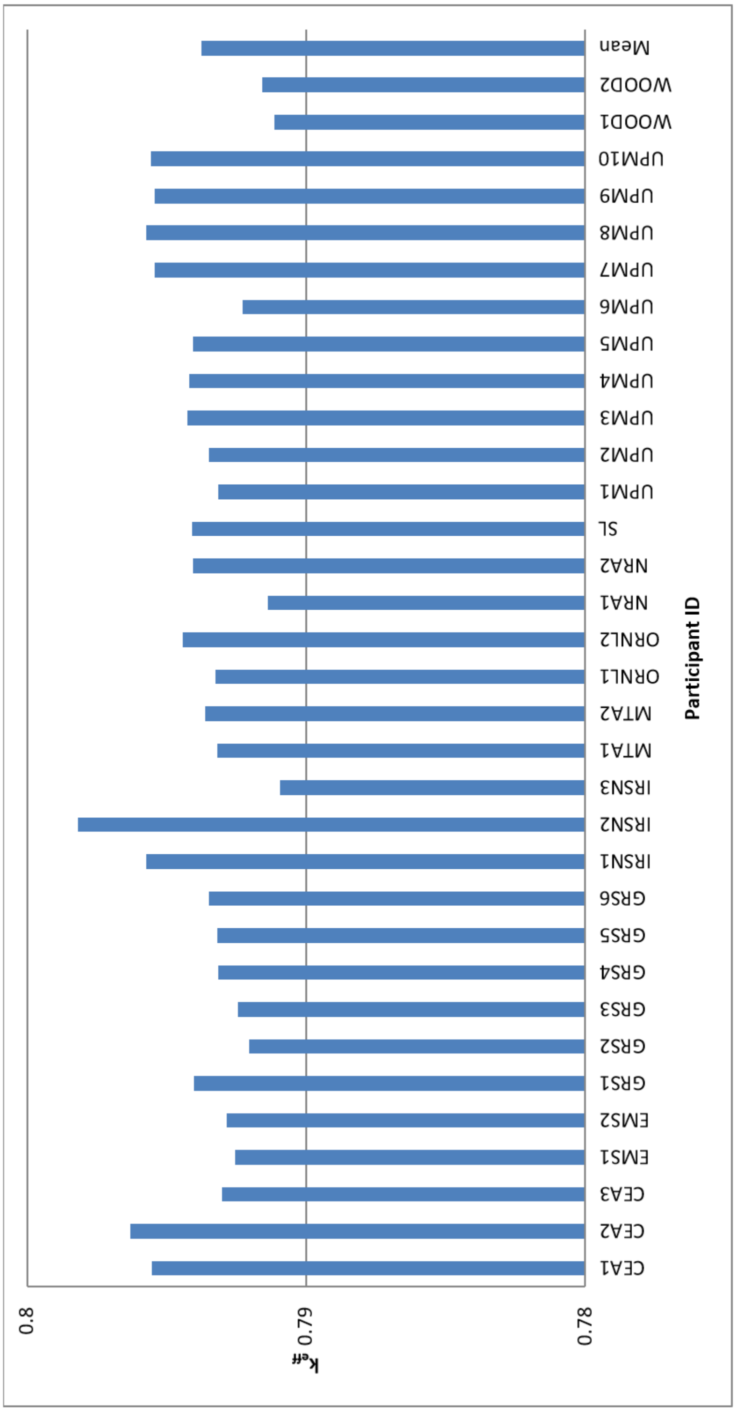
Source: NEA data, 2020.

Figure A.33. Summary graph of results for T588-SU cases



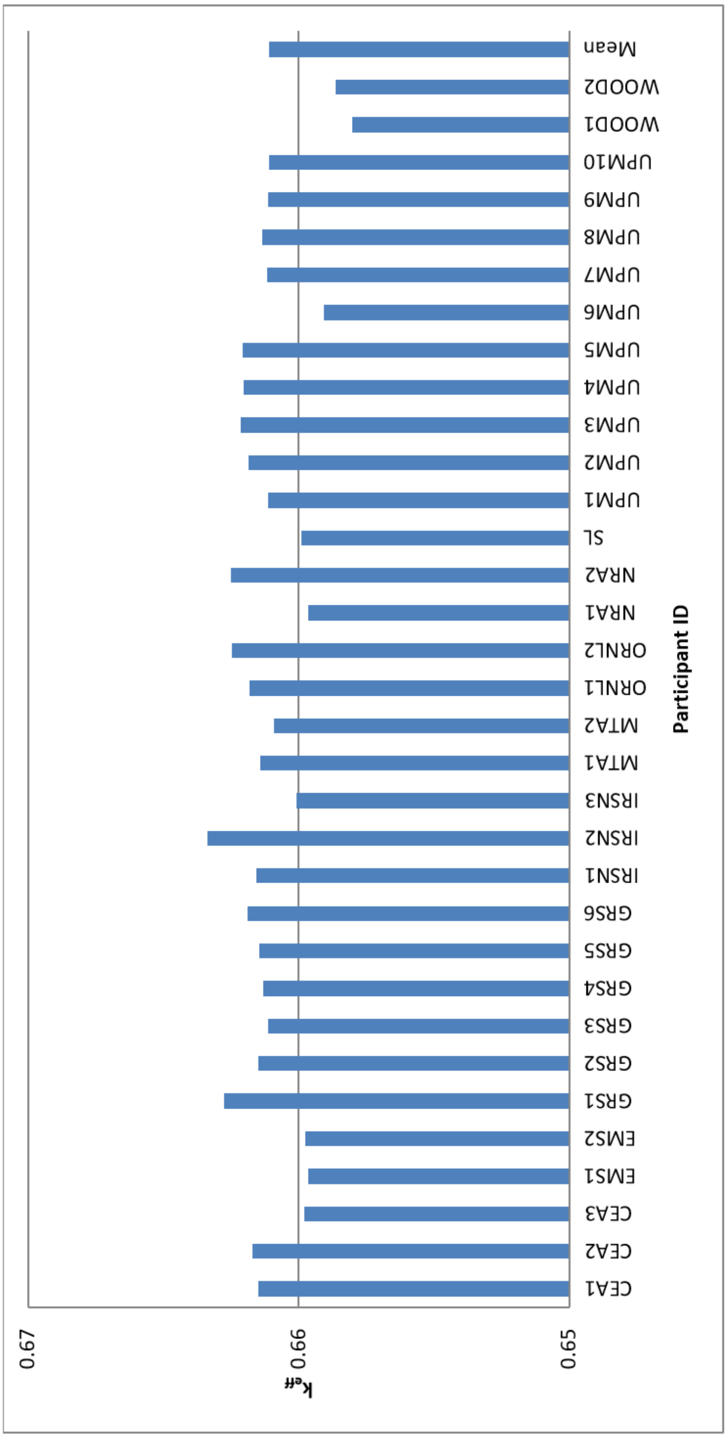
Source: NEA data, 2020.

Figure A.34. Participant results for case T588-SU-0



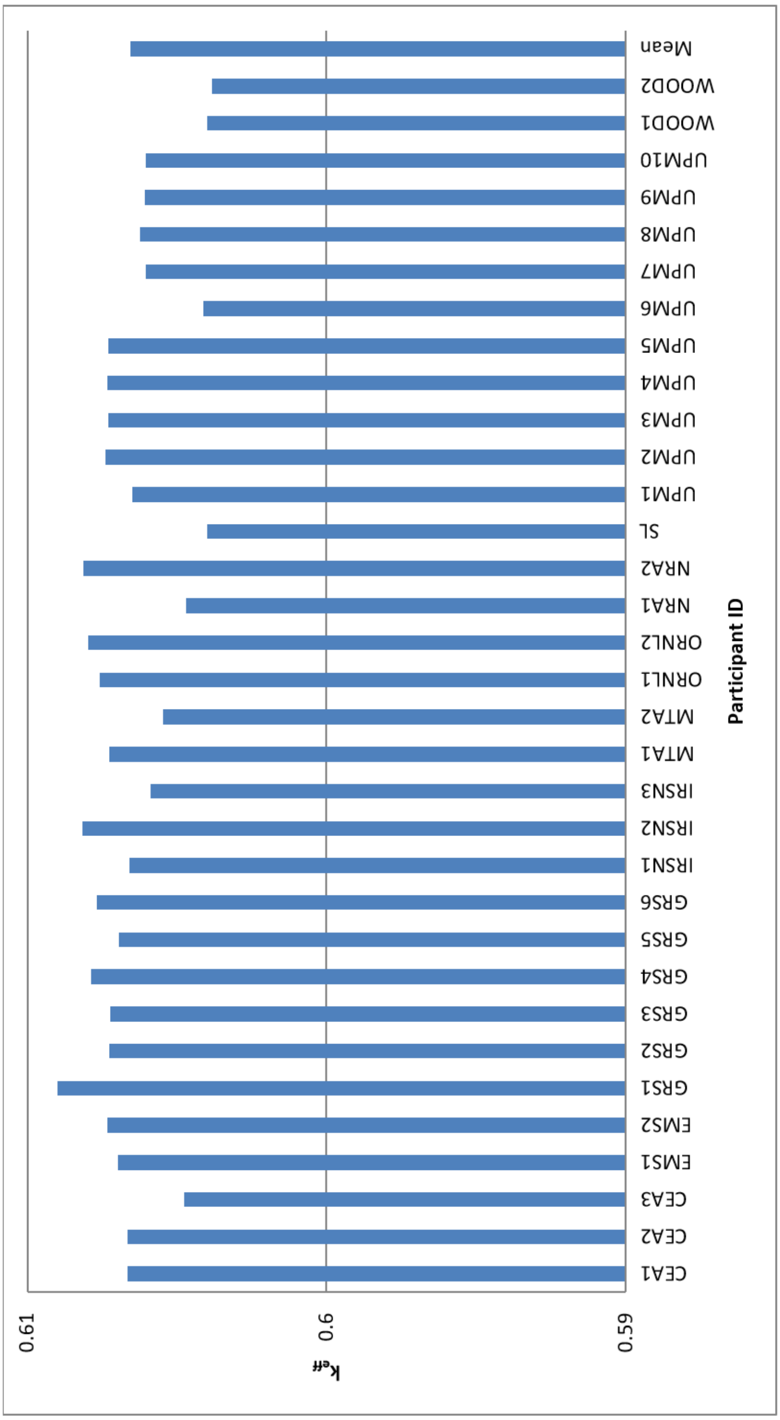
Source: NEA data, 2020.

