Chapter 7

CRITICALITY VALIDATION STUDIES

This chapter is based on two papers [1,2] presented at the last two criticality safety conferences. It reviews the benchmark analysis performed using the various codes both independently and collectively, in order to summarise the current validation status of the JEF-2.2 file for criticality purposes. A more detailed reference list to JEF documents dealing with JEF2.2 benchmarking for criticality safety studies is given at the end of this chapter.

A variety of experimental sources was considered for each class of problem to avoid experimental programme specific tendencies. Also, the use of the results from independent codes and analysis enables code specific bias effects to be minimised. Recommendations are made concerning areas where further benchmark analysis may be required and where further improvements to the source nuclear data file should be sought for the benefits of criticality assessment. Finally, results of sensitivity studies are presented showing the effect of nuclear data uncertainties on the calculation of typical criticality configurations.

Introduction

This paper summarises the outcome of an intercomparison exercise between criticality safety analysis codes used in France and the UK. The exercise covers a range of system types of interest to the criticality assessor, with experimental details being drawn from the handbook of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [3]. By this means, common modelling assumptions are made for each code, thereby eliminating a potential source of discrepancy.

The objective of this work is to reach code-independent conclusions concerning the accuracy achievable using JEF-2.2 based nuclear data libraries for criticality analysis. Monte Carlo and S_n codes were used. This allows to evaluate the effect of geometrical discretisations. Moreover, cross-section representations were used ranging from broad group structures (20 or 172 groups) to hyperfine group structure (13 193 groups) or pointwise representation.

Codes used

In France, calculations were performed with CRISTAL, the new French package for criticality safety studies. This package includes two calculation routes using JEF-2.2 nuclear data:

- A pointwise route using the Monte Carlo code TRIPOLI-4 [4] with its continuous energy JEF-2.2 library.

- A multi-group route using the combination of the nuclear data library CEA93.V4 (V3 in the S_n calculations; the difference being in the fission spectrum, which is softer in V4) derived

from JEF-2.2, the assembly code APOLLO-2.4 and the Monte Carlo code MORET-4. The 172 group (Xmas energy structure) application library CEA93.V4 was derived from JEF-2.2 and processed using NJOY-THEMIS. The assembly code APOLLO-2 is used for self-shielding (using the generalised Livolant-Jeanpierre formalism) and flux calculations (using the Pij method). Then, self-shielded cross-sections homogenised and/or collapsed are used in the Monte Carlo code MORET-4 for 3-D calculations with a general P_n-like anisotropy representation or in S_n calculations with APOLLO-2. S_n calculations are carried out using a 20 group structure, an S_8 quadrature and a P_3 approximation for H_2O anisotropic scattering.

In the UK, the comparison involves the use of MONK (version 7 or 8) together with its hyperfine energy group cross-section library (13 193 groups) and continuous energy/angle collision processing treatment. The MONK library uses solely unadjusted JEF-2.2 nuclear data as issued by the NEA Data Bank and processed using NJOY in conjunction with MONK-specific additional codes. Following the general release of JEF-2.2, the initial MONK library utilised 8 220 energy groups in common with its UKNDL-based alternative. Following early testing and intercomparison, this group scheme was extended to better represent the resonance data available in JEF-2.2 (particularly for ^{238}U) and to better model thermal fission effects in ^{239}Pu. The MONK JEF-2.2 nuclear data library has now been frozen since 1996 and has been issued to code users for field evaluation. More recently (1998), a consensus was reached in the UK nuclear industry that the library is acceptable for use in formal safety submissions as an alternative to the longer-established UKNDL-based library. It is expected that use of the UKNDL library will now gradually diminish on time scales consistent with particular organisational requirements.

Comparison results

The range of experiments for which intercomparisons have been performed is wide-ranging but varying in depth according to the availability of suitable data and the discrepancies that were investigated during the early phases of developing JEF-based libraries. The results presented here are the final intercomparisons following the completion of the development phase of the respective libraries described previously. The results of the intercomparisons are presented under the following five headings:

- Plutonium solutions.
- Highly enriched uranium solutions.
- Low enriched uranium solutions.
- Mixed uranium/plutonium solutions.
- Low enriched uranium oxide and mixed oxide systems.

In addition, for each type of system, a review of other benchmark results for the individual codes is presented where common experiments have not been analysed.

Plutonium solutions

Description of the intercomparison experiments

Comparison cases have been selected from the following ICSBEP experiments (all in the series PU-SOL-THERM):

Experiment	Laboratory	Description
001	Hanford	Water-reflected spheres, 4.67% ^{240}Pu, Pu 73.0-268.7 g/l
002	Hanford	Water-reflected spheres, 3.12% ^{240}Pu, Pu 49.8-77.1 g/l
003	Hanford	Water-reflected spheres, 1.76-3.12% ^{240}Pu, Pu 33.3-44.1 g/l
004	Hanford	Water-reflected spheres, 0.54-3.43% ^{240}Pu, Pu 26.3-39.4 g/l
005	Hanford	Water-reflected spheres, 4.05-4.40% ^{240}Pu, Pu 29.7-40.9 g/l
006	Hanford	Water-reflected spheres, 3.12% ^{240}Pu, Pu 24.8-27.0 g/l
012	Valduc	Water-reflected cuboids, 19.0% ^{240}Pu, Pu 13.0-105.0 g/l
022	Valduc	Water-reflected annular cylinders, 19.0% ^{240}Pu, Pu 28.7-165.0 g/l

Intercomparison results and discussion

The calculated results for the selected configurations are shown in Table 7.1. The results show excellent agreement between the four codes for the whole set of experiments. As the geometrical configurations of the investigated experiments are rather simple, the 2-D S_n capabilities are sufficient to accurately describe them. There being no significant difference between Monte Carlo and deterministic results, we conclude that the options used in the latter method (broad energy mesh, quadratures…) are adequate for this class of media. Also, no significant differences are noticed between pointwise and multi-group Monte Carlo codes.

