Appendix C
DESCRIPTION OF EVALUATION METHODS

For each source of calculation results and of critical values, a brief summary of the methods applied is given below. Relevant information could include:

- calculation of atomic number densities (stoichiometric formula of material, theoretical density of materials, atomic weights, Avogadro's number, isotopic composition of fissile elements, material and solution mixing relations, etc.)
- description of computation (type and version of code, cross-section-library, nuclides used)
- geometry and reflector representation
- numerical model: mesh points, convergence criteria, S_n-order, P_l-order, MC-tracking (confidence level, convergence of eigen-distribution, tracking error checks)
- validation description
- description of method for bias correction
- type of provided value: calculation-only, best-estimate.

ARH, USA

Hanford, Fluor Federal Services, Inc has recently supported a release of the classical criticality safety handbook on the web for interactive use. It is also referred to as a source for nuclide density equations and other material properties. Further work on an update is planned.

ARH-600

The criticality safety handbook ARH-600 (Atlantic Richfield Hanford) from 1968 and revised at least up to 1983 is available on the internet; http://ncsp.llnl.gov/ARH600/index.htm. Many reference values can be obtained from the curves in the handbook. The handbook is also a widely used reference for other information such as properties of fissile and other materials. The GAMTEC-II cross-section processing code (from 18 groups to 2 groups) and the HFN 1D diffusion theory code were used.

When references are made to the ARH-600, it is important to know which revision, which page and which equation, table or curve that was used. There may be multiple sources in the same revision.

Significant uncertainties are introduced from reading the curves. In some cases, results for U(100) and $U(100)O_2F_2$ were reported as $U(100)O_2$ results. They may be essentially identical in many cases, but this needs to be confirmed.

Validation was important when the handbook was released. Each section reports results from calculations on critical experiments. Some of those may be used in ICSBEP handbook benchmark models but no effort has been made in this study to determine bias corrections based on the current information on the experiments.

DIN, Germany

The German institution DIN (Deutsches Institut für Normung) has released some standards with reference values related to this study.

DIN 25403-4

The reference values for $U(100)O_2$, $U(20)O_2$, $U(5)O_2$ are given but the calculations are not described in the standard. The reference values in the standard are based on a report SR-2010 from NUKEM.

DIN 25403-5

The reference values for $Pu(100/0/0/0)O_2$ and $Pu(95/5/0/0)O_2$ are given but the calculations are not described in the standard. The reference values in the standard are based on a 1997 report from Forschungsinstitut für Kerntechnik und Energieumwandlung.

DIN 25403-6

The reference values for Pu(100/0/0/0)NH and Pu(95/5/0/0)NH are given but the calculations are not described in the standard. The reference values in the standard are based on a 1997 report from Forschungsinstitut für Kerntechnik und Energieumwandlung.

DIN 25403-8

The reference values for U(100)NH are given but the calculations are not described in the standard. The reference values in the standard are based on a report SR-2010 from NUKEM.

EMS, Sweden

The EMS (E Mennerdahl Systems) contribution EMS-S4X-238 from early 2001 was considered a first step towards a more focused validation for best-estimate value determination, rather than for direct criticality safety application. For various reasons, this continuation was not carried out. However, in September 2004, EMS was asked to complete a final evaluation and report for the study. Further calculations were necessary to carry out this work and several methods were used. The newly released code packages SCALE 5 (from RSICC in June 2004) [79] and MCNP5 releases 1.20 and 1.30 (from RSICC late November 2004) [80] were used.

The pre-compiled Windows versions of SCALE and MCNP were used. The differences between MCNP4C2, MCPNP5 release 1.20 and release 1.30 are not considered significant concerning precision of calculated values. SCALE 5 contains some improvements over SCALE 4.4 in default convergence and mesh parameters but no major differences are expected. The cross-section libraries are identical. The two SCALE 5 codes, KENOVa and XSDRNPM/S as well as MCNP5 calculate the EALF (Energy corresponding to Average Lethargy of neutrons causing Fission) parameter by default.

SCALE 5 contains a new method for calculation of nuclide densities for solutions, the Pitzer method. SCALE 4 and earlier used the ARH-600 method. Re-calculations of previous SCALE 4.4 input data for uranyl nitrate solutions caused SCALE 5 to reject the suggested densities at room temperature (293K). The user is told that the density is above the crystal density, which is not correct.

