Appendix E

VERIFICATION OF CODES AND CROSS-SECTIONS

Properties of the applications versus benchmarks

The fissionable material system applications considered in this study are geometrically simple. The material compositions are few and without impurities. Real applications often involve complicated systems that are difficult to assess exactly but can be confidently assured to be safe based on conservative approximations. Critical experiment benchmarks are usually in between; their geometry and material compositions are often specified with high accuracy. However, there are uncertainties and errors in the specifications. They are estimated, but additional uncertainties should be assumed to remain. For that reason, independent critical experiments of similar systems are valuable.

The total biases and uncertainties in the selected applications are not found only by evaluation of benchmarks based on critical experiments. The additional uncertainties primarily involve atomic number densities (or equivalent specifications) and optimisation of the moderation. Other benchmarks are needed to verify such input. Comparison of contributions, preferably independent, based on the specifications of the selected applications in this study helps to identify uncertainties and discrepancies.

Validation or verification?

The verification reported in this appendix is limited to computer codes and cross-sections. Determination of atomic number densities or equivalent information is very important and can include significant uncertainties, in particular for water-soluble fissile compositions. Determination of optimum moderation is another uncertainty source that is not directly covered in this appendix. Determination of optimum geometry shape is not expected to be complicated for the selected systems.

Convergence criteria, mesh distribution, angular quadrature, etc. can involve significant uncertainties for deterministic codes. They are considered in a few of the verification cases, where the default code input has been modified.

Convergence criteria can be very important also in Monte Carlo calculations. The total number of neutron histories is obviously important, but also removal of a sufficient number of neutron histories from the first part of the neutron tracking (the "transient" phase before convergence) can be important. Determination of k_{eff} and other values should be based on a converged source distribution of neutrons. The convergence should be established before the scoring is started. Absorption rates, fission distribution and sensitivities are usually much more sensitive than k_{eff} to early transients. Source convergence in Monte Carlo has been considered in all verification cases by removing (skipping) more initial neutron histories and often by increasing the total number of histories.

In Appendix K, atomic number density methods are evaluated. Further evaluations in Appendix L lead to an effort to validate the best-estimate values given in the main report.

Selection of benchmarks for verification

The verification cases were first selected subjectively by looking at the ICSBEP Handbook specifications from evaluations of critical experiments. The new TSUNAMI capabilities in SCALE 5 [86-88] were used later to evaluate similarities between applications and benchmarks.

- Priority is given to simple benchmarks with few material constituents, pure water moderation and reflection, no neutron absorbers and a geometry that can easily be modelled. Simplicity may reduce unknown errors. That is not necessarily always true (more material constituents could mean better chemical analysis, not more complications, etc.).

- Some benchmarks involve a chain of experiments with similar materials, equipment, measurement procedures, chemical assays, etc. They will be extremely valuable in determining trends due to the changed parameters. However, they are not independent. Priority is given to one set of results from a series of correlated experiments, in the hope that there will be a sufficient number of independent benchmarks to establish a bias and an uncertainty. The single set of results could include a combined evaluation of all correlated and similar benchmarks, leading to a smaller uncertainty than for any single benchmark.

- Whether identical or different weights are given to the selected benchmarks, the reasons should be understood and described. This conclusion is independent on whether the selection is based on reasoning alone or on a combination of reasoning with more systematic statistical and numerical evaluations.

- The verification is primarily intended for finding best-estimates of the requested values. Verification with the purpose of finding safe values would very likely be different;

- Preference is given to benchmarks with low uncertainties. A result for a single benchmark with an uncertainty of 0.0010 in k_{eff} is statistically worth the same as results for ten completely uncorrelated benchmarks, each with an uncertainty of 0.0031. The uncertainty is an important parameter in weighting the benchmarks.

- In the past, benchmark error sources often were of two types. One was chemical analysis and presence of impurities. This would usually lead to a supercritical benchmark model. Another error source type is the presence of more reflecting materials than documented. Reflection from distant walls could be inferred by k_{eff} sensitivity to array size. This error type leads to a subcritical benchmark model. The ICSBEP evaluators seem to be well aware of these potential error types.