These experiments cover a broad range of plutonium concentration, include differing levels of ^{240}Pu (albeit only two main levels ~4% and 19%) and include experiments from more than one laboratory. There is no discernible trend with plutonium concentration but some possible indication of an increase in calculated result for cases with the higher ^{240}Pu content – however, as this marks the difference between laboratories, this apparent discrepancy may have other causes.

Compared with the experimental value of unity, however, the calculated results are consistently on average ~500 pcm high (about 300 pcm for cases with ^{240}Pu content lower than 5% and about 600 pcm for ^{240}Pu content of 19%). Given the diversity of the systems studied and their origin and the different code systems used in our analysis, it is concluded that over-prediction is a code-independent commentary on the accuracy of the JEF-2.2 files for plutonium.

Other benchmark results

Additional configurations from the ICSBEP experiments have been calculated using MONK, and the results confirm the level of agreement previously observed. Other experiments analysed include further Hanford spheres (with various reflectors) and a high burn-up plutonium case from Hanford (cylinders of solution with 42.9% ^{240}Pu and plutonium concentrations between 40.6 and 140.0 g/l). The results from these cases again follow the general trend, with the high burn-up case adding credence to the suggestion of higher calculated values for higher ^{240}Pu contents. For the complete set

Table 7.1. Calculated results for the selected configurations

k_{eff} values with statistical uncertainty are in parentheses

Experiment	C_{Pu} (g/l)	APOLLO-2/ MORET-4	APOLLO-2/S_n	TRIPOLI-4	MONK-7/ MONK-8
001/1	73	1.0038 (0.0010)	1.0032	1.0032 (0.0009)	1.0018 (0.0010)
001/2	96	1.0051 (0.0010)		1.0055 (0.0010)	1.0050 (0.0010)
001/3	119	1.0073 (0.0010)	1.0078	1.0072 (0.0010)	1.0070 (0.0010)
001/4	132	1.0040 (0.0010)		1.0020 (0.0010)	0.9986 (0.0010)
001/5	140	1.0063 (0.0010)	1.0068	1.0049 (0.0010)	1.0044 (0.0010)
001/6	268	1.0063 (0.0010)	1.0075	1.0036 (0.0010)	1.0062 (0.0010)
002/1	49.8	1.0038 (0.0010)			1.0012 (0.0010)
002/3	59.1	1.0022 (0.0010)			1.0034 (0.0010)
002/7	77.1	1.0066 (0.0010)			1.0027 (0.0010)
003/1	33.3	1.0024 (0.0010)			0.9996 (0.0010)
003/3	37.4	1.0052 (0.0010)			1.0044 (0.0010)
003/6	44.1	1.0064 (0.0010)			1.0059 (0.0010)
004/2	26.3	0.9987 (0.0010)	1.0004	0.9994 (0.0010)	0.9975 (0.0010)
004/3	27.2	1.0031 (0.0010)	1.0025	1.0003 (0.0010)	1.0007 (0.0010)
004/5	27.6	1.0029 (0.0010)		0.9982 (0.0010)	0.9984 (0.0010)
004/6	28.6	1.0022 (0.0010)	1.0027	1.0040 (0.0010)	1.0011 (0.0010)
004/8	29.9	1.0024 (0.0010)		1.0010 (0.0010)	1.0007 (0.0010)
004/11	39.4	1.0000 (0.0010)	1.0004	1.0008 (0.0010)	0.9992 (0.0010)
005/1	29.6	1.0037 (0.0010)			1.0027 (0.0010)
005/5	36.0	1.0046 (0.0010)			1.0049 (0.0010)
005/7	40.9	1.0040 (0.0010)			1.0007 (0.0010)
006/2	25.6	1.0049 (0.0010)			1.0003 (0.0010)
012/1	19.7	1.0026 (0.0010)	1.0036		1.0053 (0.0010)
012/3	16.7	1.0076 (0.0010)			1.0067 (0.0010)
012/5	13.2	1.0076 (0.0010)			1.0082 (0.0010)
012/6	105	1.0099 (0.0010)	1.0069		1.0077 (0.0010)
012/9	31.9	1.0135 (0.0010)			1.0102 (0.0010)
012/11	21.7	1.0075 (0.0010)	1.0054		1.0069 (0.0010)
012/13	13.2	1.0071 (0.0010)	1.0089		1.0102 (0.0010)
022/1	152	1.0023 (0.0010)			1.0018 (0.0010)
022/2	104	1.0041 (0.0010)			1.0053 (0.0010)
022/3	62	1.0059 (0.0010)			1.0041 (0.0010)
022/4	51	1.0066 (0.0010)			1.0043 (0.0010)
022/5	40.9	1.0048 (0.0010)			1.0034 (0.0010)
022/6	36	1.0068 (0.0010)			1.0045 (0.0010)
022/7	33.1	1.0071 (0.0010)			1.0052 (0.0010)
022/8	30.8	1.0090 (0.0010)			1.0058 (0.0010)
022/9	28.7	1.0078 (0.0010)			1.0078 (0.0010)

of experiments calculated using MONK (over one hundred configurations), the mean over-prediction is 460 pcm. If the low (<5%) and high ^{240}Pu content cases are separated, the mean over-predictions are 320 pcm and 670 pcm respectively.

Highly enriched uranium solutions

Description of the intercomparison experiments

The investigated experiments originate from different programmes carried out at Oak Ridge, Rocky Flats and IPPE Obninsk. All these experiments are described in the ICSBEP Handbook using the identification name HEU_SOL_THERM. Details are given in Table 7.2.