Figure A.35. Participant results for case T588-SU-30



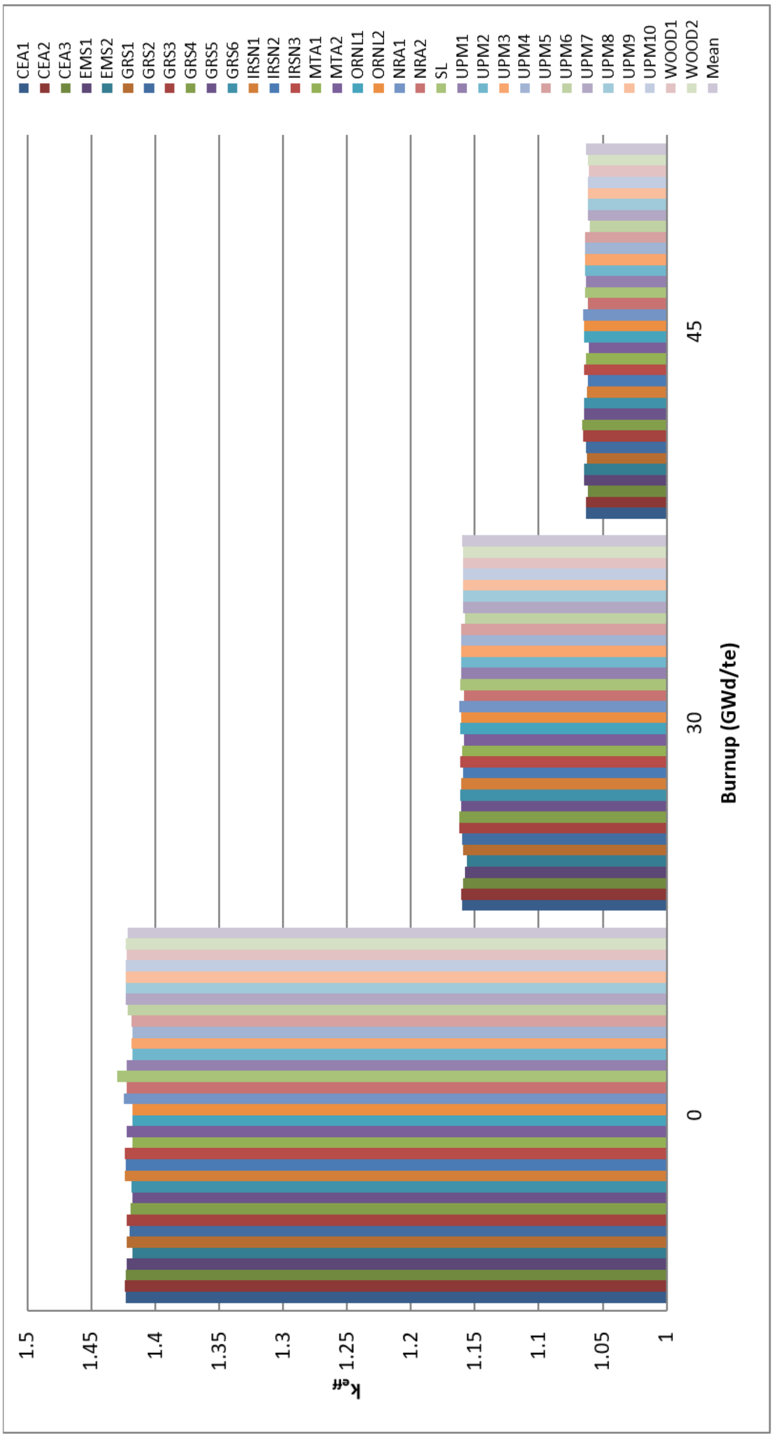
Source: NEA data, 2020.

Figure A.36. Participant results for case T588-SU-45



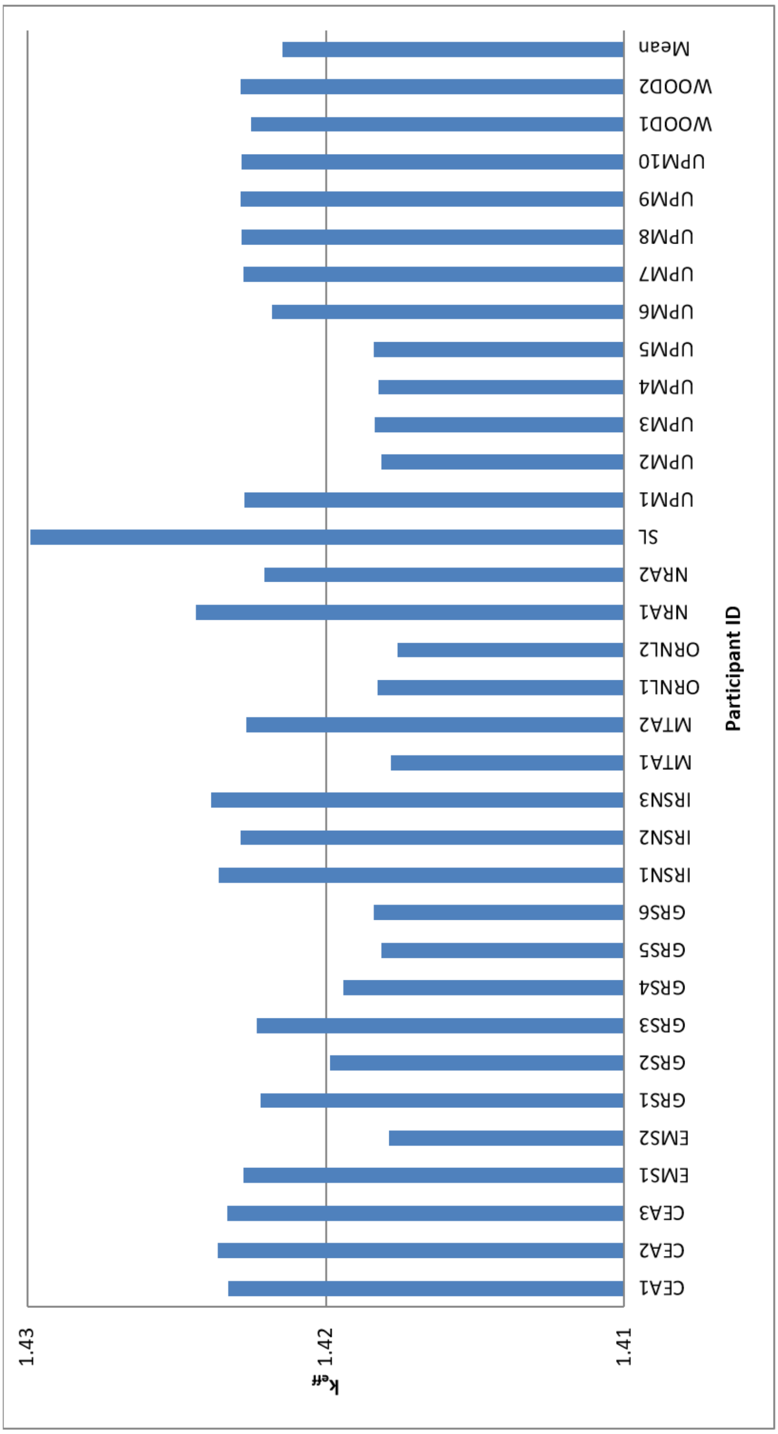
Source: NEA data, 2020.

Figure A.37. Summary graph of results for T588-INF cases



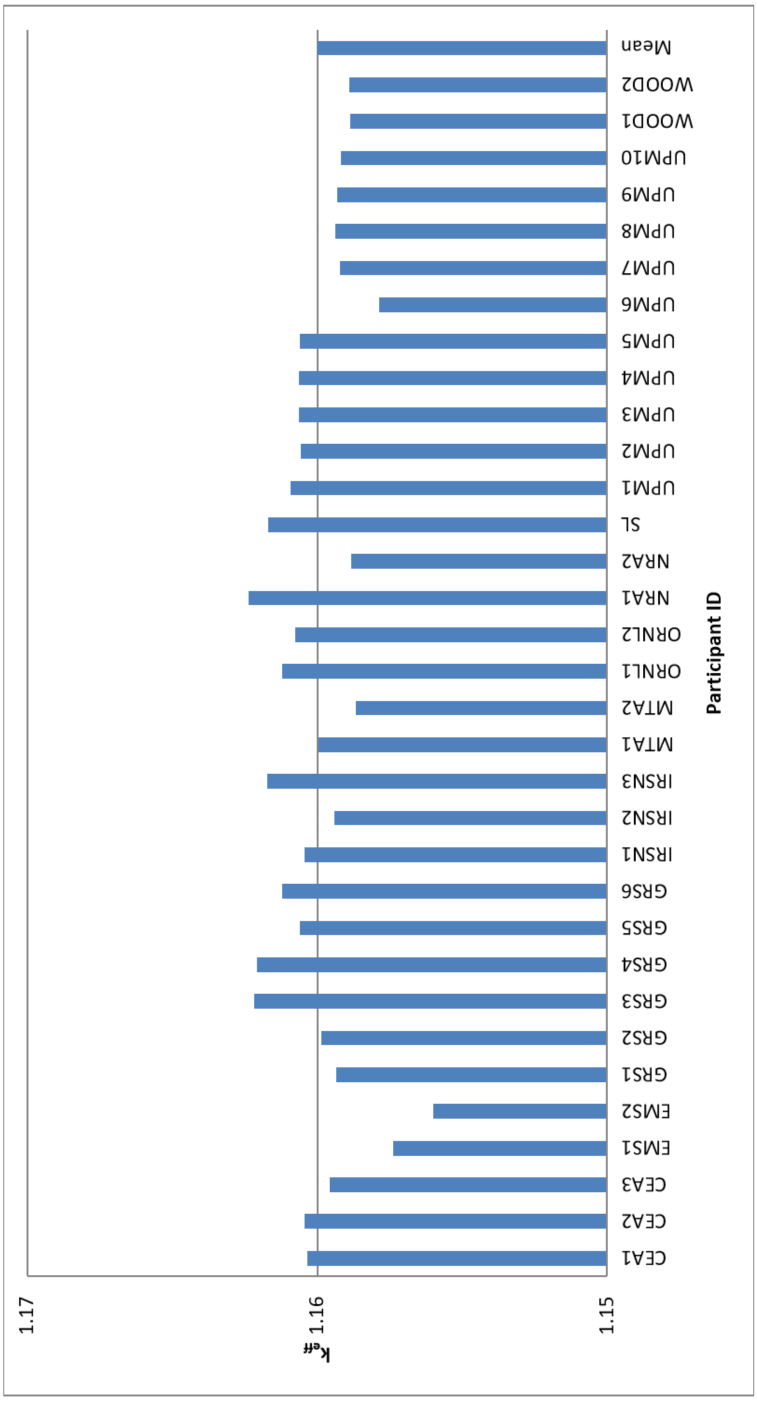
Source: NEA data, 2020.