Both EMS and ORNL had used this temperature (293K) for their contributions. At the default temperature of 300K, the results were very different but still not correct. For plutonium nitrate solutions, the problem occurred also for 298K, the temperature at which many parameters are determined. Eventually it has become clear that the problem is not with the Pitzer method but in the SCALE implementations of first the ARH-600 and then the Pitzer methods for solution densities. The solution methods are used to determine the crystal densities instead of using the theoretical density of the crystal (salt). ORNL is aware of the problem and is considering a prevention of calculations with actinide concentrations above the solubility limit. The user is already warned by SCALE if the solubility limit is exceeded.

The nuclide density input data for the MCNP5 dioxide systems were based on SCALE 4 calculations in 2000. However, for solutions, the optimum actinide element densities from 2000 were used in SCALE 5 to generate new nuclide densities for MCNP5. This means that the new Pitzer method was applied to MCNP5 input. As is pointed out above and elsewhere, there is a serious problem with the SCALE 5 implementation of the Pitzer method. The temperature was changed from 293K to 300K for low-enriched systems when the SCALE 5 nuclide densities to be used by MCNP5 were determined. The densities are still not correct.

For MCNP5 calculations, not all benchmark nuclides or elements were available in the same cross-section release (identifier .XXc). Since the purpose was to validate the cross-sections for the reference value applications, missing cross-sections were taken from later releases, in particular from ENDF/B-VI.8 (KAERI).

EMS-S1K-27

A few calculations were made with an older calculation method. A modification of SCALE1 codes with a SCALE-0 version of the 27-group cross-section library was installed by EMS on an IBM PC AT computer with 640 kb RAM in 1985 [93]. The SCALE-0 library was replaced with a SCALE-3 library in February 1986. The reason was a problem pointed out during a NEA working group study on dissolution, including gadolinium experiments. The gadolinium cross-section (27^{th} group) in SCALE was changed by several orders of magnitude after SCALE-0. The change in cross-section format should probably have been accompanied by the new version of NITAWL for treating the revised format properly. However, EMS used the SCALE-1 version of NITAWL with the SCALE-3 version of the 27-group library. Benchmarking did not indicate any large or inconsistent error.SCALE-1 contained KENO-V rather than -Va. Due to memory constraints with the Intel 80286 computer chip (segmented) and operating system limitations (640 kb RAM including space for the operating system), the size of each generation in KENO-V was often limited to 100. It was replaced in 1988 with an 80386 version with fewer restrictions. The 1985 version was used in many projects, including NEA criticality studies, licensing and other research.

A few reference value applications have been calculated with the 1985 SCALE 1 PC-version and the SCALE-3 27-group library. The statistics were 330 000 neutrons of which 30 000 were skipped (100 neutrons per generation). The optimum moderation fissile material and water fractions were based on SCALE 4 calculations, but the number densities were generated with SCALE 1.

EMS-S4-CSAS

The first release of SCALE 4 for mainframe computers was installed by EMS on a PC in 1992. The 27 group burnup library was required for the NEA working group studies. This implementation was used in this study only to calculate pre-SCALE-5 number densities, based on the ARH-600 methods.

EMS-S4X-238

In 2000 and early 2001, a PC-based, ORNL-compiled executable version of SCALE 4.4 together with the 238 group ENDF/B-V cross section library were used by EMS. The 1D deterministic transport code XSDRNPM/S was used to calculate the minimum critical values. Default convergence parameters were used and this turned out to be insufficient in some cases. Some uncertainties in the results remain due to this issue.

Optimum moderation was determined for a few densities close to the optimum and then using interpolation to get the optimised value. XSDRNPM search techniques were used to calculate parameters (sphere radius, cylinder diameter, and slab thickness) for specified k_{eff} values. Thus, linear interpolation based on sensitivity of k_{eff} to a parameter was not used.

Validation was not carried out in detail. Agreement with some results from calculations carried out by ORNL, the developer of the method, was judged sufficient to assume that the methods were essentially identical. A validation report by ORNL was then used to derive biases and uncertainties for each fissile material. The validation base included many complicated systems as well as benchmarks with large uncertainties, giving a large spread of results for most material types.