- The results are displayed in table and chart formats in Appendix F. The charts were created automatically, using Microsoft Excel. A legend is displayed in each sub-section and applies to all charts in that sub-section. Trend lines are inserted for trial use only. The equations generated are not reliable for so few and often very uncertain data points. Extrapolation is certainly not recommended. Discussion of bias and uncertainty determination for all systems and methods is covered in Appendix I.

Input data for benchmarks

Time and resources did not allow independent generation of input data for the benchmarks. Input files were taken from the DVD containing the ICSBEP Handbook, 2004 edition or from Appendix A of the benchmark specifications in the Handbook. The input data have not been checked properly to be trusted for verification of safety applications. A major purpose of using these input files is that they give excellent information on differences due to cross-sections.

The references to the ICSBEP handbook benchmarks should be easy to recognise. In the tables and figures, the identification of methods has been shortened to reduce space. The identifications may vary but in general M stands for MCNP and S for SCALE with the version number following directly (M5, S5, etc.). The cross-section library is specified by the number of energy groups (e.g. 238, 27, and 44) or a letter (E for ENDF/B, J for JENDL and JF or only F for JEF(F)) plus release number for the source library for evaluated continuous energy cross-sections (e.g. E50 means ENDF/B-5.0, F22 means JEF2,2, etc.).

Values may be added late during the evaluation. The purpose is to give additional information on the methods. All results are not necessarily included in the charts or in the evaluations. However, a selection of methods that is considered essential has been identified and the corresponding results are included, when available. The "major 6" methods include those that have been bias-corrected and use the latest cross-section library available for the method.

The major 6 methods are:

- EMS-S5K-238. The cross-sections are old but the verification appears appropriate and the results appear to respond to the physics variations of the benchmark and reference systems. This is not always true for the 44-group and 27-group libraries

- EMS-M5-E7P and EMS-M5-E68. These are the latest ENDF/B cross-sections available. The only plutonium isotope available in the preliminary ENDF/B-VII library is ^{239}Pu. Rather than mixing the libraries for plutonium with other isotopes, the ENDF/B-VI.8 library was used. This library was obtained from KAERI, S. Korea for evaluation.

- EMS-M5-J33. Revision 1 of the JENDL-3.3 library was released during 2004.

- EMS-M5-F30. Dr. Yolanda Rugama prepared a sub-set of JEFF-3.0 in ACE-format (used by MCNP) containing the nuclides involved in the reference systems.

- Serco-Mk8-F22. Serco used bias-corrections based on a reasonable verification.

- IPPE-04 or ABBN93. In addition to handbook values from 1984, IPPE submitted new results both for the reference systems and for the benchmark systems. IPPE claims that the verification using KENOVa is valid for the XSDRNPM/S calculations of reference systems when the same ABBN93 library is used. This is credible since the same conclusion was reached for those codes within the SCALE 5 system and the 238-, 44- and 27-group libraries.

Sometimes, values using one of the 6 methods are not available. This will be noted by referring to the selection as the "major 5".

The IRSN-CR-Isop-172 and IRSN-CrV0-20 methods are verified and validated for criticality safety but not quite for best-estimate evaluations. Even so, they usually have small biases and are considered when the best-estimate results are determined.

The Japanese handbook values are bias-corrected, but it seems as if the validation is not so successful for best-estimate evaluations. One reason is that the validation was carried out a long time ago, long before the first version of the ICSBEP handbook was available. The biases in the benchmarks, as documented at that time, were not always clear. A new Data Collection Release 2 that will reduce the problems is expected soon.

The EMS-S4X-238 values are bias-corrected. However, the verification from ORNL appears too "broad" to be used for best-estimate evaluations of the reference systems. Sometimes a large positive bias correction suggested by the ORNL verification report is changed into a negative bias-correction when more focused verification is carried out.