Figure A.38. Participant results for case T588-INF-0



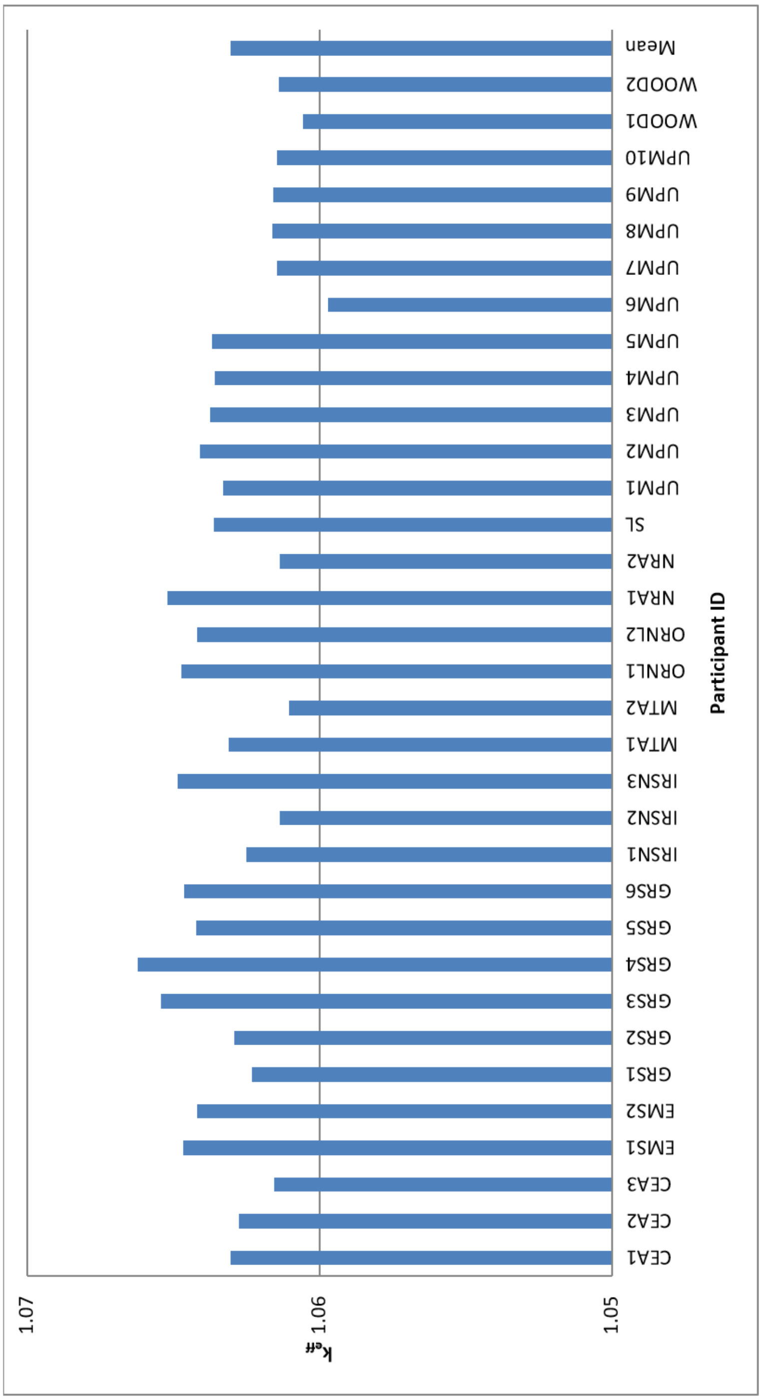
Source: NEA data, 2020.

Figure A.39. Participant results for case T588-INF-30



Source: NEA data, 2020.

Figure A.40. Participant results for case T588-INF-45



Source: NEA data, 2020.

Table A.11. Mean of participant results for each case type

	INF			SU		
	Burn-up (GWd/te)					
Temperature (K)	0	30	45	0	30	45
233	1.48082	1.22542	1.11717	0.90477	0.75459	0.68732
253	1.48004	1.22428	1.11650	0.90342	0.75302	0.68594
293	1.48700	1.23208	1.12405	0.92910	0.77449	0.70550
333	1.48393	1.22841	1.12125	0.92181	0.76799	0.69998
588	1.42146	1.16000	1.06303	0.79375	0.66109	0.60656

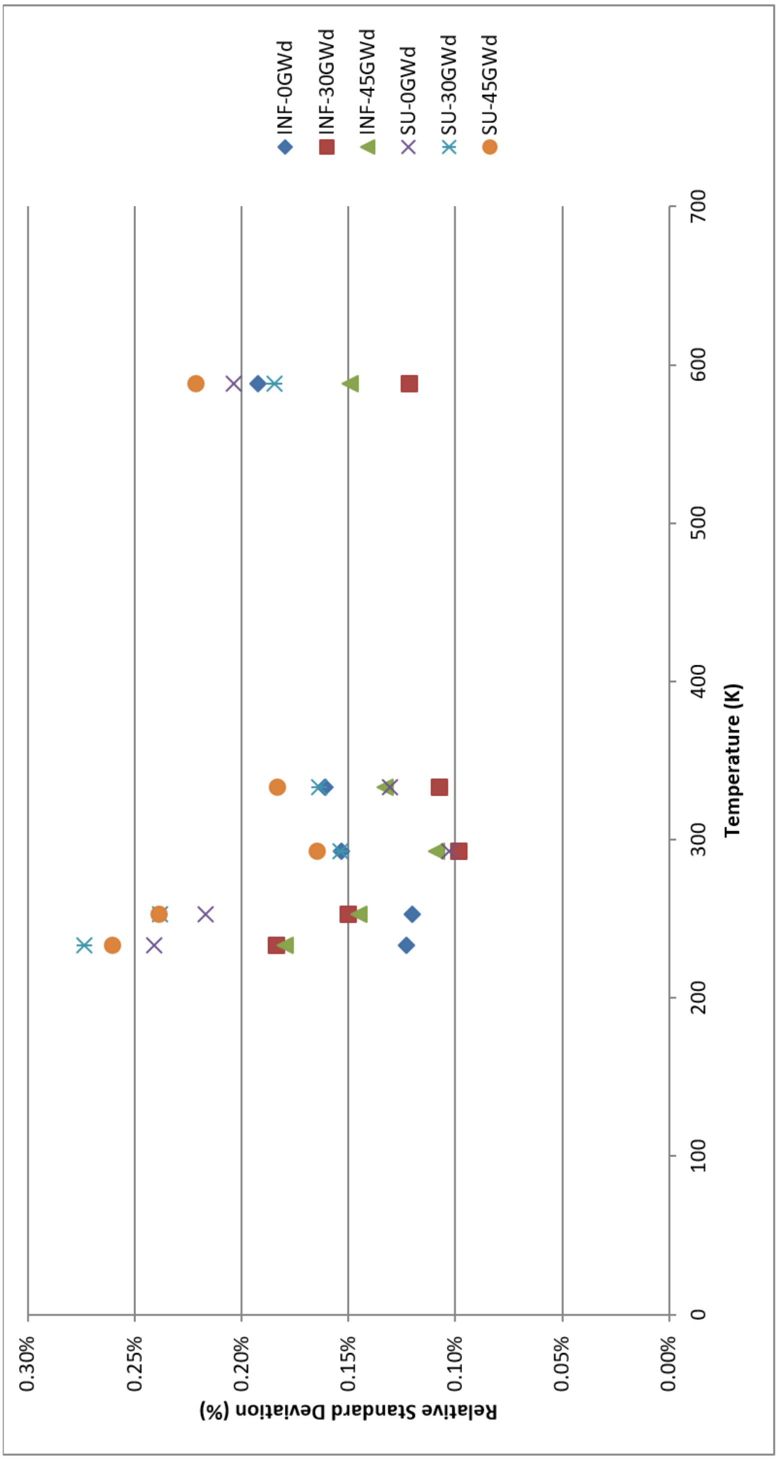
Source: NEA data, 2020.

Table A.12. Relative standard deviation (%) associated with participant results for each case type

	INF			SU		
	Burn-up (GWd/te)					
Temperature (K)	0	30	45	0	30	45
233	0.12%	0.18%	0.18%	0.24%	0.27%	0.26%
253	0.12%	0.15%	0.14%	0.22%	0.24%	0.24%
293	0.15%	0.10%	0.11%	0.10%	0.15%	0.16%
333	0.16%	0.11%	0.13%	0.13%	0.16%	0.18%
588	0.19%	0.12%	0.15%	0.20%	0.18%	0.22%

Source: NEA data, 2020.

Figure A.41. Graph of relative standard deviation (%) associated with participant results



Source: NEA data, 2020.

Table A.13. Mean result for each case type by nuclear data library

Case Type	Temperature (K)	Burn-up (GWd/te)	Data Library						
			ENDF/B-VII.1	ENDF/B-VIII.0	JEF 2.2	JEFF-3.1.1	JEFF-3.1.2	JEFF-3.3	JENDL-4.0
INF	233	0	1.47966	1.47950	-	-	1.48370	1.48176	1.48281
		30	1.22171	1.22632	-	-	1.22505	1.22641	1.22463
		45	1.11464	1.11855	-	-	1.11437	1.11764	1.11611
	253	0	1.47967	1.47842	-	-	1.48266	1.48090	1.48242
		30	1.22159	1.22491	-	-	1.22314	1.22505	1.22431
		45	1.11477	1.11763	-	-	1.11385	1.11678	1.11566
	293	0	1.48846	1.48434	1.49260	1.48872	1.48864	1.48679	1.48980
		30	1.23184	1.23243	1.23150	1.23068	1.23112	1.23208	1.23316
		45	1.12423	1.12477	1.12290	1.12145	1.12192	1.12404	1.12455
	333	0	1.48487	1.48144	1.49110	1.48550	1.48547	1.48394	1.48667
		30	1.22817	1.22895	1.22860	1.22705	1.22688	1.22820	1.22935
		45	1.12128	1.12226	1.11960	1.11879	1.11844	1.12103	1.12216
	588	0	1.42208	1.41823	1.42990	1.42254	1.42270	1.42308	1.42342
		30	1.15972	1.16039	1.16170	1.15871	1.15889	1.15971	1.16097
		45	1.06327	1.06421	1.06360	1.06063	1.06097	1.06197	1.06381
SU	233	0	0.90255	0.90380	-	-	0.90381	0.90788	0.90362
		30	0.75232	0.75423	-	-	0.75232	0.75723	0.75341
		45	0.68599	0.68705	-	-	0.68496	0.68949	0.68587
	253	0	0.90230	0.90213	-	-	0.90256	0.90629	0.90255
		30	0.75142	0.75241	-	-	0.75077	0.75544	0.75247
		45	0.68475	0.68561	-	-	0.68333	0.68802	0.68500
	293	0	0.92888	0.92889	0.92850	0.92822	0.92752	0.93046	0.92856
		30	0.77421	0.77491	0.77210	0.77282	0.77202	0.77549	0.77452
		45	0.70572	0.70588	0.70290	0.70352	0.70322	0.70644	0.70480
	333	0	0.92158	0.92153	0.92000	0.92119	0.92008	0.92342	0.92120
		30	0.76752	0.76840	0.76560	0.76662	0.76556	0.76903	0.76804
		45	0.70022	0.70042	0.69810	0.69820	0.69686	0.70087	0.69936
	588	0	0.79297	0.79359	0.79410	0.79266	0.79136	0.79600	0.79213
		30	0.66118	0.66165	0.65990	0.65943	0.65833	0.66162	0.66073
		45	0.60707	0.60745	0.60400	0.60445	0.60391	0.60656	0.60625