A more focused approach to validation for each selected fissile system would improve the bias corrections and reduce the uncertainties.

EMS-S5X-238

This is essentially the same method as used in 2000 (XSDRNPM/S with 238-group cross-sections). However, default input data for convergence was tightened in SCALE 5. Further, mesh and angular quadrature input were improved over the default input in SCALE 5. For spheres, the ISN parameter was increased by the evaluator to 64 and for cylinders and slabs to 32 or 64 for all fast systems and for some slow systems. The mesh distribution was improved for fast slab systems and for a few slow slab systems by setting the size factor SZF to 0.5. The improvements were significant.

A 30 cm water reflector was used. However, it was found that 20 cm is sufficient and that some previous improvements by using a 30 cm reflector were more related to inadequate mesh or angular quadrature settings than the actual reflection from the extra 10 cm of water.

A few benchmarks based on 1-dimensional spherical models were calculated. However, they were not evaluated directly for biases and uncertainties. Instead, comparisons between SCALE1X (XSDRNPM/S) and SCALE25 (KENOVa) calculations were made. They show that there are essentially no differences between XSDRNPM/S and KENOVa calculations when the same cross-section library is used. The improved mesh and angular quadrature input mentioned above are important for getting agreement.

EMS-S5X-27

The same method and input data as for EMS-S5X-238 were used, except for the 27-group ENDF/B-IV cross-section library.

EMS-S5X-44

The same method and input data as for EMS-S5X-238 were used, except for the 44-group ENDF/B-V cross-section library.

EMS-S5K-238

The same method and input data as for EMS-S5X-238 were used, except that the KENOVa Monte Carlo code was used rather than the 1D XSDRNPM/S code. A major difference in input data compared with default input, both for validation and for the reference value applications, is that more neutrons were tracked and, in particular, more initial neutrons were skipped. The number of tracked neutrons was set with the goal of obtaining a statistical uncertainty of 0.0005 or lower. This was achieved for the reference value applications but not always for benchmarks.

EMS-S5K-27

The same method and input data as for EMS-S5K-238 were used, except for the 27-group ENDF/B-IV cross-section library.

EMS-S5K-44

The same method and input data as for EMS-S5K-238 were used, except for the 44-group ENDF/B-V cross-section library.

EMS-M5-E50

MCNP5 with the LANL ENDF/B-V cross-section sets identified with .50c was used. A problem with the ^{239}Pu set was observed; see EMS-M5-E5F below. Most calculations were made with the MCNP5 release 1.20. The older S(α,β) thermal scattering data set lwtr.01t was used.

As with KENOVa Monte Carlo calculations, the number of skipped initial neutron histories was increased during the validation process, compared with examples in the ICSBEP Handbook. For many of the older examples the total number of neutrons was also increased significantly. The number of tracked neutrons was set with the goal of obtaining a statistical uncertainty of 0.0005 or lower. This was achieved for the reference value applications, but not always for benchmarks.

The material input specifications were based on the optimisation process carried out in 2000, using the EMS-S4X-238 method. The optimum parameters are not so sensitive to small changes in the neutron spectrum so this approximation is not considered significant. However, this conclusion has not been verified. For solutions, the number densities were calculated with SCALE 5 as mentioned above.

EMS-M5-E5F

Exactly the same as EMS-M5-E50, except that the ^{239}Pu cross-section set .50c was replaced with the .55c set. Both are used in the examples of the ICSBEP handbook but the .55c is more frequent. The .50c set is an interim version while the .55c is the final version (according to Russ Mosteller, LANL). It was decided to use both sets in the validation and reference value applications.

EMS-M5-E62

MCNP5 and the LANL ENDF/B-VI-2 cross-section sets identified as .60c were used. Other sets such as .62c and .49c had been used with MCNP4C2 previously, without giving significant differences. The older S(α,β) thermal scattering data set lwtr.01t was used

EMS-M5-E66

MCNP5 and the LANL ENDF/B-VI.6 cross-sections identified as .66c were used consistently for all nuclides. The LANL library contains some more recent ENDF/B-VI.8 cross-sections for non-fissionable nuclides but they were not used in this method. The new S(α,β) thermal scattering data set lwtr.60t was used

EMS-M5-E68

MCNP5 and an ENDF/B-VI.8 library processed by KAERI, S. Korea (obtained through private communication) in the autumn of 2002 were used. The new S(α,β) thermal scattering data set lwtr.60t from LANL was used.