Table 7.2. Description of investigated experiments with the reference to the series numbers in the ICSBEP classification

Experiment	Laboratory	Description
001	Rocky Flats	Different diameters bare cylindrical vessels containing 93% enriched uranium nitrate solutions; the uranium concentration range extends from 55 g/l to 358 g/l.
002	Rocky Flats	Different diameters concrete-reflected cylindrical vessels containing 90% enriched uranium nitrate solutions; the uranium concentration is 144 g/l or 335 g/l.
009-012	Oak Ridge	Water reflected spheres of various diameters containing 93% enriched uranium fluoride solutions; the uranium concentration range extends from 20 to 696 g/l.
013	Oak Ridge	Bare spheres containing boron poisoned nitrate solutions with U concentrations ranging from 20 g/l to 28 g/l and boron concentration from 0 g/l to 0.23 g/l.
014-019	IPPE-Obninsk	Water reflected cylindrical tanks (of variable diameters and heights) containing gadolinium poisoned uranium (enrichment 90%) nitrate solutions; the uranium concentration range extends from 68 g/l to 447 g/l. Gadolinium-free configurations were also investigated at different uranium concentrations. For the poisoned cases, Gd concentration ranges from 0.1 g/l to 2 g/l and generally increases with uranium concentration.

Intercomparison results and discussion

Table 7.3 shows the results obtained by the different codes. The differences (X2-X1), between TRIPOLI-4 (X1) and APOLLO-2/MORET-4 (X2) results are between -250 pcm and 420 pcm with a tendency of the latter system of codes to give higher results. The difference between the two codes does not show any visible trend, neither with uranium concentration nor with Gd content.

The differences (X2-X1) between TRIPOLI-4 (X1) and MONK-7/8 (X2) range from -460 pcm to 260 pcm with a tendency of the latter code to give lower results. The difference between the two codes does not show any visible trend, neither with uranium concentration nor with Gd content.

As a consequence, APOLLO-2/MORET-4 gives results that are systematically higher than those obtained with MONK-7/8. The differences range from 30 pcm to 700 pcm without any visible trend with uranium concentration and Gd content. The origin of these differences has not yet been investigated.

Table 7.3. Results obtained by the different codes

Experiment	C(U) / C(Gd) g/l	APOLLO-2/ MORET-4	APOLLO-2/S_n	TRIPOLI-4	MONK-7/ MONK-8
001/1	146	1.0057 (0.0010)		1.0068	
001/2	347	1.0052 (0.0010)		1.0032	
001/3	143	1.0100 (0.0010)		1.0067	
001/4	358	1.0089(0.0010)		1.0083	
001/5	55	1.0042 (0.0010)		1.0034	
001/6	60	1.0085 (0.0010)		1.0076	
001/7	137	1.0082 (0.0010)		1.0040	
001/8	146	1.0042 (0.0010)		1.0058	
001/9	358	1.0049 (0.0010)		1.0029	
001/10	64	0.9987 (0.0010)		0.9970	
002/1	144	1.0129 (0.0010)			
002/2	144				
002/3	335	1.0088 (0.0010)			
002/4	335				
002/5	144				
002/6	144				
002/7	335	1.0089 (0.0010)			1.0075 (0.0010)
002/8	335				1.0151 (0.0010)
002/9	60				1.0048 (0.0010)
002/10	60				1.0096(0.0010)
002/11	144	1.0109 (0.0010)			1.0063 (0.0010)
002/12	144				1.0158 (0.0010)
002/13	335	1.0075 (0.0010)			
002/14	335				
009/1	696	1.0101 (0.0010)		1.0077 (0.0020)	1.0067 (0.0010)
009/2	543	1.0106 (0.0010)		1.0078 (0.0020)	1.0052 (0.0010)
009/3	349	1.0061 (0.0010)		1.0042 (0.0020)	1.0044 (0.0010)
009/4	213	1.0017 (0.0010)		0.9991 (0.0020)	0.9953 (0.0010)
010/1	102	1.0050 (0.0010)		1.0019 (0.0020)	1.0021 (0.0010)
010/2	104	1.0049 (0.0010)		1.0018 (0.0020)	1.0016 (0.0010)
010/3	109	1.0060 (0.0010)		1.0026 (0.0020)	0.9990 (0.0010)
010/4	112	1.0030 (0.0010)		0.9994 (0.0020)	0.9973 (0.0010)
011/1	53	1.0109 (0.0010)		1.0068 (0.0010)	1.0028 (0.0010)
011/2	52	1.0067 (0.0010)		1.0025 (0.0010)	1.0020 (0.0010)
012/1	22	1.0034 (0.0010)		1.0033 (0.0010)	1.0006 (0.0010)
013/1	20	1.0031 (0.0010)		1.0004 (0.0010)	0.9970 (0.0010)
013/2	24	1.0023 (0.0010)		0.9988 (0.0010)	0.9986 (0.0010)
013/3	27	0.9974 (0.0010)		0.9945 (0.0010)	0.9971 (0.0010)
013/4	28	0.9994 (0.0010)		0.9973 (0.0010)	0.9940 (0.0010)

Table 7.3. Results obtained by the different codes (*cont.*)