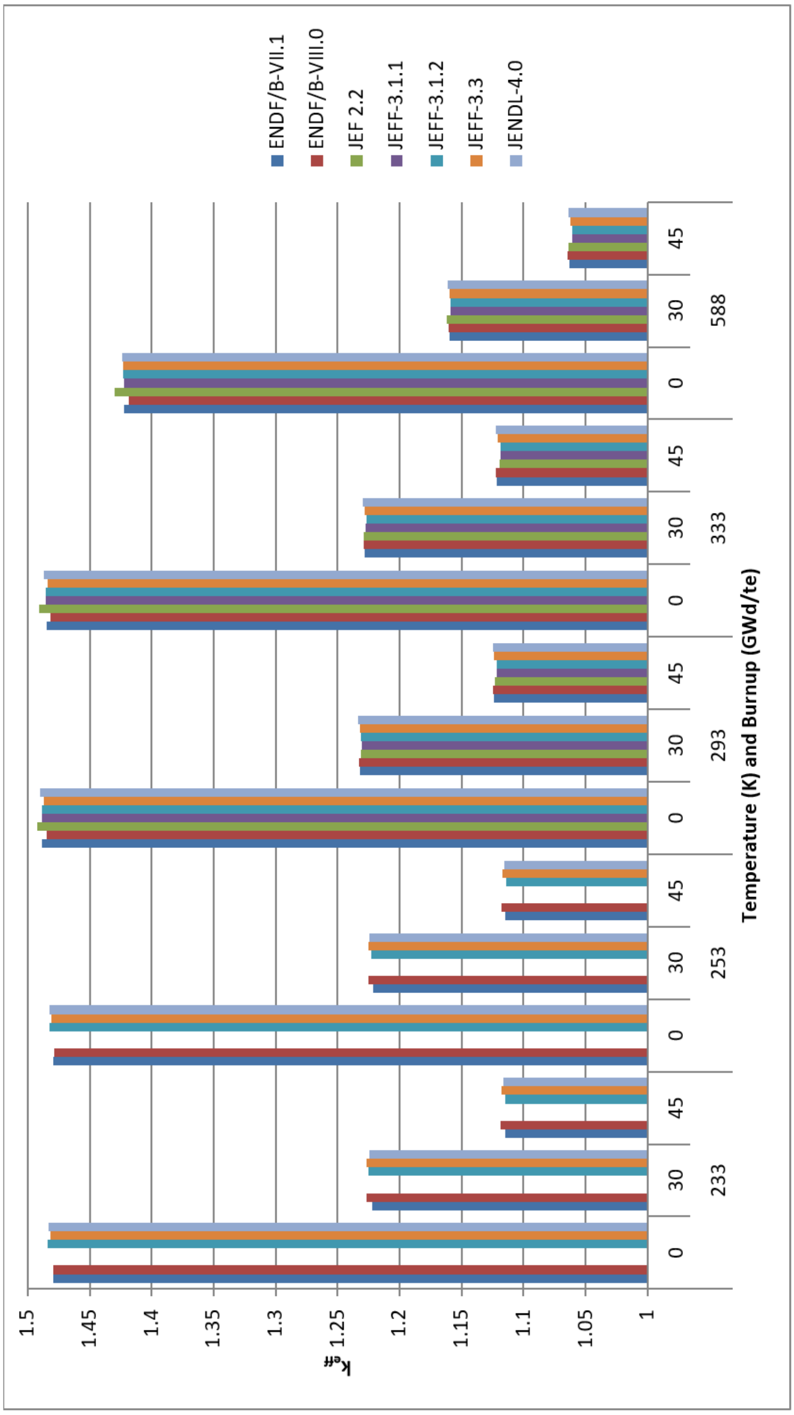
Source: NEA data, 2020.

Table A.14. Relative standard deviation (%) on each case per nuclear data library

			Data Library					
Case Type	Temperature (K)	Burn-up (GWd/te)	ENDF/B-VII.1	ENDF/B-VIII.0	JEFF-3.1.1	JEFF-3.1.2	JEFF-3.3	JENDL-4.0
INF	233	0	0.10%	0.08%	-	0.03%	0.02%	0.14%
		30	0.15%	0.14%	-	0.04%	0.03%	0.28%
		45	0.16%	0.09%	-	0.03%	0.04%	0.28%
	253	0	0.10%	0.05%	-	0.02%	0.02%	0.12%
		30	0.15%	0.11%	-	0.05%	0.03%	0.26%
		45	0.11%	0.06%	-	0.03%	0.04%	0.26%
	293	0	0.08%	0.03%	0.05%	0.03%	0.03%	0.03%
		30	0.13%	0.10%	0.05%	0.04%	0.04%	0.10%
		45	0.11%	0.04%	0.06%	0.00%	0.04%	0.14%
	333	0	0.12%	0.06%	0.04%	0.02%	0.02%	0.05%
		30	0.13%	0.12%	0.07%	0.01%	0.04%	0.11%
		45	0.13%	0.07%	0.09%	0.05%	0.04%	0.16%
	588	0	0.08%	0.03%	0.07%	0.02%	0.03%	0.08%
		30	0.14%	0.13%	0.10%	0.00%	0.05%	0.16%
		45	0.15%	0.08%	0.12%	0.06%	0.06%	0.20%
SU	233	0	0.06%	0.06%	-	0.10%	0.04%	0.25%
		30	0.16%	0.10%	-	0.07%	0.04%	0.33%
		45	0.11%	0.08%	-	0.04%	0.03%	0.44%
	253	0	0.08%	0.05%	-	0.03%	0.05%	0.18%
		30	0.14%	0.08%	-	0.04%	0.03%	0.25%
		45	0.05%	0.03%	-	0.02%	0.06%	0.37%
	293	0	0.05%	0.02%	0.02%	0.01%	0.08%	0.07%
		30	0.11%	0.09%	0.06%	0.02%	0.09%	0.07%
		45	0.08%	0.01%	0.06%	0.02%	0.07%	0.22%
	333	0	0.04%	0.03%	0.06%	0.00%	0.09%	0.20%
		30	0.11%	0.09%	0.10%	0.03%	0.10%	0.21%
		45	0.10%	0.05%	0.09%	0.08%	0.08%	0.26%
	588	0	0.09%	0.07%	0.07%	0.04%	0.12%	0.21%
		30	0.15%	0.11%	0.08%	0.06%	0.11%	0.23%
		45	0.19%	0.05%	0.08%	0.02%	0.12%	0.29%

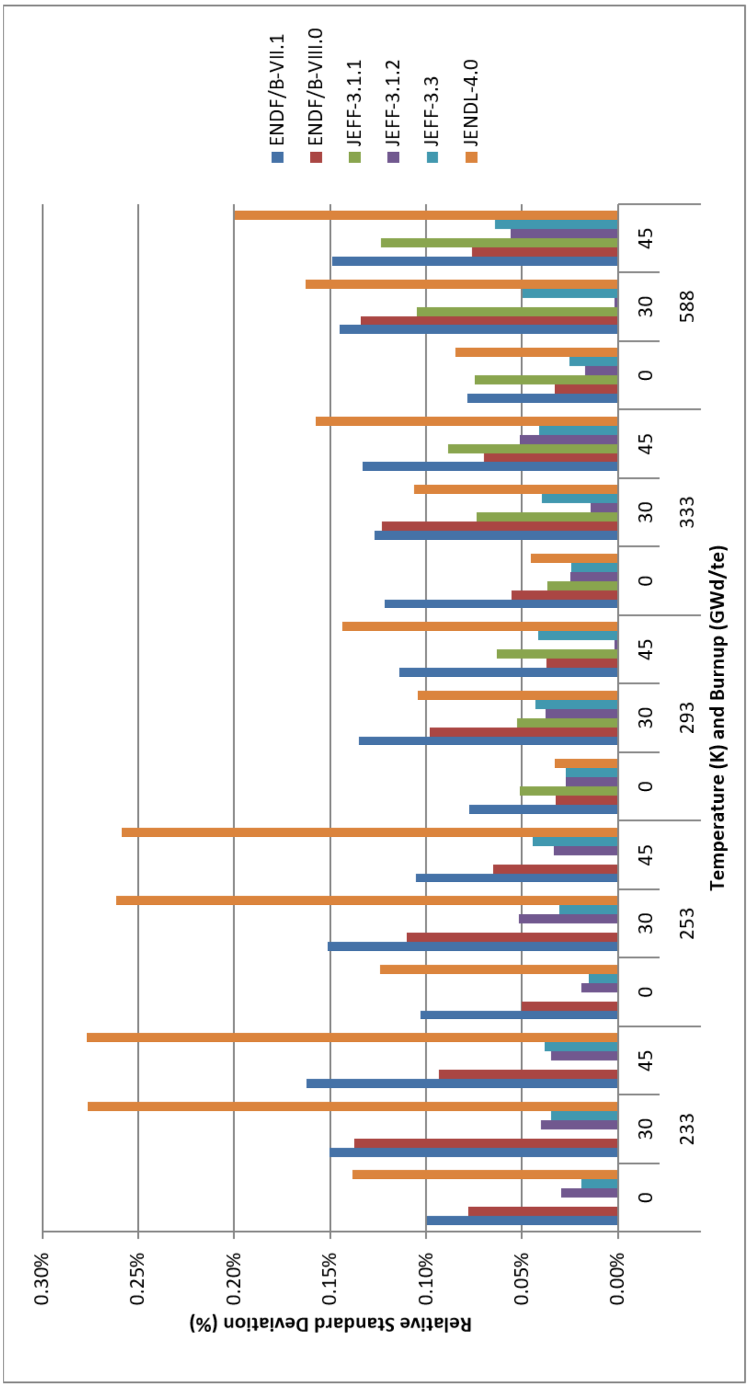
Source: NEA data, 2020.