Selected ICSBEP Handbook benchmarks

Table E1. Fast HEU systems

ICSBEP id.	Description	Case	Model
HEU-MF-001	Bare U(94) metal sphere, LANL 1950's. Small uncertainty	1	Godiva
			Shell
HEU-MF-004	Water-reflected U(96) metal sphere, LANL 1976. Small uncertainties	1	3D
			1D
HEU-MF-008	Bare U(90) metal sphere, VNIITF 1982. Similar to HEUMF-018	1	
HEU-MF-015	Bare U(96) metal sphere, VNIITF 1984. Similar to HEUMF-065	1	
HEU-MF-018	Bare U(90) metal sphere, VNIIEF 1962. Small uncertainties	1	Detail
		1	Simple
HEU-MF-020	Polyethylene-reflected U(90) metal sphere, VNIIEF 1962	1	Detail
		1	Simple
HEU-MF-065	Bare U(96) metal cylinder, VNIITF 1987. Small uncertainty	1	

Table E2. Thermal compound and metal HEU systems

ICSBEP id.	Description	Case
HEU-CT-011	Four clusters of square-pitched 21x21 lattices of $U(80)O_2$ + Al fuel rods, stainless steel clad and water-moderated. Kurchatov 1997. Large uncertainty.	1
		2
		3
HEU-MT-011	Arrays of U(93) - aluminium alloy plates. Water-moderated and –reflected. Valduc 1969. Small uncertainties.	1
		3
		5
		7
		35
		37
		39
		41

Table E3. Thermal HEU solution systems

ICSBEP id.	Description	Case
HEU-ST-001	Minimally reflected cylinders of U(93)NH-solution. Rocky Flats 1976. Large uncertainties.	01 02 03 04 05 06 07 08 09 10
HEU-ST-009	Water-reflected 6.4 litre spheres of $U(93)O_2F_2$ solutions. ORNL 1954 and 1958. Large uncertainties.	1 2 3 4
HEU-ST-010	Water-reflected 9.7 litre spheres of $U(93)O_2F_2$ solutions. ORNL 1950.	1 2 3 4
HEU-ST-011	Water-reflected 17 litre spheres of $U(93)O_2F_2$ solutions. ORNL 1954 and 1957.	1 2
HEU-ST-012	Water-reflected 91 litre sphere of $U(93)O_2F_2$ solution. ORNL 1958. Large uncertainty	1
HEU-ST-025	Water-reflected cylinder with U(89)NH solution. IPPE 1987.	1
HEU-ST-027	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Large uncertainty	1
HEU-ST-028	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Large uncertainty (case 9)	1 9
HEU-ST-029	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Very large uncertainty	1
HEU-ST-030	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Very large uncertainty (case 4).	1 4
HEU-ST-033	Concrete-reflected annular cylinders with U(89)NH solution. Rocky Flats 1980. Extremely large uncertainties.	11A-S 11B-S
HEU-ST-035	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Large uncertainties.	1 5 7
HEU-ST-036	Water-reflected cylinder with U(89)NH solution. IPPE 1969. Large uncertainty.	1
HEU-ST-037	Water-reflected cylinder with U(89)NH solution. IPPE 1961. Large uncertainty.	1 3 6
HEU-ST-038	Two interacting slab tanks with U(93)NH solution. LANL 1988.	1
HEU-ST-042	Bare large-diameter cylinders of U(93)NH solution. ORNL 1950. Large uncertainties.	1 2 3 4 5 6 7 8
HEU-ST-043	Bare large-diameter cylinders of $U(93)O_2F_2$ solutions. ORNL 1957.	1 2 3