EMS-M5-E7P

MCNP5 and the preliminary ENDF/B-VII set of cross-sections (identified by .69c) supplied by LANL in the Release 1.30 of MCNP5 were used. The only plutonium isotope included is ^{239}Pu. Default (no specification of the version) cross-sections were used for all nuclides. This means that some ENDF/B-VI.8 cross-sections (e.g. for hydrogen and oxygen) were used. The new S(α,β) thermal scattering data set lwtr.60t from LANL was also used.

EMS-M5-F22

MCNP5 and a JEF 2.2 cross-section library processed by ENEA [84], Italy were used. The S(α,β) thermal scattering data set is from the same JEF 2.2 library.

EMS-M5-F30

MCNP5 and a limited set of cross-sections from JEFF-3.0, processed in December 2004 by Dr. Yolanda Rugama, OECD/NEA for this evaluation, were used. The new S(α,β) thermal scattering data set lwtr.60t from LANL was used together with the JEFF-3.0 cross sections. The JEFF-3.0 cross-sections were limited to those used in the reference value calculations. Other nuclides were necessary for the benchmark calculations. Cross-sections from the ENDF/B-VI.8 library (KAERI) were used to allow validation of the uranium and plutonium isotopes together with water and nitrogen.

EMS-M5-J32

MCNP5 and a JENDL-3.2 cross-section library processed by JAERI [81] were used. The older S(α,β) thermal scattering data set lwtr.01t from LANL was used together with the JENDL-3.2 data.

EMS-M5-J33

MCNP5 and a JENDL-3.3 revision 1 cross-section library, processed by JAERI [82], were used. The new S(α,β) thermal scattering data set lwtr.60t from LANL was used together with the JENDL3.3 data.

GRS, Germany

GRS-HzK-98

Most of the GRS (Gesellschaft für Anlagen- und Reaktorsicherheit) values are obtained from the GRS Handbuch zur Kritikalität [19]. Values are calculation results based on older methods such as GAMTEC-II together with DTF-IV and SCALE 4/XSDRNPM together with 27-group cross-sections. Sometimes results by both methods are included in the handbook. The contributed results for $U(100)O_2$ are based on a low maximum uranium density. Since the optimum values are for full density material, these values have been removed from the evaluation.

GRS-M4-E50

A method based on MCNP4A with ENDF/B-V continuous cross sections.

GRS-S4X-44

A method based on SCALE 4.3 and XSDRNPM/S with 44group ENDF/BV cross sections.

IPPE, Russia

The IPPE methods and calculations are described [35] with some more detail than other methods since the IPPE methods may not be as familiar to criticality safety specialists in countries outside of Russia. In the future, similar information about other methods should be compiled and compared to explain and reduce the spread of results. It is noted that the chemical forms for PuNH in the two IPPE contributions appear to be different. In IPPE-84 there are six water molecules in the crystal form while IPPE-ABBN93 and other sources are based on only five water molecules in the crystal form. In criticality safety references, it is usually assumed that the number five should be used. The chemical properties of soluble fissionable materials are important for safety.

IPPE-84.

The originally reported data (IPPE-84) were taken from a Russian criticality safety handbook issued in 1984. All the reported data are given in the handbook as the minimal critical values with infinite water reflector. The data are calculation values.

The values for the uranium systems were calculated with the KRAB-1 one-dimensional code, using the S_n-method in S_8-approximation. The ABBN-78 26-group cross sections were used. The order of cross section scattering anisotropy was P_1.

The uncertainties for the uranium systems are estimated in the handbook as follows: The handbook says that for the uranium systems, the calculation approach gives basically conservative results, i.e. the calculation values of minimum critical parameters are less than experimental values practically in the whole region of existence.

The total uncertainty of the calculations of critical parameters for the uranium systems with high enrichment (more than 5%) weakly depends on uranium concentration, almost does not depend at all on the type of mixture and does not exceed 0.5% in k_{eff}, 2% in critical dimension, and 6% in critical mass. For the systems with low enrichment at moderation ratios of $H/^{235}U<20$ and $H/^{235}U>800$, the uncertainty of calculation is comparable with the uncertainty for the systems with high enrichment.