Experiment	C(U) / C(Gd) g/l	APOLLO-2/ MORET-4	APOLLO-2/S_n	TRIPOLI-4	MONK-7/ MONK-8
014/1	70 0	0.9994 (0.0010)		0.9979 (0.0010)	
014/2	70/0.1			1.0126 (0.0010)	
014/3	70/0.19			1.0203 (0.0010)	
015/1	100				
015/2	100/0	0.9946 (0.0010)		0.9933	
015/3	100				
015/4	100/0.20			1.0162	
015/5	100/0.4			1.0143	
016/1	150/0	0.9951 (0.0010)		0.9976	
016/2	150/0.30			1.0110	
016/3	150/0.53			1.0305	
017/1	200/0	0.9967 (0.0010)		0.9969	
017/2	200			0.9862	
017/3	200/0	0.9849 (0.0010)		0.9838	
017/4	200			1.0015	
017/5	200/0.50			1.0104	
017/6	200/0.50			1.0094	
017/7	200			1.0107	
017/8	200/0.80			1.0095	
018/1	300/0	0.9986 (0.0010)	0.9934	0.9973	0.9943 (0.0010)
018/2	300		0.9865		0.9900 (0.0010)
018/3	300/0	0.9939 (0.0010)	0.9904	0.9964	0.9922 (0.0010)
018/4	300/0.50	1.0054 (0.0010)	1.0015	1.0044	1.0030 (0.0010)
018/5	300		0.9965		0.9989 (0.0010)
018/6	300/0.50	1.0009 (0.0010)	0.9963	0.9995	0.9960 (0.0010)
018/7	300/0.98	1.0125 (0.0010)	1.0117	1.0143	1.0097 (0.0010)
018/8	300		1.0129		1.0136 (0.0010)
018/9	300/0.98	1.0129 (0.0010)	1.0101	1.0138	1.0093 (0.0010)
018/10	300		1.0258		1.0274 (0.0010)
018/11	300/1.4	1.0322 (0.0010)	1.0284	1.0309	1.0289 (0.0010)
018/12	300	1.0256 (0.0010)	1.0222	1.0253	1.0214 (0.0010)
019/1	400/0	1.0061 (0.0010)		1.0041	
019/2	400/0.65	1.0072 (0.0010)		1.0073	
019/3	400/1.16	1.0062 (0.0010)		1.0045	

The results obtained with APOLLO-2/S_n are systematically lower than those obtained with Monte Carlo (up to 500 pcm). This may originate from the difference in the library version (V3 in S_n and V4 in multi-group Monte Carlo, the difference being attributed to fission spectrum).

The comparison between calculations and experiments shows important scatter of the C-E values. Of special concern are the results obtained for experiments performed at IPPE Obninsk. C-E values of 2 000 pcm or 3 000 pcm are obtained even with low Gd concentrations. The scatter obtained

at 0 Gd concentration (C-E between -1 620 pcm and 420 pcm) may be an indication of experimental problems (there is more than 1 300 pcm difference between two experiments at the same U and Gd concentrations differing only by geometrical dimensions). For the other experiments, calculations show a general tendency to k_{eff} over-prediction, especially for high U concentrations (up to about 1 000 pcm). However, the differences between code results and between experimental programmes make it difficult to assign an overall C-E value and to clearly infer to nuclear data.

Low enriched uranium solutions

Description of the intercomparison experiments

Different experimental programmes involving low enriched uranium solutions were carried out at Los Alamos (SHEBA reactor), Oak Ridge, NUCEF (STACY facility) and Obninsk (IPPE). The investigated experiments are all described in the ICSBEP handbook in the volume devoted to LEU_SOL_THERM. As shown in Table 7.4, two series experiments involved 5% enriched uranium fluoride solutions and two other series involved 10% enriched uranium nitrate solutions. The ranges of concentration of the different programmes are rather complementary, which does not ensure consistency checks.

Table 7.4. Description of experimental programmes involving low enriched uranium solutions

Experiment	Laboratory	Description
001	LANL SHEBA	Bare cylinder containing a 5% enriched UO_2F_2 solution with a uranium concentration of 978 g/l.
002	Oak Ridge	Water reflected spheres containing 4.9% enriched UO_2F_2 solutions; the uranium concentration range extends from 452 g/l to 492 g/l.
003	IPPE Obninsk	10% enriched $UO_2(NO_3)_2$ solutions contained in a bare spherical tank; the uranium concentration range extends from 168 g/l to 296 g/l.
04	STACY NUCEF	Water reflected cylindrical tank containing a 10% enriched $UO_2(NO_3)_2$ solution; the uranium concentration range extends from 225 g/l to 310 g/l.

Intercomparison results and discussion

Table 7.5 shows the results obtained by the different codes. Differences up to 500 pcm are found, and for some STACY experiments up to 700 pcm. These latter differences are probably due to differences in benchmark models, as the evaluation work by ICSBEP for this series of experiments was not definitively completed at the time of this comparison.

Compared to experimental results we observe some scatter. The calculation of the SHEBA experiment (the highest studied U concentration) gives a rather large overestimation (of the order of 1 500 pcm). Unfortunately, it was not possible to provide independent experimental evidence in this concentration range. The evaluation of an old experimental programme performed at Valduc which covers an extended uranium concentration range (up to 1 300 g/l) would be very beneficial.