Figure A.42. Graph of results for INF cases by nuclear data library



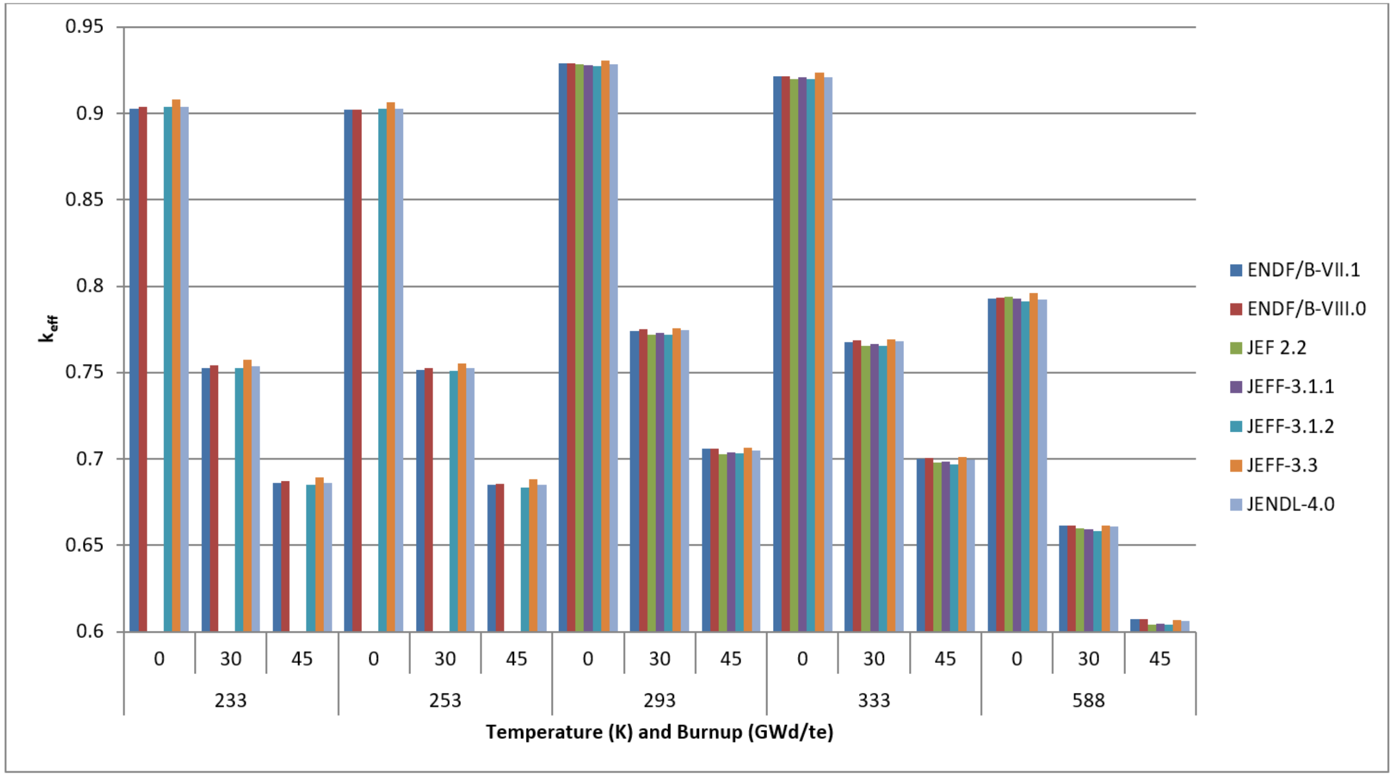
Source: NEA data, 2020.

Figure A.43. Graph of relative standard deviation (%) for INF cases by nuclear data



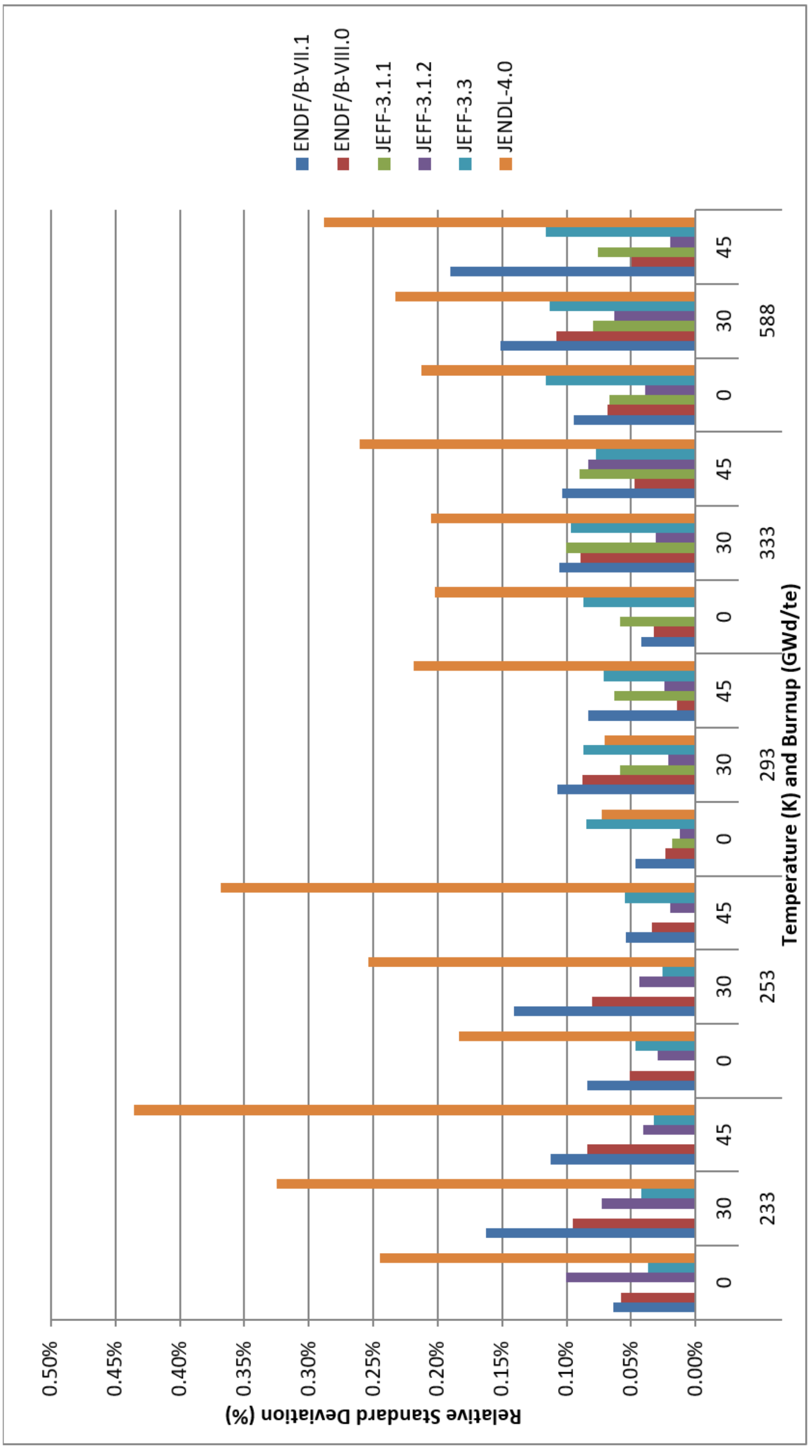
Source: NEA data, 2020.

Figure A.44. Graph of results for SU cases by nuclear data library



Source: NEA data, 2020.

Figure A.45. Graph of relative standard deviation (%) for SU cases by nuclear data library



Source: NEA data, 2020.

Table A.15. Mean result by use of bound H data (233K and 253K cases)

Temperature (K)	Case Type	Burn-up (GWd/te)	Bound H Data	
			H_1_H_2O	H_1_ICE
233	INF	0	1.48208	1.48513
		30	1.22434	1.2283
		45	1.11645	1.120403
	SU	0	0.90326	0.90839
		30	0.75363	0.75784
		45	0.68708	0.68977
253	INF	0	1.48178	1.48449
		30	1.22416	1.2277
		45	1.11578	1.118992
	SU	0	0.90301	0.90675
		30	0.75258	0.75574
		45	0.68529	0.68851

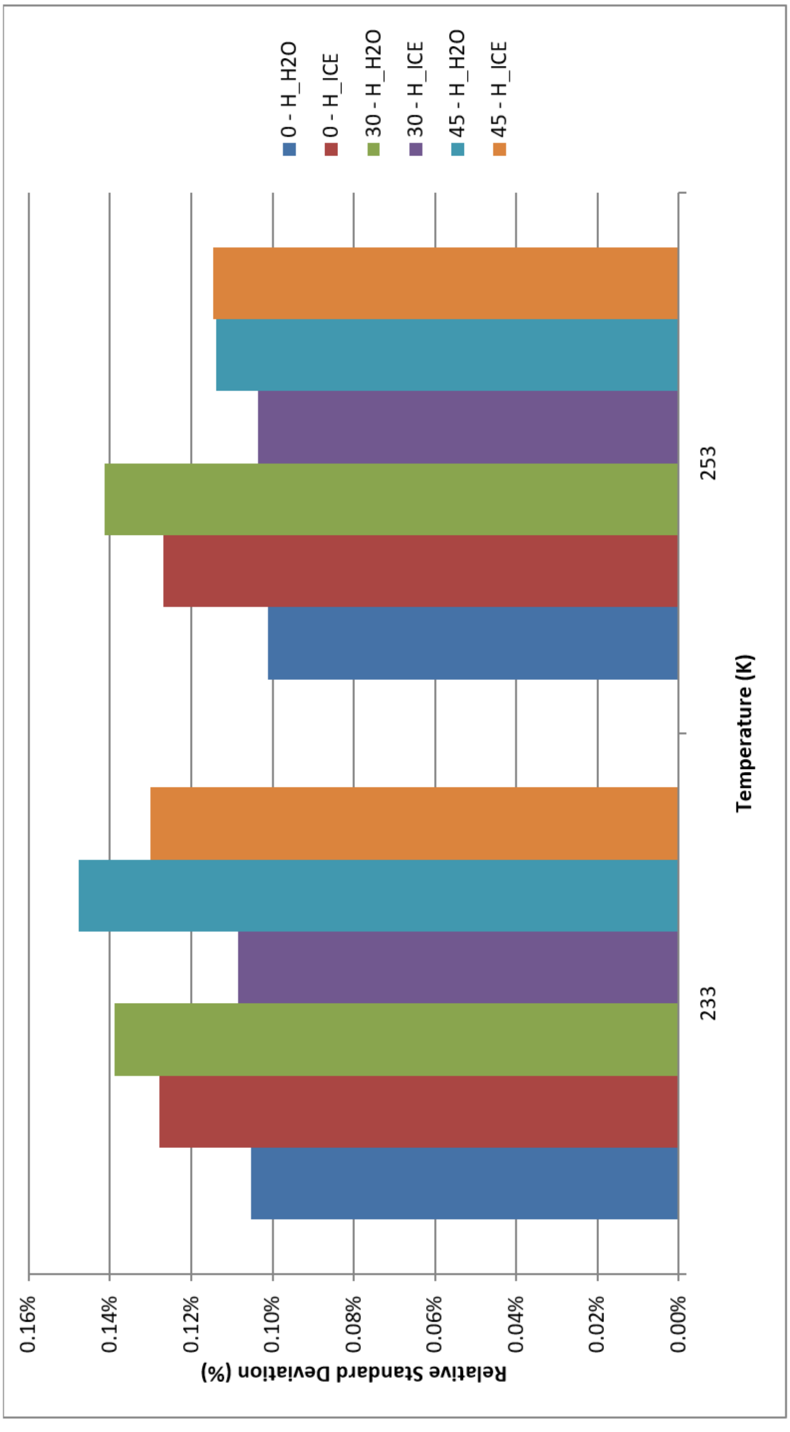
Source: NEA data, 2020.