Table E4. Thermal LEU compound and solution systems

ICSBEP id.	Description	Case
LEU-CT-001	Water-moderated $U(2.35)O_2$ rods in square-pitched arrays. PNL 1977.	1 2
LEU-CT-002	Water-moderated $U(4.31)O_2$ rods in square-pitched arrays. PNL 1977.	1 4
LEU-CT-013	Water-moderated $U(4.31)O_2$ rods in square-pitched arrays. PNL 1980. Steel and water reflection.	1
LEU-CT-014	Water-moderated and –reflected $U(4.31)O_2$ rods in square-pitched arrays. PNL 1982.	1 6
LEU-CT-039	Incomplete arrays of water-moderated and –reflected $U(4.738)O_2$ rods in square-pitched arrays. Valduc 1978.	1
LEU-CT-049	MARACAS: $U(5)O_2$ powder, heterogeneously moderated and reflected by polyethylene. Valduc 1983. Large uncertainty.	1-Simple
LEU-CT-061	Water-moderated and –reflected $U(4.4)O_2$ hexagonal-pitched lattices of fuel rods (VVER). Kurchatov 1993.	1
LEU-CT-070	Water-moderated and –reflected $U(6.5)O_2$ hexagonal-pitched lattices of fuel rods (VVER). Kurchatov 1989.	1
LEU-ST-001	Unreflected $U(5)O_2F_2$+H_2O cylindrical assembly (Sheba-II). LANL 1994.	1
LEU-ST-003	Full and truncated bare spheres of U(10)NH solutions in water. IPPE 1965. Large uncertainties.	1 2 3 4 5 6 7 8 9
LEU-ST-007	Bare cylinder of U(10)NH solution in water. NUCEF 1995. Small uncertainties.	1 2 3 4 5
LEU-ST-016	Water-reflected slabs of U(10)NH solution in water. NUCEF 1997. Small uncertainties.	1 2 3 4 5 6 7
LEU-ST-017	Bare slabs of U(10)NH solution in water. NUCEF 1997. Small uncertainties.	1 2 3 4 5 6
LEU-ST-020	Water-reflected cylinder of U(10)NH solution in water. NUCEF 1998. Small uncertainties.	1 2 3 4
LEU-ST-021	Bare cylinder of U(10)NH solution in water. NUCEF 1998. Small uncertainties.	1 2 3 4

Table E5. Fast Pu metal systems

ICSBEP id.	Description	Case	Model
Pu-MF-001	Bare Pu(95/5/0/0) metal sphere, LANL 1950.	1	
Pu-MF-002	Bare Pu(76/20/3/0.4) metal sphere, LANL 1964.	1	
Pu-MF-003	Bare, unmoderated Pu(93.5/6/0.5/0) metal button array. LLNL 1965.	1	
		2	
		3	
		4	
		5	
Pu-MF-005	Tungsten-reflected Pu(95/5/0/0) metal sphere, LANL 1958. Small uncertainty.	1	
Pu-MF-011	Water-reflected Pu(94.5/5/0.5/0) metal (alpha-phase) sphere, LANL 1968. Small uncertainty.	1	
Pu-MF-016	Water-flooded 3x3x3 array of 3-kg Pu(94/6/0/0) metal cylinders. Rocky Flats 1982. Large uncertainty.	1	
Pu-MF-022	Bare Pu(98/2/0/0) metal (delta-phase) sphere, VNIIEF 1956.	1	Simplified
Pu-MF-029	Bare Pu(88.5/9/1.5/0) metal (alpha-phase) sphere, VNIIEF 1965.	1	Simplified
Pu-MF-037	Water-flooded 2x2x2 arrays of 3-kg Pu(94/6/0/0) metal cylinders. Rocky Flats 1973. Large uncertainties.	1	
		5	
		7	
		10	
		12	
		15	
		16	

Table E6. Thermal Pu solution systems

ICSBEP id.	Description	Case
Pu-ST-009	Bare Pu(97/3/0/0)NH solution sphere, PNL 1978. Large uncertainties.	1
		2
		3
Pu-ST-014	Pu(95/4/0/0)NH solution cylinders, interacting in air without reflection. Valduc 1968. Large uncertainties.	1
		2
Pu-ST-015	Pu(95/4/0/0)NH solution cylinders, interacting in air without reflection. Valduc 1968. Large uncertainties.	1
		2
Pu-ST-022	Pu(74/19/6/1)NH solution in an annular cylinder tank with water reflection. Valduc 1973.	1
		2
		3
		4
		5
		6
		7
		8
		9
Pu-ST-025	Water-reflected slabs of Pu(95/5/0/0)NH, Pu(76/18/5/1)NH and Pu(72/23/4/1)NH solutions. PNL 1967. Large uncertainties.	1
		7
		14
		21
		28
		34
		39
Pu-ST-026	Bare slabs of Pu(95/5/0/0)NH, Pu(76/18/5/1)NH and Pu(72/23/4/1)NH solutions. PNL 1967. Large uncertainties.	1
		4
		9
		15
		17