Table 7.5. Results obtained by the different codes

Experiment	C(U) g/l	APOLLO-2/ MORET-4	TRIPOLI-4	MONK-7/ MONK-8
001/1	978	1.0111 (0.0010)	1.0141 (0.0010)	1.0101 (0.0010)
002/1	452	0.9964 (0.0010)	0.9970 (0.0010)	0.9988 (0.0010)
002/2	492	0.9943 (0.0010)	0.9952 (0.0010)	0.9945 (0.0010)
002/3	492	0.9960 (0.0010)	1.0012 (0.0010)	0.9963 (0.0010)
003/1	296	0.9979 (0.0010)	0.9988 (0.0010)	
003/2	264	0.9945 (0.0010)	0.9963 (0.0010)	
003/3	260	0.9998 (0.0010)	1.0012 (0.0010)	
003/4	255	0.9931 (0.0010)	0.9952 (0.0010)	
003/5	203	0.9967 (0.0010)	0.9955 (0.0010)	
003/6	197	0.9975 (0.0010)	0.9977 (0.0010)	
003/7	193	0.9956 (0.0010)	0.9944 (0.0010)	
003/8	171	0.9998 (0.0010)	0.9984 (0.0010)	
003/9	168	1.0000 (0.0010)	0.9962 (0.0010)	
004/1	310	1.0009 (0.0010)	1.0036 (0.0009)	1.0003 (0.0010)
004/29	290	1.0004 (0.0010)	1.0028 (0.0009)	1.0012 (0.0010)
004/33	270	0.9975 (0.0010)	1.0020 (0.0009)	0.9958 (0.0010)
004/34	253	1.0021 (0.0010)	1.0013 (0.0009)	1.0022 (0.0010)
004/46	241	1.0049 (0.0010)	1.0035 (0.0010)	0.9996 (0.0010)
004/51	233	0.9990 (0.0010)	1.0030 (0.0008)	1.0008 (0.0010)
004/54	225	1.0065 (0.0010)	1.0025 (0.0009)	0.9991 (0.0010)

Most of the other C-E values fluctuate within ±500 pcm (to be compared with experimental uncertainties of about 400 pcm), the maximum absolute difference being around 700 pcm and the average being as low as -120 pcm. There is no visible trend with U concentration.

Mixed uranium and plutonium solutions

Description of the intercomparison experiments

The investigated experiments, taken from ICSBEP benchmarks (in the series MIX_SOL_THERM), cover a wide range of plutonium and uranium concentrations, including different U/(U + Pu) ratios. A short description of these experiments is given in Table 7.6.

Table 7.6. Description of the intercomparison experiments for mixed uranium and plutonium solutions

Experiment	Laboratory	Description
002	Pacific Northwest Laboratory	Water reflected cylinder; Pu/(U + Pu) 22.9 and 52.11%; ^{nat}U; 8.3% ^{240}Pu; Pu 11.73-12.19 g/l
003	Aldermaston (UK)	Water reflected cylinder; Pu/(U + Pu) 30.7%; ^{nat}U; 5.63% ^{240}Pu; Pu 17.50-101.3 g/l
004	PNL	Water reflected and unreflected cylinder; Pu/(U + Pu) 39.68%; ^{nat}U; 8.3 % ^{240}Pu; Pu 41.69-172.82 g/l

Intercomparison results and discussion

The calculated k_{eff} for the selected experiments are given in Table 7.7. First of all, it should be noted that the k_{eff} values calculated by the four codes are in good agreement. The discrepancies between the results of Monte Carlo calculations are within the uncertainties. For the experiments in series MSTH_002, S_n results fit also with the others. However, for the unreflected experiments MSTH_004_65, 70 and 77, the deterministic calculations show some differences with the other codes (average discrepancy of -300 pcm). The simplified geometrical model adopted for these calculations could explain this under-prediction since the "room return" effect is not accurately accounted for.

Table 7.7. Calculated k_{eff} for the selected experiments

Statistical uncertainty in parentheses

Experiment	C_{U+Pu} (g/l)	APOLLO-2/ MORET-4	APOLLO-2/S_n	TRIPOLI-4	MONK
002/58	22.93	1.0028 (0.0010)	1.0026	1.0015 (0.0010)	1.0017 (0.0010)
002/59	22.51	1.0040 (0.0010)		1.0011 (0.0010)	1.0027 (0.0010)
002/61	53.23	1.0028 (0.0010)	1.0020	1.0011 (0.0010)	1.0003 (0.0010)
003/01	329.8	1.0114 (0.0010)		1.0092 (0.0010)	1.0075 (0.0010)
003/02	329.8	1.0115 (0.0010)		1.0076 (0.0010)	1.0086 (0.0010)
003/03	329.8	1.0090 (0.0010)		1.0072 (0.0010)	1.0081 (0.0010)
003/04	329.8	1.0018 (0.0010)		1.0003 (0.0010)	0.9998 (0.0010)
003/05	102.88	1.0054 (0.0010)		1.0023 (0.0010)	1.0023 (0.0010)
003/06	102.88	1.0074 (0.0010)		1.0074 (0.0010)	1.0071 (0.0010)
003/07	102.88	1.0019 (0.0010)		1.0030 (0.0010)	1.0022 (0.0010)
003/08	60.81	1.0082 (0.0010)		1.0064 (0.0010)	1.0051 (0.0010)
003/09	60.81	1.0025 (0.0010)		1.0040 (0.0010)	1.0035 (0.0010)
003/10	57.1	1.0057 (0.0010)		1.0031 (0.0010)	1.0013 (0.0010)
004/65	105.07	0.9963 (0.0010)	0.9928	0.9975 (0.0010)	
004/66	105.54	0.9950 (0.0010)	0.9957	0.9949 (0.0010)	
004/69	293.71	0.9955 (0.0010)	0.9947	0.9967 (0.0010)	
004/70	293.43	0.9963 (0.0010)	0.9926	0.9951 (0.0010)	
004/77	435.35	0.9969 (0.0010)	0.9936	0.9944 (0.0010)	
004/78	435.37	0.9944 (0.0010)	0.9947	0.9947 (0.0010)	

Considering the C-E discrepancies, the three experimental series give contradictory trends (about 100 pcm discrepancy for series 002, from 200-900 pcm for series 003 and -560 to -250 pcm for series 004). More questionable are the results of experiment series 003 for which one sees an important decrease of the calculated k_{eff} for some specific experiments. Indeed, while the results of experiments 003/01, 003/02, 003/03 are fairly consistent (about 1% high) the result for experiment 003/04 is 800 pcm lower. Bearing in mind that all these experiments were made with the same solution, but with different internal cylinder radius, it is likely that the differences do not come from Pu cross-sections. The same situation is found for experiments 003/05, 003/06 on the one hand and 003/07 on the other hand and finally between 003/08 and 003/09. If one looks more closely, it is always the configuration with the largest internal radius (and thus the lowest critical height) that gives

lower results. As there is a polyethylene reflector on the top of the solution, a possible correlation that may explain this behaviour is that when the reactivity effect of this reflector becomes important, other causes of discrepancy are introduced.