Table A.16. Relative standard deviation (%) of result by use of bound H data (233K and 253K cases)

Temperature (K)	Case Type	Burn-up (GWd/te)	Bound H Data	
			H_1_H_2O	H_1_ICE
233	INF	**0**	0.11%	0.13%
		30	0.14%	0.11%
		45	0.15%	0.13%
	SU	**0**	0.07%	0.22%
		30	0.14%	0.24%
		45	0.20%	0.22%
253	INF	**0**	0.10%	0.13%
		30	0.14%	0.10%
		45	0.11%	0.11%
	SU	**0**	0.09%	0.23%
		30	0.13%	0.23%
		45	0.16%	0.22%

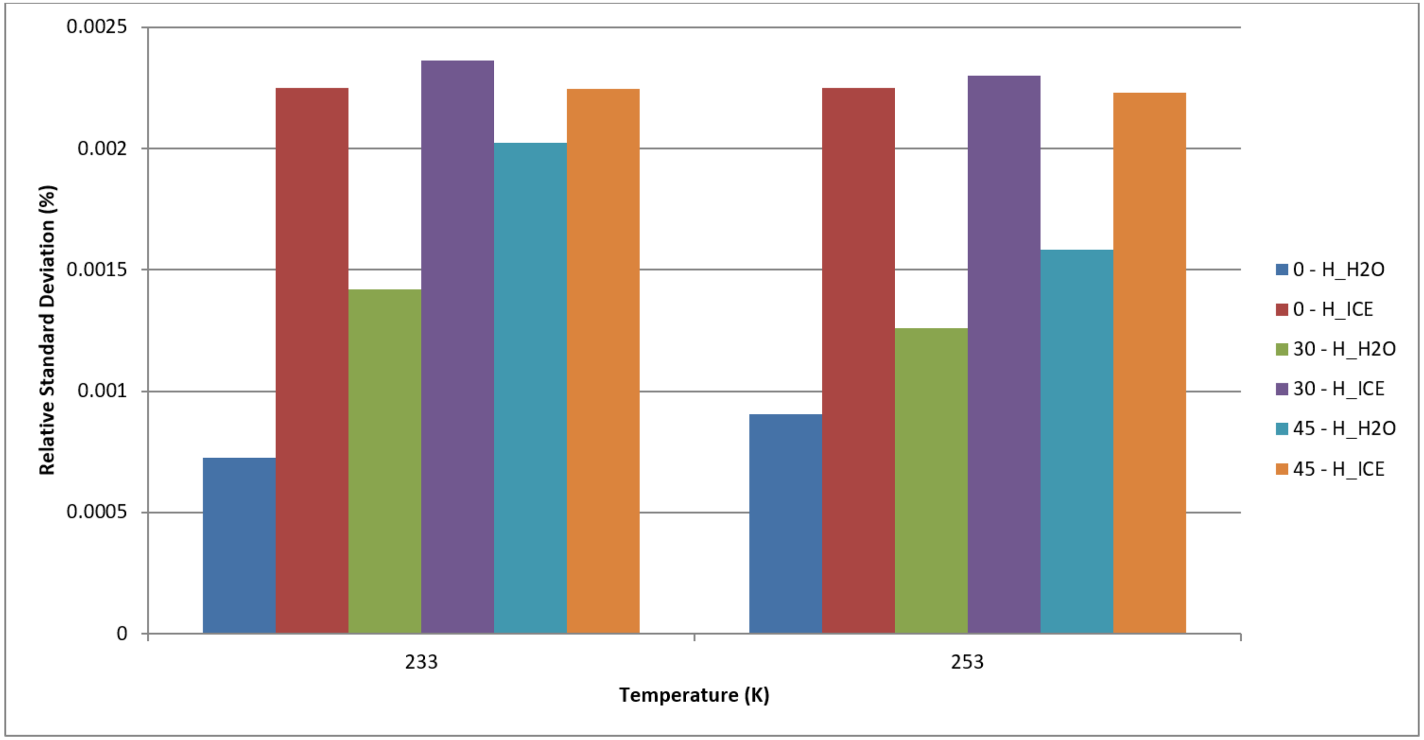
Source: NEA data, 2020.

Figure A.46. Relative standard deviation on result by burn-up and bound H (233K and 253K INF cases)



Source: NEA data, 2020.

Figure A.47. Standard deviation on result by bound H (233K and 253K SU cases)



Source: NEA data, 2020.

Table A.17. Mean result for INF cases where more than one code has used the same nuclear data library

	Temperature (K)	233			253			293			333			588		
	Burnup GWd/te	0	30	45	0	30	45	0	30	45	0	30	45	0	30	45
Data Library																
ENDF/B-VII.1	AVERAGE	1.47966	1.22171	1.11464	1.47967	1.22159	1.11477	1.48846	1.23184	1.12423	1.48487	1.22817	1.12128	1.42208	1.15972	1.06327
	MCNP 6.1							1.48909	1.23386	1.12516	1.48592	1.22985	1.12225	1.42272	1.16093	1.06329
	MCNP 6.1.1							1.48929	1.23161	1.12203	1.48662	1.22835	1.11975	1.42265	1.15866	1.06103
	MCNP 6.2							1.48906	1.22992	1.12497						
	SCALE 6.2.2	1.47917	1.22225	1.11420	1.47926	1.22219	1.11443	1.48758	1.23244	1.12397	1.48359	1.22814	1.12094	1.42145	1.16045	1.06354
	SCALE 6.2.3	1.48114	1.22011	1.11594	1.48088	1.21977	1.11578	1.48903	1.23018	1.12550	1.48590	1.22641	1.12286	1.42275	1.15739	1.06465
ENDF/B-VIII.0	AVERAGE	1.47950	1.22632	1.11855	1.47842	1.22491	1.11763	1.48434	1.23243	1.12477	1.48144	1.22895	1.12226	1.41823	1.16039	1.06421
	MCNP 6.1	1.47946	1.22655	1.11840	1.47839	1.22520	1.11738	1.48451	1.23294	1.12478	1.48128	1.22924	1.12191	1.41830	1.16073	1.06394
	MCNP 6.1.1	1.48146	1.22799	1.11944	1.47882	1.22569	1.11852	1.48417	1.23248	1.12462	1.48317	1.23047	1.12379	1.41781	1.15995	1.06312
	MCNP 6.2	1.47884	1.22228	1.11810	1.47852	1.22157	1.11759	1.48439	1.22895	1.12470	1.48087	1.22464	1.12161	1.41787	1.15598	1.06419
	OpenMC	1.48075	1.22800	1.11985	1.47871	1.22550	1.11780	1.48432	1.23251	1.12476	1.48159	1.22940	1.12264	1.41814	1.16061	1.06421
	SCALE 6.2.2	1.47788	1.22515	1.11670	1.47868	1.22466	1.11789	1.48481	1.23305	1.12561	1.48229	1.22957	1.12294	1.41940	1.16209	1.06621
	SCALE 6.2.3	1.47912	1.22666	1.11897	1.47798	1.22529	1.11760	1.48376	1.23256	1.12448	1.48075	1.22910	1.12216	1.41792	1.16099	1.06447
JEFF-3.1.1	AVERAGE							1.48872	1.23068	1.12145	1.48550	1.22705	1.11879	1.42254	1.15871	1.06063
	MCNP 6.1							1.48818	1.23022	1.12095	1.48511	1.22641	1.11809	1.42179	1.15785	1.05970

Source: NEA data, 2020.

Table A.17. Mean result for INF cases where more than one code has used the same nuclear data library (cont.)

	Tripoli 4.9							1.48926	1.23114	1.12195	1.48588	1.22769	1.11949	1.42329	1.15957	1.06155
JEFF-3.1.2	**AVERAGE**	1.48370	1.22505	1.11437	1.48266	1.22314	1.11385	1.48864	1.23112	1.12192	1.48547	1.22688	1.11844	1.42270	1.15889	1.06097
	MONK 10B	1.48401	1.22470	1.11409	1.48286	1.22269	1.11358	1.48835	1.23145	1.12193	1.48521	1.22675	1.11803	1.42252	1.15887	1.06055
	MONK 11 (Dev)	1.48339	1.22540	1.11464	1.48246	1.22358	1.11411	1.48892	1.23079	1.12190	1.48573	1.22700	1.11884	1.42287	1.15890	1.06139
JEFF-3.3	**AVERAGE**	1.48176	1.22641	1.11764	1.48090	1.22505	1.11678	1.48679	1.23208	1.12404	1.48394	1.22820	1.12103	1.42308	1.15971	1.06197
	MCNP 6.1	1.48154	1.22603	1.11728	1.48078	1.22474	1.11635	1.48656	1.23165	1.12364	1.48364	1.22783	1.12064	1.42282	1.15927	1.06152
	MORET 5.D.1	1.48207	1.22667	1.11791	1.48101	1.22524	1.11741	1.48697	1.23268	1.12437	1.48425	1.22832	1.12121	1.42323	1.15992	1.06193
	Tripoli 4	1.48186	1.22699	1.11791	1.48081	1.22539	1.11709	1.48681	1.23204	1.12441	1.48404	1.22866	1.12177	1.42326	1.16034	1.06305
	Tripoli 4.9	1.48192	1.22685	1.11831	1.48123	1.22559	1.11694	1.48734	1.23261	1.12461	1.48440	1.22895	1.12153	1.42361	1.16043	1.06276
JENDL-4.0	**AVERAGE**	1.48281	1.22463	1.11611	1.48242	1.22431	1.11566	1.48980	1.23316	1.12455	1.48667	1.22935	1.12216	1.42342	1.16097	1.06381
	MORET 5.D.1	1.48513	1.22830	1.11931	1.48449	1.22770	1.11863	1.49005	1.23381	1.12559	1.48724	1.22995	1.12358	1.42384	1.16171	1.06485
	MVP3	1.48208	1.22396	1.11586	1.48178	1.22390	1.11549	1.49011	1.23400	1.12537	1.48685	1.23024	1.12273	1.42436	1.16237	1.06521
	CASMO5	1.48122	1.22163	1.11315	1.48099	1.22134	1.11287	1.48923	1.23168	1.12269	1.48593	1.22785	1.12018	1.42206	1.15882	1.06136

Source: NEA data, 2020.