The values for the plutonium systems were calculated with the KRAB-1 one-dimensional code. The ABBN-78 26-group cross sections were used. Order of cross section scattering anisotropy was P_1.

The uncertainties for the plutonium systems are estimated in the handbook as follows: The handbook says that the approach used for the processing of the cross sections led to significant errors in the values of critical parameters for the plutonium systems at the moderation range of 500>H/Pu>20. The error of calculation of k_{eff} is about 5%, critical dimension – 15%, and critical mass – 45%. At the same time, the use in the calculations of the P_1-approximation led to errors in accounting for anisotropy of the neutron flux that fully compensate the mentioned errors.

The result is that the critical parameters of homogeneous plutonium systems with H/Pu>20 are calculated with an acceptable accuracy (the uncertainty is no more than 5% for critical dimension). This conclusion is supported by results of calculations of experiments.

Concentrations for the homogeneous mixture of uranium dioxide with water were calculated using the equation:

$$\mathrm{H/U} = \frac{238 - 3\,x_5}{9}\left(\frac{1}{C_{\mathrm{U}}} - 0.103\right)$$

where x_5 uranium enrichment, $Cu = 0.8814\gamma_{UO_2}$ – uranium concentration, γ_{UO_2} – density of uranium dioxide assumed to be 10.96 g/cm^3.

Concentrations for the homogeneous mixture of uranyl nitrate hexahydrate $[UO_2(NO_3)_2 \cdot 6H_2O]$ with water were calculated using the equation:

$$\mathrm{H/U} = 26.14/C_{\mathrm{U}} - 19.65 \quad \left(C_{\mathrm{U}} \le 1.33\ \mathrm{g/cm^3}\right)$$

The density of $UO_2(NO_3)_2 \cdot 6H_2O$ was assumed to be 2.807 g/cm^3.

Concentrations for the homogeneous mixture of plutonium dioxide with water were calculated using the equation:

$$\mathrm{H/Pu} = 26.59/C_{\mathrm{Pu}} - 2.629$$

where $C_{Pu} = 0.8814\gamma_{PuO_2}$ – plutonium concentration, γ_{PuO_2} – density of plutonium dioxide is assumed to be 11.46 g/cm^3. According to IPPE an appendix of the Handbook gives a density of 11.44 g/cm^3 which explains why this value was used in 2004.

Concentrations for the homogeneous mixture of plutonium nitrate hexahydrate $[Pu(NO_3)_4 \cdot 6H_2O]$ with water were calculated using the equation:

$$\mathrm{H/Pu} = 26.556/C_{\mathrm{Pu}} - 9.4$$

The density of $Pu(NO_3)_4 \cdot 6H_2O$ was assumed to be 2.9 g/cm^3.

IPPE-04, IPPE-ABBN93 or just ABBN93

The IPPE-ABBN93 data are new calculations performed specially for this project. The 299-group ABBN-93.01a cross-sections were used for the calculations. The order of the cross section scattering anisotropy was P5. The temperature was 300K. The code used for the calculations was XSDRNPM from the ORNL SCALE-4.3 package. The S_{16}-approximation was used. The thickness of the water reflector in the calculations was 30 cm. Mesh size was 0.5 cm in the reflector and from 0.03 to ~0.5 cm in the core. Atomic weights and Avogadro's number used for the atomic densities calculations were taken from the ICSBEP Handbook. The following chemical formulas of the compounds and the densities were used for the atomic density calculations:

- UO_2 – 10.96 g/cm^3
- $UO_2(NO_3)_2 \cdot 6H_2O$ – 2.807 g/cm^3
- PuO_2 – 11.44 g/cm^3 (this value has been confirmed – 11.46 is the established value)
- $Pu(NO_3)_4 \cdot 5H_2O$ – 2.9 g/cm^3
- H_2O – 1 g/cm^3

The atomic densities were calculated as a mechanical mixture of the compound and water.

IRSN (formerly IPSN), France

IRSN (formerly IPSN) contributed data from three major sources; a 1978 handbook, a 1996 internal compilation and recent calculations using the CRISTAL code system. Validation has always been important, but the actual biases and uncertainties are not specifically documented together with the contributions. On the other hand, IRSN tries to validate the whole system, including nuclide density calculations. This is a necessary procedure to assure safety.