The results of series 004 are systematically low. This could originate from the fact that a concrete reflector is present. This may disturb the trends one may wish to extract for U and Pu cross-sections in JEF-2.2.

In conclusion, the experiments considered in this section do not allow us to derive clear tendencies about the ability of JEF-2.2 to predict the results of mixed uranium and plutonium solutions. The calculation of additional "clean" experiments is required.

Other benchmark results

Additional configurations from the above ICSBEP experiments have been calculated using MONK. Other experiments analysed cover similar U:Pu ratios but with different fissile concentrations. The mean value overall for MONK/JEF from the 58 configurations is 1.0001 ± 0.0084, but there remains some evidence of a correlation between calculated k_{eff} and H:(Pu + U).

Low enriched uranium and mixed oxide systems

Description of the intercomparison experiments

Experiments are described in ICSBEP benchmarks in the series LEU_COMP_THERM (LCTH) and MIX_COMP_THERM (MCTH).

Experiment	Laboratory	Description
LCTH/007	Valduc	Water-reflected uranium dioxide fuel rods 4.75% ^{235}U
LCTH/006	JAERI	Water-reflected uranium dioxide fuel rods 2.6% ^{235}U
LCTH035/B1	JAERI	Water-reflected uranium dioxide fuel rods 2.6% ^{235}U, 70 ppm boron
LCTH035/B2	JAERI	Water-reflected uranium dioxide fuel rods 2.6% ^{235}U, 148 ppm boron
LCTH035/C1	JAERI	Water-reflected uranium dioxide fuel rods 2.6% ^{235}U, 64.5 ppm gadolinium
MCTH004/2	JAERI	Water-reflected mixed plutonium-uranium fuel rods

Intercomparison results and discussion

The calculated k_{eff} for the selected experiments are given in Table 7.8. The results show good agreement between the codes for UOX and MOX fuels. Due to the discretisations used in the S_n method, the S_n results are higher than the Monte Carlo ones but the discrepancies are quite constant.

For the well thermalised UOX lattices studied, there is a good C-E agreement. We can notice that there is no discernible trend either with ^{235}U enrichment or with moderation ratio.

For the MOX fuels, the C-E comparison shows a slight underestimation but only one experimental programme has been calculated so we must be careful not to conclude too quickly.

Table 7.8. Calculated k_{eff} for the selected experiments

Statistical uncertainty in parentheses

Experiment	APOLLO-2/ MORET-4	APOLLO-2/S_n	TRIPOLI-4	MONK
LCTH007/1	0.9982 (0.0010)	1.0064	1.0019 (0.0010)	0.9960 (0.0010)
LCTH007/2	1.0014 (0.0010)	1.0102	1.0027 (0.0010)	0.9968 (0.0010)
LCTH007/3	0.9995 (0.0010)	1.0073	0.9985 (0.0010)	0.9960 (0.0010)
LCTH006/3	1.0017 (0.0010)	1.0059	0.9980 (0.0010)	
LCTH006/4	1.0005 (0.0010)	1.0019	1.0006 (0.0010)	
LCTH006/8	1.0019 (0.0010)	1.0056	0.9997 (0.0010)	
LCTH006/13	1.0021 (0.0010)	1.0059	0.9981 (0.0010)	
LCTH006/18	1.0023 (0.0010)	1.0067	0.9986 (0.0010)	
LCTH035/B1	0.99910 (0.0010)	1.0051	0.9990 (0.0010)	
LCTH035/B2	0.99770 (0.0010)	1.0028	0.9985 (0.0010)	
LCTH035/C1	0.99575 (0.0010)	0.9971	0.9911 (0.0010)	
MCTH004/2	0.9966 (0.0010)	0.9986	0.9933 (0.0010)	0.9937 (0.0010)
MCTH004/5	0.9989 (0.0010)	1.0001	0.9954 (0.0010)	0.9953 (0.0010)
MCTH004/8	1.0002 (0.0010)	1.0014	0.9994 (0.0010)	0.9944 (0.0010)
MCTH004/10	0.9996 (0.0010)	1.0012	0.9971 (0.0010)	0.9945 (0.0010)

Other benchmark results

Additional configurations from the above experiments have been calculated using MONK. For eight of the nine uranium lattice experiments studied (71 configurations in total, excluding the apparently anomalous lead-reflected set), the mean k_{eff} is 0.9994 ± 0.0034. The MONK/JEF-2.2 results for lead-reflected lattice from Valduc are significantly higher than the measurements, even though the fuel rods involved are the same as those used in other experiments where good agreement is observed. This suggests that there are errors/uncertainties in the JEF-2.2 lead data, particularly as similar discrepancies have been reported by other analysts (see JEF/DOC-604).

For the mixed oxide lattices, six systems in total have been studied using MONK with four different plutonium compositions in the fuel. For these experiments (63 configurations in total), the mean k_{eff} is 0.9962 ± 0.0032, which confirms the slight underestimation observed previously.