Table A.18. Mean result for SU cases where more than one code has used the same nuclear data library

	Temperature (K)	233			253			293			333			588		
	Burnup GWd/te	0	30	45	0	30	45	0	30	45	0	30	45	0	30	45
Data Library																
ENDF/B-VII.1	AVERAGE	0.90255	0.75232	0.68599	0.90230	0.75142	0.68475	0.92888	0.77421	0.70572	0.92158	0.76752	0.70022	0.79297	0.66118	0.60707
	MCNP 6.1							0.92883	0.77482	0.70595	0.92161	0.76847	0.70045	0.79316	0.66112	0.60649
	MCNP 6.1.1							0.92936	0.77455	0.70451	0.92185	0.76710	0.69885	0.79361	0.66091	0.60546
	MCNP 6.2							0.92874	0.77297	0.70578						
	SCALE 6.2.2	0.90250	0.75283	0.68605	0.90241	0.75189	0.68463	0.92879	0.77469	0.70593	0.92155	0.76778	0.70041	0.79284	0.66180	0.60783
	SCALE 6.2.3	0.90269	0.75079	0.68579	0.90197	0.75001	0.68509	0.92890	0.77306	0.70599	0.92134	0.76621	0.70077	0.79255	0.65966	0.60699
ENDF/B-VIII.0	AVERAGE	0.90380	0.75423	0.68705	0.90213	0.75241	0.68561	0.92889	0.77491	0.70588	0.92153	0.76840	0.70042	0.79359	0.66165	0.60745
	MCNP 6.1	0.90378	0.75431	0.68699	0.90199	0.75252	0.68554	0.92886	0.77507	0.70589	0.92160	0.76865	0.70056	0.79390	0.66199	0.60741
	MCNP 6.1.1	0.90362	0.75444	0.68738	0.90294	0.75257	0.68542	0.92893	0.77477	0.70586	0.92218	0.76885	0.70077	0.79318	0.66142	0.60727
	MCNP 6.2	0.90368	0.75235	0.68704	0.90231	0.75079	0.68560	0.92891	0.77313	0.70590	0.92108	0.76643	0.70032	0.79286	0.65975	0.60733
	OpenMC	0.90463	0.75502	0.68791	0.90216	0.75260	0.68587	0.92872	0.77474	0.70571	0.92136	0.76838	0.70039	0.79317	0.66147	0.60694
	SCALE 6.2.2	0.90259	0.75389	0.68565	0.90138	0.75223	0.68542	0.92917	0.77599	0.70600	0.92152	0.76874	0.69959	0.79316	0.66133	0.60789
	SCALE 6.2.3	0.90421	0.75464	0.68729	0.90233	0.75286	0.68584	0.92889	0.77504	0.70585	0.92135	0.76837	0.70040	0.79384	0.66213	0.60777
JEFF-3.1.1	AVERAGE							0.92822	0.77282	0.70352	0.92119	0.76662	0.69820	0.79266	0.65943	0.60445
	MCNP 6.1							0.92810	0.77250	0.70320	0.92081	0.76607	0.69775	0.79228	0.65906	0.60412

Source: NEA data, 2020.

Table A.18. Mean result for SU cases where more than one code has used the same nuclear data library (cont.)

	Tripoli 4.9							0.92834	0.77314	0.70383	0.92157	0.76716	0.69864	0.79303	0.65980	0.60477
JEFF-3.1.2	AVERAGE	0.90381	0.75232	0.68496	0.90256	0.75077	0.68333	0.92752	0.77202	0.70322	0.92008	0.76556	0.69686	0.79136	0.65833	0.60391
	MONK 10B	0.90317	0.75193	0.68515	0.90237	0.75100	0.68323	0.92760	0.77190	0.70310	0.92007	0.76572	0.69645	0.79114	0.65803	0.60399
	MONK 11 (Dev)	0.90445	0.75270	0.68476	0.90274	0.75054	0.68342	0.92744	0.77213	0.70334	0.92008	0.76539	0.69727	0.79158	0.65862	0.60382
JEFF-3.3	AVERAGE	0.90788	0.75723	0.68949	0.90629	0.75544	0.68802	0.93046	0.77549	0.70644	0.92342	0.76903	0.70087	0.79600	0.66162	0.60656
	MCNP 6.1	0.90784	0.75704	0.68942	0.90622	0.75538	0.68785	0.93005	0.77503	0.70604	0.92302	0.76859	0.70048	0.79555	0.66119	0.60610
	MORET 5.D.1	0.90772	0.75721	0.68944	0.90602	0.75532	0.68798	0.93111	0.77621	0.70705	0.92436	0.76985	0.70146	0.79697	0.66249	0.60738
	Tripoli 4	0.90786	0.75742	0.68961	0.90675	0.75567	0.68832	0.93071	0.77561	0.70675	0.92311	0.76903	0.70087	0.79554	0.66149	0.60667
	Tripoli 4.9	0.90839	0.75784	0.68977	0.90662	0.75574	0.68845	0.93056	0.77577	0.70653	0.92347	0.76914	0.70130	0.79631	0.66172	0.60667
JENDL-4.0	AVERAGE	0.90362	0.75341	0.68587	0.90255	0.75247	0.68500	0.92856	0.77452	0.70480	0.92120	0.76804	0.69936	0.79213	0.66073	0.60625
	MORET 5.D.1	0.90603	0.75610	0.68887	0.90425	0.75450	0.68737	0.92795	0.77417	0.70516	0.91969	0.76699	0.69912	0.79095	0.66007	0.60590
	MVP3	0.90167	0.75131	0.68290	0.90095	0.75071	0.68235	0.92845	0.77423	0.70311	0.92062	0.76727	0.69767	0.79139	0.65964	0.60470
	CASMO5	0.90317	0.75281	0.68585	0.90246	0.75219	0.68529	0.92929	0.77515	0.70613	0.92328	0.76985	0.70129	0.79406	0.66249	0.60814

Source: NEA data, 2020.

Appendix B. Description of the calculation method used by the participants

1) CEA1

Institute and country:

CEA-Saclay, France.

Participants:

Yi-Kang Lee.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

TRIPOLI-4.

Number of neutron energy group:

Continuous energy.

Description of your code system:

TRIPOLI-4 Monte Carlo transport code.

Description of any preparation methods used to generate the results:

GALILEE nuclear data processing system was used to generate library for TRIPOLI-4 criticality calculations.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293L, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Interpolation option of TRIPOLI-4 was used.

Any results omitted:

No.

2) CEA2

Institute and country:

CEA-Cadarache, France.

Participants:

Marion Tiphine and Coralie Carmouze.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

TRIPOLI-4.

Number of neutron energy group:

Continuous energy.

Description of your code system:

TRIPOLI-4.11 Monte Carlo transport code.

Description of any preparation methods used to generate the results:

The JEFF-3.3 nuclear data evaluation has been used and data has been processed with GALILEE V0-3.2 for cross-sections computations and CALENDF to generate the probability tables.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Hydrogen data were available at 233K and 253K. At 293K, 333K and 588K, nearest point data were used for hydrogen:

294K for the 293K calculation.

324K for the 333K calculation.

574K for the 588K calculation.

Any results omitted:

No.

3) CEA3

Institute and country:

CEA-Cadarache, France.

Participants:

Marion Tiphine and Coralie Carmouze.

Neutron data library:

JEFF-3.1.1.

Neutron data processing code or method:

TRIPOLI-4.

Number of neutron energy group:

Continuous energy.

Description of your code system:

TRIPOLI-4.11 Monte Carlo transport code.

Description of any preparation methods used to generate the results:

The JEFF-3.1.1 nuclear data evaluation has been used and data has been processed with GALILEE V0-3.0.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Hydrogen data were available at 233K and 253K. At 293K, 333K and 588K, nearest point data were used for hydrogen:

294K for the 293K calculation.

324K for the 333K calculation.

574K for the 588K calculation.

Any results omitted:

No.

4) IRSN1

Institute and country:

Institut de Radioprotection et de Sûreté Nucléaire, France.

Participants:

Nicolas Leclaire and Mathieu Milin.

Neutron data library:

JEFF-3.3 evaluation is used for all elements.

Neutron data processing code or method:

MORET 5.D.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MORET 5.D.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

The JEFF-3.3 nuclear data library was used for all elements at the temperatures indicated in the benchmark.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Hydrogen data were available at 233K, 253K and 293K. At 333K and 588K, nearest point data were used for hydrogen:

323.6K for the 333K calculation.

573.6K for the 588K calculation.

Any results omitted:

No.

5) IRSN2

Institute and country:

Institut de Radioprotection et de Sûreté Nucléaire, France.

Participants:

Nicolas Leclaire and Mathieu Milin.

Neutron data library:

JEFF-3.3 except for hydrogen and its S(α,β) thermal scattering cross sections for which the ENDF/B-VIII.0 evaluation is used.

Neutron data processing code or method:

MORET 5.D.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MORET 5.D.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

The JEFF-3.3 nuclear data library was used for all elements at the temperatures indicated in the benchmark. As a result, the IRSN GAIA 1.1.1 tool based on NJOY2016.35 was used to process the ENDF files (cross-sections + thermal scattering data) at these temperatures and generate ACE formatted files for use in the Monte Carlo calculation.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Hydrogen data were available at 233K, 253K and 293K. At 333K and 588K, nearest point data were used for hydrogen:

323.6K for the 333K calculation.

573.6K for the 588K calculation.

Any results omitted:

No.

6) IRSN3

Institute and country:

Institut de Radioprotection et de Sûreté Nucléaire, France.

Participants:

Nicolas Leclaire and Mathieu Miln.

Neutron data library:

JENDL-4.0 with Hydrogen in ice S(α,β)data from JEFF-3.3.

Neutron data processing code or method:

MORET 5.D.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MORET 5.D.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

The IRSN GAIA 1.1.1 tool based on NJOY2016.35 was used to process the ENDF files (cross-sections and thermal scattering data) at these temperatures and generate ACE formatted files for use in the Monte Carlo calculation.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE from JEFF-3.3.

A brief description of any steps taken to provide temperature correction:

As thermal scattering data of hydrogen in water are only available at 296K, 350K, 400K, 450K, 500K and 600K, the data of 350K and 600K were used by the MORET 5.D.1 code, respectively for experiments at 333K and 588K. No interpolation is therefore performed.

Any results omitted:

No.

7) GRS1

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VII.1.

Neutron data processing code or method:

SCALE 6.2.2.

Number of neutron energy group:

56 energy groups.

Description of your code system:

SCALE 6.2.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction and temperature correction for $S(\alpha,\beta)$ thermal scattering.

Any results omitted:

No.

8) GRS2

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VII.1.

Neutron data processing code or method:

SCALE 6.2.2.

Number of neutron energy group:

252 energy groups.

Description of your code system:

SCALE 6.2.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction and temperature correction for S(α,β) thermal scattering.

Any results omitted:

No.

9) GRS3

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VII.1.

Neutron data processing code or method:

SCALE 6.2.2.

Number of neutron energy group:

Continuous energy.

Description of your code system:

SCALE 6.2.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction and temperature correction for S(α,β) thermal scattering.

Any results omitted:

No.

10) GRS4

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

SCALE 6.2.2.

Number of neutron energy group:

Continuous energy.

Description of your code system:

SCALE 6.2.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

Processed from ENDF files using the AMPX-Package delivered with SCALE6.2.2.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE (ENDF-BVIII.0) for 233K and 253K.

H1_H_2O (ENDF-BVII.1) for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction and temperature correction for S(α,β) thermal scattering.

Any results omitted:

No.

11) GRS5

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

OpenMC.

Number of neutron energy group:

Continuous energy.

Description of your code system:

OpenMC Monte Carlo code.

Description of any preparation methods used to generate the results:

HDF-5 format library converted from original Ace-library using python script provided by OpenMC distribution.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction, and temperature interpolation for the resolved and unresolved temperature ranges along with temperature correction for $S(\alpha,\beta)$ thermal scattering.

Any results omitted:

No.

12) GRS6

Institute and country:

Gesellschaft für Anlagen- und Reaktorsicherheit, Germany.