IRSN validation shows that there are positive biases (about 0.005% in Δk) both when all methods are covered and when only older methods are selected. The biases are slightly lower for the older methods but the spread of results is larger.

The IRSN position on the issue of reference values related to this study is explained in [59]. The intention has not been to determine the best possible value but to demonstrate the safety of the complete procedure. A few results that IRSN consider more accurate, obtained with TRIPOLI 4.1 and JEF 2.2 as well as ENDF/B-VI cross sections in continuous energy form, show significant differences. Further, calculations with the full 172 group library, rather than with the collapsed 20-group set, show some deviations that indicate that the full library may give more accurate values.

Two different versions of CRISTAL were used in the contributions to this study. For uranium and plutonium nitrate systems, version V0 with the CEA93 V4 JEF-2.2 based cross-section library was used. A 20-group collapsed set of the 172 group library was used. The deterministic code APOLLO2, an S_n code was used to obtain k_{eff}. The order n was 8, anisotropy was P_3 for water, P_1 for U and Pu).

For uranium and plutonium dioxide systems, version V1.0 with the CEA93 V6 JEF-2.2 based cross-section library was used. The full 172 group library was used. The deterministic code APOLLO2 (S_n code, the order n was 32, P_5 anisotropy) was used to obtain k_{eff}.

The geometry mesh distribution for all plutonium dioxide systems and for uranium dioxide systems with 100% ^{235}U was set to 10 points per cm of fissile material. For other uranium dioxide as well as for all uranium and plutonium nitrate systems the number of mesh points was 1 per cm of fissile material.

A significant contribution to biases for nitrate systems is the nuclide density calculation methods. IRSN has shown that older methods can give significant errors and that the new extended isopiestic law developed by IRSN and included in CRISTAL is quite accurate, in particular for the systems covered by this study. For older IRSN reference value evaluations of PuNH systems, the densities corresponding to minimum critical masses are good. For PuNH systems corresponding to minimum critical geometry (volume, cylinder, slab), the old method densities lead to serious underestimations, up to 3.4% in k_{eff} were found and they could even be higher.

ICSBEP handbook benchmarks were used [39-40] to compare the results based on direct benchmark specifications, on the isopiestic law and on the ARH-600 (1968 version)/Leroy-Jouan laws for solutions. Five series of benchmarks were selected: PU-SOL-THERM-001 (6 configurations), LEU-SOL-THERM-004 (7 configurations), LEU-SOL-THERM-016 (7 configurations), HEU-SOL-THERM-001 (10 configurations), and MIX-SOL-THERM-003 (10 configurations). The HEU-SOL-THERM-001 and LEU-SOL-THERM-016 have also been selected for the reference value evaluation in this study. The APOLLO2-MORET4 system was used. The results are important and should be used as a basis for further studies.

IRSN contributed the results as best-estimates, even though it is clear that there are biases and uncertainties. The importance of making more accurate determinations was not considered sufficient to motivate further validation at the time. Biases and uncertainties for various fissile systems are discussed and rough numerical values were given in the IRSN presentations to the expert group.

The IRSN methods as referred to in this report are specified as follows:

IRSN-CR-Spec

The nuclide densities specified in ICSBEP benchmarks were used [39-40] with the CRISTAL V0 package route APOLLO2 (Sn code, the order n was 8, P_3 anisotropy) and the CEA93 V4 172 group cross-section library. This method was used during validation work only.

IRSN-CR-Isop-172

The new extended isopiestic (isopiestic law only below the solubility limit with volume addition above the solubility limit) law [39-40] was used to calculate nuclide densities for use with the CRISTAL V0 package route APOLLO2 (Sn code, the order n was 8, P_3 anisotropy) and the CEA93 V4 172 group cross-section library (JEF 2.2). This method is separated from the method IRSN-Cr-V020 below by using the full 172-group rather than the 20-group collapsed set used in APOLLO2 calculations of reference values.