Summary of results

The findings of this study can be summarised as follows:

- *Plutonium solutions*
  No observable trend of the C-E results with spectrum hardness was observed. Some evidence of calculation over-prediction was obtained with a tendency to increase with ^{240}Pu content. The overall C-E were of 300 pcm for ^{240}Pu content lower than 5% and of 600 pcm for ^{240}Pu content of 19%.

- *Low enriched uranium solutions*
  The agreement is quite good between calculations and results for low and intermediate concentrations. At very high concentrations, the only available benchmark indicates an over-prediction of about 1 000 pcm. Additional experimental evidence is required and could be provided by a re-evaluation of old Valduc UO_2F_2 experiments.

- *Highly enriched uranium solutions*
  A clear evidence of over-prediction was obtained with a trend to increase with uranium concentration, reaching about 1 000 pcm. Other investigations showed the same trend for wet uranium powders as those encountered in fuel fabrication process. These over-predictions are likely to be cancelled with the JEFF3T (ENDF/BVI-Release 5) ^{235}U evaluation.

- *Mixed uranium and plutonium solutions*
  It was not possible to conclude, as the different investigated experiments provided contradictory trends. The results suggested possible experimental biases and a need for "cleaner" configurations was stressed (the ones considered contained polyethylene and concrete).

- *Low-enriched uranium lattices*
  A general good agreement was found. A slight tendency to under-predict was obtained with MONK. It is also believed that the new ^{235}U evaluation adopted in JEFF3T (originated from ENDF/BVI-Release 5) would lead to less good results for some of the tight lattices.

- *Mixed oxide lattices*
  An under-prediction of about 400 pcm was observed. Here also, there is a need for more precise experiments.

Inconsistencies between different experimental programmes were noted in many cases. The status of experimental uncertainties is not always obvious in the experimental evaluations, especially the confidence interval defined by this uncertainty. Possible correlations and systematic errors could not be discarded.

W. Bernnat, *et al*. [5] performed a comparative study of the performance of different libraries (ENDF/B-V, -VI, JENDL-3.2 and JEF-2.2) using the MCNP-4B code. As far as JEF-2.2 is concerned, the conclusions are not always consistent with the results presented in this paper. For instance, an under-prediction of about -400 pcm was found by Bernnat, *et al*. for highly enriched solutions while an over-prediction (up to 1 000 pcm) is obtained in this paper. The same situation is found for plutonium solutions for which we conclude to an over-prediction of about 500 pcm in average while Bernnat, *et al*. do not observe a tendency to over-prediction. More detailed comparisons are required to understand these discrepancies. When comparing the results obtained with different evaluations, Bernnat, *et al*. observe some significant discrepancies (up to 600 pcm) due to differences in the nuclear data of important nuclides. Elastic scattering of ^{16}O in the slowing-down region is responsible for about 250 pcm of this difference and the same amount of difference comes from the data of ^{235}U, ^{238}U and ^{239}Pu.

Effect of nuclear data uncertainties

The effect of microscopic data uncertainties on the calculation of integral parameters could be assessed using error propagation formulae defined later. We will limit ourselves here to the effective

multiplication factor, which is the main parameter investigated in criticality analysis. The following definitions are introduced first:

- S: column vector whose elements are the sensitivity coefficients defined as the relative variation of k_{eff} due to relative change of nuclear data item x_i:

$$S_i = \frac{\Delta k/k}{\Delta x_i/x_i}$$

- V: symmetric matrix called the correlation matrix whose elements are defined as:

$$V_{ij} = \sigma_i \mathrm{cov}(x_i, x_j)\sigma_j$$

where σ_i is the uncertainty (standard deviation) of a nuclear data item x_i and $\mathrm{cov}(x_i,x_j)$ is the correlation (covariance term) between two nuclear data items.

Nuclear data items considered in this preliminary sensitivity analysis are: the number of neutrons emitted by fission, cross-sections for fission, capture, scattering (P_0 term only) and (*n*,*xn*) reactions. Sensitivity and correlation coefficients are given for each nuclear data item and in each group belonging to a 15 group energy mesh. Sensitivity coefficients have been calculated using the assembly code APOLLO-2 with the fundamental mode assumption. The correlation coefficients are those defined by E. Fort, *et al*. [6] and used for the adjustment of the JEF-2.2 based application library ERALIB-1 for fast neutron reactors.

The *a priori* uncertainty *u* on k_{eff} due to nuclear data uncertainties is defined as:

$$u^2 = S^T V S$$

which can be split into different terms in order to evaluate the contribution of each nuclide and each reaction. This uncertainty is to be considered in the sense of a standard deviation, i.e. the square of *u* is the summation of the square of independent contributions. In the following, *u* will be expressed in pcm (10^{-5}).

In order to evaluate the effect of energy correlation in nuclear data (covariance terms), the *a priori* uncertainty was calculated with all available terms of matrix *V* and also considering only a diagonal matrix (no correlation terms). The following materials were investigated:

- Plutonium nitrate solutions.
- Highly enriched uranium nitrate solutions.
- Highly enriched uranium fluoride solutions.
- Low enriched and moderated uranium powders.
- Low moderated mixed oxide powders.
- Arrays of UO_2 pins.

The results are reported in Table 7.9. The effect of nuclear data uncertainties on calculated integral parameters ranges from about 500 pcm up to 1 400 pcm. Also, we clearly see that the covariance data have an important effect on the calculated a priori uncertainty and neglecting the correlation coefficients tends to underestimate the effect of nuclear data uncertainties on the calculated integral parameter. Unfortunately, it is difficult to collect these data since evaluated files describe them for a few nuclides only. For the other nuclides rough estimates are used assuming that the correlation coefficients are of the kind described below for the 15 group structure used:

$$\mathrm{cov}(x_i, x_i) = 1$$

$$\mathrm{cov}(x_i, x_{i+1}) = 0.66$$

$$\mathrm{cov}(x_i, x_{i+2}) = 0.33$$

$$\mathrm{cov}(x_i, x_j) = 0 \text{ for the other terms}$$

When individual contributions to the *a priori* uncertainty are considered (data not shown) we can classify nuclides and reactions in the order of importance for each configuration. This can be summarised as follows:

- For homogeneous solutions (nitrate, fluoride) the most important contribution to the uncertainty comes from water crosssections – both capture (from 200 pcm to 1 400 pcm) and scattering (from 500 to 700 pcm); for well thermalised solutions, the water capture effect dominates.