Participants:

Fabian Sommer, Matthias Behler and Volker Hannstein.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MCNP 6.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Doppler broadening correction and temperature correction for S(α,β) thermal scattering using nearest temperature point.

Any results omitted:

No.

13) MTA1

Institute and country:

Centre for Energy Research, Hungarian Academy of Sciences, Hungary.

Participants:

Gabor Hordosy.

Neutron data library:

ENDF/B-VIII.0.

Neutron data processing code or method:

MCNP 6.1.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MCNP 6.1.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

^{238}U thermal scattering the nearest table or interpolation from two calculations was used, details given bellow. All other cross-section tables were prepared by makxsf for the required temperature.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

As for low temperature, there are thermal scattering data for ice for 233K and 253K. Isotopic cross-sections are given for 0.1K and 250K. For 233K, two k_{eff} calculations were performed using the 0.1K and the 250K ^{238}U data, and the results were interpolated to 233K.

For higher temperatures, the isotopic cross-sections are given for 293K and 600K, the thermal scattering data are given in ~25K steps. For ^{238}U cross-sections the tables given for 293K were used in the cases of 293K and 333K, and the tables given for 600K were used in the cases of 588K. Other isotopic cross-sections were prepared by makxsf. For the cases of 333K two calculations were performed by the nearest $S(\alpha,\beta)$ tables, and the results were interpolated to 333K. Similar procedure was used for 588K.

Any results omitted:

No.

14) MTA2

Institute and country:

Centre for Energy Research, Hungarian Academy of Sciences, Hungary.

Participants:

Gabor Hordosy.

Neutron data library:

ENDF/B VII.

Neutron data processing code or method:

MCNP 6.1.1.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MCNP 6.1.1 Monte Carlo code.

Description of any preparation methods used to generate the results:

Data prepared using makxsf.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

There is no thermal scattering data for ice, so only the cases with 293K, 333K and 588K temperature were investigated. For room temperature the libraries for 293K or 300K were used. For 333K and 588K the libraries were prepared by the makxsf utility distributed together by MCNP. makxsf Doppler broadens the resolved resonance data to a higher temperature, interpolates any unresolved resonance probability tables to the new temperature and interpolates $S(\alpha,\beta)$ thermal scattering kernel data to the new temperature.

For 333K and 588K the isotopic cross-sections were prepared from the libraries made for 300K and 600K, and the thermal scattering data were prepared from the libraries made for 293K and 350K, or 550K and 600K, respectively.

Any results omitted:

233K and 253K.

15) NRA1

Institute and country:

Nuclear Regulation Authority, Japan.

Participants:

Shigeki Shiba and Toshisha Yamamoto.

Neutron data library:

JENDL-4.0.

Neutron data processing code or method:

MVP3.

Number of neutron energy group:

Continuous energy.

Description of your code system:

Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

-

Any results omitted:

No.

16) NRA2

Institute and country:

Nuclear Regulation Authority, Japan.

Participants:

Shigeki Shiba and Toshisha Yamamoto.

Neutron data library:

JENDL-4.0.

Neutron data processing code or method:

CASMO5.

Number of neutron energy group:

19 Groups.

Description of your code system:

Deterministic Code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

-

Any results omitted:

No.

17) UPM1

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

ENDF/B VII.1.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

128 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 32 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K interpolated from 323.6K and 573.6K using IAEA/Barioloche TSL library generation.

Any results omitted:

233K and 253K.

18) UPM2

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

128 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 32 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K interpolated from 323.6K and 573.6K using IAEA/Barioloche TSL library generation.

Any results omitted:

No.

19) UPM3

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

64 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 16 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

20) UPM4

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

256 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 64 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

21) UPM5

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

ENDF/B VIII.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

512 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 64 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

22) UPM6

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

JEFF-3.1.1.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

128 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 32 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

233K and 253K.

23) UPM7

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

128 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 32 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

24) UPM8

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

64 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 16 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

25) UPM9

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

256 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 64 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

26) UPM10

Institute and country:

University of Madrid, Spain.

Participants:

Oscar Cabellos.

Neutron data library:

JEFF-3.3.

Neutron data processing code or method:

MCNP 6.1.

Number of neutron energy group:

512 energy groups.

Description of your code system:

MCNP 6.1 Monte Carlo code, 64 angular groups.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

Results for 333K and 588K generated using nearest temperature points 323.6K and 573.6K respectively.

Any results omitted:

No.

27) EMS1

Institute and country:

E Mennerdahl Solutions, Sweden.

Participants:

Dennis Mennerdahl.

Neutron data library:

ENDF/B-VII.1.

Neutron data processing code or method:

SCALE 6.2.3 Monte Carlo code.

Number of neutron energy group:

Continuous energy.

Description of your code system:

SCALE 6.2.3 CSAS5 (KENO Va) with ENDF/B-VII.1 continuous-energy cross-sections were used to calculate all cases.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O.

A brief description of any steps taken to provide temperature correction:

The built-in (default option, DBX=2) Doppler broadening of cross-sections were used.

The SCALE 6.2.3 calculations were made with default values and temperatures as specified.

Any results omitted:

No.

28) EMS2

Institute and country:

E Mennerdahl Solutions, Sweden.

Participants:

Dennis Mennerdahl.

Neutron data library:

ENDF/B-VIII.0.

Neutron data processing code or method:

MCNP 6.2.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MCNP6.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K, 588K.

A brief description of any steps taken to provide temperature correction:

The MCNP6.2 calculations were made with “pseudo materials”, i.e. weighted mixtures of the cross-sections at the two nearest library temperatures. The weighting follows the procedure established by Conlin, Brown and Mosteller in LANL-UR-05-6225.

The MCNP6.2 thermal scattering data, i.e. $S(\alpha,\beta)$ for four of the six temperatures 233K, 253K, 293K (very close to 294K), 333K, 450K and 588K were directly available in the ENDF/B-VIII.0 library. For each of the two temperatures 333K and 588K, two MCNP6.2 calculations were with the nearest library temperatures (324K + 350K and 574K + 600K respectively).

Any results omitted:

No.

29) EMS3

Institute and country:

E Mennerdahl Solutions, Sweden.

Participants:

Dennis Mennerdahl.

Neutron data library:

ENDF/B-VII.1.

Neutron data processing code or method:

MCNP 6.2.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MCNP6.2 Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O for 293K.

A brief description of any steps taken to provide temperature correction:

-

Any results omitted:

233K, 253K, 333K and 588K.

30) SL

Institute and country:

Sellafield Ltd, United Kingdom.

Participants:

James Ryan.

Neutron data library:

JEF-2.2.

Neutron data processing code or method:

MONK 9A.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MONK 9A Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_H_2O for 293K, 333K and 588K.

A brief description of any steps taken to provide temperature correction:

-

Any results omitted:

233K and 253K.

31) WOOD1

Institute and country:

Wood, United Kingdom.

Participants:

David Hanlon.

Neutron data library:

JEFF-3.1.2.

Neutron data processing code or method:

MONK 10B.

Number of neutron energy group:

Continuous energy.

Description of your code system:

MONK 10B Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K and 588K.

A brief description of any steps taken to provide temperature correction:

MONK10B Release Update 0: S(α,β) thermal scattering data for water or ice were used, with the code choosing the closest temperature data available on the library to that requested in the calculation input. Bound nuclides H1_H_2O (^{1}H in light water), H1_ICE (^{1}H bound in ice) and O_ICE (^{16}O bound in ice) all have S(α,β) tabulations at 193.0, 233.0, 263.0, 273.15, and 293.6K, plus higher temperatures. Exceptions to this are H1_H_2O, which has a minimum available temperature of 273.15K, and H_ICE/O_ICE, which has a maximum available temperature 273.15K.

For both MONK10B Release Update 0 and MONK11 Dev: The built-in default option is for the code to perform Run-time Doppler Broadening (RDB) of cross-sections to the requested input temperature if this is more than 0.5K away from a library temperature. If within 0.5K then the library temperature data are used. Available library temperatures are 193.0, 233.0, 263.0, 273.15, 293.6, 500.0, 1 000.0, 1 500.0, 2 000.0, 3 500.0, 5 000.0, 10 000.0, 20 000.0, 40 000.0 and 80 000.0K.

Any results omitted:

No.

32) WOOD2

Institute and country:

Wood, United Kingdom.

Participants:

David Hanlon.

Neutron data library:

JEFF-3.1.2.

Neutron data processing code or method:

MONK 11 (Dev).

Number of neutron energy group:

Continuous energy.

Description of your code system:

MONK 11 Development version Monte Carlo code.

Description of any preparation methods used to generate the results:

-

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K and 588K.

A brief description of any steps taken to provide temperature correction:

MONK11 Dev: S(α,β) thermal scattering data for water or ice were used with stochastic interpolation of the data to the temperature requested in the calculation input.

For both MONK10B Release Update 0 and MONK11 Dev: The built-in default option is for the code to perform Run-time Doppler Broadening (RDB) of cross-sections to the requested input temperature if this is more than 0.5K away from a library temperature. If within 0.5K then the library temperature data are used. Available library temperatures are 193.0, 233.0, 263.0, 273.15, 293.6, 500.0, 1 000.0, 1 500.0, 2 000.0, 3 500.0, 5 000.0, 10 000.0, 20 000.0, 40 000.0 and 80 000.0K.

Any results omitted:

No.

33) ORNL1

Institute and country:

Oak Ridge National Laboratories, United States.

Participants:

BJ Marshall, D Bowen and B Rearden.

Neutron data library:

ENDF/B-VIII.

Neutron data processing code or method:

SCALE 6.2.3.

Number of neutron energy group:

Continuous energy.

Description of your code system:

SCALE 6.2.3 Monte Carlo code.

Description of any preparation methods used to generate the results:

AMPX was used to generate a library based on the ENDF files.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K and 588K.

A brief description of any steps taken to provide temperature correction:

Doppler broadening methods for continuous-energy calculations are described. 1D and 2D data were broadened to the requested temperature, unless that temperature was within +/- 4K of a library temperature. Thus H1_ICE is not broadened since it is evaluated explicitly at 233.15K and 255.15K in ENDF/B-VIII. H1_H_2O is used without broadening at 293.6K.

Any results omitted:

No.

34) ORNL2

Institute and country:

Oak Ridge National Laboratories, United States.

Participants:

BJ Marshall, D Bowen and B Rearden.

Neutron data library:

ENDF/B-VIII.

Neutron data processing code or method:

SCALE 6.2.3.

Number of neutron energy group:

252 energy group.

Description of your code system:

SCALE 6.2.3 Monte Carlo code.

Description of any preparation methods used to generate the results:

AMPX was used to generate a library based on the ENDF files.

What bound data has been selected (i.e. H1_ICE/H1_H_2O):

H1_ICE for 233K and 253K.

H1_H_2O for 293K, 333K and 588K.

A brief description of any steps taken to provide temperature correction:

Doppler broadening for the multi-group calculations are performed by interpolating using the square root of the absolute temperature.

Any results omitted:

No.