IRSN-Pre-Iso

This method, sometimes referred to by IRSN as “the ARH-600 law” (1968 release of the ARH600 handbook) for PuNH and as the Leroy-Jouan law for UNH, was used [39-40] to calculate nuclide densities for use with the CRISTAL V0 package route APOLLO2 (S_n code, the order n was 8, P_3 anisotropy) and the CEA93 V4 172 group cross-section library (JEF 2.2).

IRSN-CrV0-20

The isopiestic law was used [40] to calculate nuclide densities for use with the CRISTAL V0 package route APOLLO2 (S_n code, the order n was 8, P_3 anisotropy) and the CEA93 V4 20 group sub-set of the 172 group cross-section library (JEF 2.2).

The default mesh distribution is set to 1 point per cm in the fissionable material, 2 points per cm in the first 5 cm of the reflector and 1 point per cm further out. The default convergence criterion is 10^{-5}. The report [40] contains several evaluations of interest to the expert group. Influence of different reflectors, including a water layer between the fissile material and the reflector is calculated.

Many of the results were not included in a formal report but contributed in a compilation, including number densities. These number densities would be useful in a continued evaluation study, including effects of different nuclide density calculation methods.

IRSN-CrV1-172

A recent update of the CRISTAL package to version V1.0 and of the 172 group cross-section library to V6 was used to calculate reference values for uranium and plutonium dioxide systems. In addition to using the full 172-group library, the angular quadrature order was increased to 32 and the anisotropy order was increased to P_5. For all plutonium dioxide systems and for uranium dioxide systems with 100% ^{235}U, the number of mesh points in the fissile material was increased to 10 per cm.

IRSN-78-CEA

The 1978 criticality standard [21] is based on calculations with the 1D S_n code DTF-IV (the angular quadrature order n was 4) and various CEA cross-section sets. Results for UNH with low-enriched uranium are identical to a table in the German Handbook.

IRSN-96

In a 1996 internal IRSN report using similar methods (DTF-IV) as for the 1978 standard, a compilation of reference values was made. The report does not explain how the values were determined but gives references to other internal IRSN documents.

JAERI, Japan

JAERI contributed results from two versions of the Japanese Criticality Safety Handbook. The handbooks give best-estimate critical values based on validation and bias correction. The JACS code system was used to calculate the handbook data.

JAERI-H-88

The first version of the Japanese Handbook [22] was released in 1988, with a translation into English published in 1995. The Data Collection contains the reference values and is included as a second part of the translation. The Handbook contains many different kinds of useful information about methods, materials, etc. The reference values were calculated with a code system, JACS, developed by JAERI.

The handbook contains information on calculation and validation of the JACS system for different fissionable materials. The reference values in the handbook are bias-corrected. It is possible to derive the direct calculation results from the validation information. The following information (explained in Appendix D of the handbook) for simple systems as revised in 1987 (Table 2.3) in the handbook (as opposed to Table 5.3 in the Data Collection, revised 1985):

- Homogeneous, low-enriched uranium: The critical value is 0.991, giving a bias of -0.009. A standard deviation of 0.004 is reported.
- Homogeneous, high-enriched uranium: The critical value is 0.985, giving a bias of -0.015. A standard deviation of 0.013 is reported.
- Homogeneous plutonium: The critical value is 1.008, giving a bias of +0.008. A standard deviation of 0.011 is reported.
- There is no separation of fast and slow systems for high-enriched uranium and for plutonium.

Appendix C of the handbook contains a large number of calculation results for benchmarks used in the validation of the JACS system. This was long before the first ICSBEP Handbook was released. It would be interesting to identify these benchmarks according to the ICSBEP Handbook identifications. A source for improvement is the better knowledge of biases and uncertainties of the benchmarks today.

It is interesting to note that there are no data for the U(20)NH material that was used to fabricate the fuel for the JOYO reactor and that was handled at JCO for many years, before the release of the first version of the handbook. NUPEC contributed calculations for this material type separately.

JAERI-H-99

The second version of the JAERI handbook [23] was released in Japanese in 1999. A translation into English was released in 2001 [24]. A second release of the Data Collection is expected soon. The handbook contains some revised reference values. Values of Handbook version 2 are identical to version 1 except those for low-enriched homogeneous uranium fuels, which were based on a published report [106].