- For low moderated uranium powders, three equally important contributions (each about 400 pcm) are observed: water scattering, ^{238}U capture and ^{235}U (fission and capture).

- For low moderated uranium and plutonium powders the most important contribution comes from ^{239}Pu (from 700 pcm to 1 000 pcm) followed by ^{241}Pu and ^{240}Pu (about 250 pcm).

- For UO_2 pin arrays we find a situation that is comparable to homogeneous powders: water scattering, ^{238}U capture and ^{235}U fission are equally important (about 300 pcm). When the moderation ratio is very high, water capture becomes, as for solutions, the dominant component (about 600 pcm) followed by the previous ones (about 200 pcm).

These results clearly indicate that the variety of configurations encountered in criticality safety leads to a variety of sensitivity profiles. This fact is very important when adjustment procedures are considered since it provides a means of separating the main parameters and minimising compensating effects, thereby facilitating the extraction of pertinent microscopic information from integral experiments. As far as we are aware, this issue has not been extensively investigated specifically for the field of criticality safety and might represent a new challenge in the near future. It should also be noted that the magnitude of the nuclear data uncertainties for the types of material studied in the inter-code comparison exercises are consistent with the differences observed between calculation and experiment. This suggests that data adjustments within the experimental uncertainties could be used to reduce the calculated bias.

Table 7.9. The *a priori* uncertainty calculated with all available terms of matrix *V* and also considering only a diagonal matrix

Material →	Nitrate plutonium solutions	Nitrate uranium solutions	UO_2F_2 solutions	UO_2 wet powders	MOX wet powders	UO_2 pins
u (in pcm)	700-1 400	700-900	800-1 200	650	1 000	550-700
u without correlation terms (in pcm)	500-1 300	500-750	700-1 200	540	700	400-600

Conclusions

Within the JEFF project, there have been constant efforts to organise the validation work and to share the results. The participants in intercomparison exercises obtained beneficial feedback, ending by improvements in both the nuclear data file and computer codes. The results obtained by the different codes are more and more close but there still remain some problems to be addressed (self-shielding problems in multi-group calculations with structural material reflectors Fe, Ni, effect of the delayed neutron component on the fission spectrum, etc.).

This study shows that, in general, non-adjusted JEF-2.2 based libraries are performing quite well for criticality applications; at least as good, or even better, than adjusted libraries based on former versions (JEF-1, ENDF/B-IV and V). Some areas need more refinements, e.g. plutonium solutions, highly enriched and concentrated uranium solutions, structural materials reflected configurations (lead, iron, etc.). The next version of the evaluation file in preparation (JEFF-3) already integrates some of this feedback and will certainly go a step forward in the improvement of calculation predictions.

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[6] E. Fort, *et al.*, "Realisation and Performance of the Adjusted Nuclear Data ERALIB1 for Calculating Fast Reactor Neutronics", Proc. PHYSOR'96, Mito, pp. F.21-F.30 (1996).

Annex

List of JEF Documents Related to JEF-2.2 Benchmarking for Criticality Safety Studies

JEF/DOC-430 Benchmarking JEF2.2 with MONK; N.R. Smith, D. Hanlon and A.K. Ziver.

JEF/DOC-461 Some Provisional Results from the 1993/94 UK JEF-2.2 Benchmarking Programme; N.T.Gulliford, D. Hanlon, G.A. Wright.

JEF/DOC-462 The UK JEF International Benchmarking Programme: Current Status and Future Programme (Draft); N.T. Gulliford.

JEF/DOC-481 UK Integral Benchmark Programme for JEF (Draft), June 1994; N.T. Gulliford.

JEF/DOC-525 A Contribution to the Criticality Benchmark Qualification of JEF-2.2; A. Nouri, G. Poullot, G. Courtois.

JEF/DOC-526 Contribution to JEF.2 Qualification of Pu Solution Calculations; A. Santamarina, B. Roque.

JEF/DOC-544 Calculation of Pu Solutions Based on JEF-2 Files Analysis of the VALDUC Benchmark Experiments; B. Roque, A. Santamarina, C. Mattera.

JEF/DOC-545 Inter-Code Comparison for Nitrate Plutonium Solutions using JEF-2.2; A. Nouri, N. Smith.

JEF/DOC-595 Validation of Thermal Pu JEF-2.2 Data – The PNL and VALDUC Benchmarks; A. Hogenbirk.

JEF/DOC-596 Inter-Code Comparisons for Highly Enriched Uranium Fluorine Benchmarks; N. Smith, A. Nouri.

JEF/DOC-604 Water Moderated and Lead Reflected UO_2 Pins Array: A Benchmark Test for Lead Cross-Sections; A. Nouri, G. Poullot, N. Smith.

JEF/DOC-620 Inter-Code Comparison for Uranium and Plutonium Homogeneous Solutions Using JEF-2.2; A. Nouri, N. Smith.

JEF/DOC-639 Updated JEF-2.2 Pu data – The Effect on Several Benchmarks; A. Hogenbirk.

JEF/DOC-696 Overview of JEF-2.2 Qualification for Criticality Calculations; A. Nouri, N. Smith.