An example of a serious error in version 2 is based on Figure 4.5 in [106]. The figure does not show the minimum value, since the curve does not go low enough in uranium concentration. The lowest value is quoted in version 2 as the minimum critical value. This value was also reported to the expert group. The error had been found by JAERI earlier but no correction was made. During the final evaluation, the error was pointed out by the evaluator and soon confirmed as well as explained by JAERI [48]. The error is serious since even the “safe” value is supercritical.

The Moeken model for nitrate nuclide densities that was used in the first release of the Data Collection will be replaced in the second release. For UNH-solution with uranium enrichments of 3 and 4% ^{235}U by mass of uranium, the new mass and volume reference values are more than 10% smaller than release one as reported to the OECD/NEA expert group.

The second version of the handbook was prepared before the JCO accident (September 30, 1999). Like the first version, it does not contain data for U(20)NH material.

A second version of the Data Collection that was issued in relation to the first issue of the Japanese Handbook has been announced [48] but was not yet released at the end of 2005.

NUPEC, Japan

NUPEC-S4X-44

NUPEC used SCALE 4.3 and the 44-group library to calculate minimum critical mass and volume for U(20)NH. This complements the data from the Japanese handbooks (JAERI-H-88 and H99). Validation was not reported but can be found in several published reports from other sources.

ORNL, USA

ORNL-S4X-238

SCALE 4.3 and the 238-group ENDF/B-V cross-section library were used by ORNL [52]. The convergence criteria were tightened compared with the default values in SCALE 4.3. Information on the calculation procedures and on nuclide density determination methods is provided in the ORNL report. Only calculated results were included in the ORNL submittal; no bias and uncertainty estimates were made. However, the ORNL report refers to a published ORNL report on validation [78]. This was also used by EMS in its 2001 contribution [29] to obtain bias corrections.

The reference values submitted by ORNL were not always for optimum systems. The nearest calculation value was chosen and sometimes this caused significant deviations (e.g. 3% in mass). Differences between EMS-S4X-238 results ("evaluated" interpolation was used) and ORNL results may either be due to this or to the better convergence criteria used by ORNL. Differences for fast systems between the ORNL results and the SCALE 5 results from EMS may also be due to a tighter mesh for slab systems and a higher angular quadrature order for spheres and cylinders in the EMS evaluations.

Serco Ass., United Kingdom

Serco Ass. made the calculations with the code system MONK [55], [56] and [57]. Two different versions, MONK-8A and MONK-8B were used together with continuous energy cross sections. The differences in the methods are negligible for the fissile systems selected. MONK-8A was used in the determination of reference values for critical masses and concentrations while MONK-8B was used for determination of reference values for critical volumes, cylinder diameters and slab thicknesses.

The WIMS system was used in preparatory calculations to support the optimisation.

The cross-section library DICE96 (point data) used by Serco is based on JEF-2.2.

Serco Ass. reported validation efforts and supplied bias-corrected critical values and uncertainties. Calculation of nuclide densities is described in the contributed papers. As an example, the maximum uranium concentration in UNH is 1.257 kg/l (slightly higher for some reference values). This does not seem to be correct. For PuNH, the corresponding maximum plutonium concentration is 1.20 kg/l. This information is valuable for continued studies of differences between methods. Like the IRSN reports, Serco mentions that plutonium solutions are likely to contain mixtures of Pu(III), Pu(IV) and Pu(VI), where III, IV and VI are valence numbers. This influences the reference values. Only Pu(IV) was assumed in the calculations.

The Serco validation shows that for uranium and reference values for volumes, cylinders and slabs there are no trends against enrichment ^{235}U and no trends against energy. The mean k_{eff} value was

1.0016. The bias correction is thus -0.0016 for all uranium systems. The uncertainty is estimated from a simple statistical evaluation based on the maximum benchmark uncertainty and the number of benchmarks (13 systems with 80 configurations). This uncertainty is combined with the MONK uncertainty.

For uranium and reference values for masses and concentrations, a similar procedure carried out earlier gave a slightly lower bias correction; -0.0014.

For plutonium, evaluation of thirteen independent systems with over 100 configurations indicates a k_{eff} overestimation by about 0.5%. No definite trend could be determined related to energy or to the plutonium isotope distribution. A flat bias correction of -0.5% was assumed. Two experimental systems were excluded due to likely discrepancies in some specifications. This evaluation covers all plutonium reference values.