ACHIEVING INDUSTRY ACCEPTANCE OF A JEF2.2 NUCLEAR DATA LIBRARY FOR MONK

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Abstract

An identified requirement of the UK nuclear industry has been to move to a position of employing data libraries based on the international library JEF, so that advantage can be taken of more modern nuclear data evaluations. Since the release of a frozen version of the library (JEF2.2) a programme of work has been undertaken in the UK to develop nuclear data libraries for use in reactor physics, shielding and criticality application codes and to provide benchmark evidence to support their use. For criticality, this has involved developing a hyper-fine group energy library for the MONK code and undertaking a large programme of comparison calculations for selected international experiments. This paper summarise the work involved in arriving at the current stage whereby use of MONK in conjunction with a JEF2.2-based library is accepted within the UK nuclear industry. The support of BNFL and British Energy during the course of this work is gratefully acknowledged.

Introduction

Modern nuclear criticality safety analysis places great reliance on calculations performed using computer codes, in particular those employing the Monte Carlo method of solution. In the United Kingdom the acknowledged standard Monte Carlo code for criticality safety assessment is MONK [1]. The accuracy achievable with MONK is ultimately governed by the accuracy of the nuclear data employed and their representation within the code nuclear data library. For some time the MONK nuclear data library has been largely based on the frozen United Kingdom Nuclear Data Library (UKNDL). An identified requirement of the UK nuclear undustry has been to move to a position of employing libraries based on the international library JEF, so that advantage can be taken of modern nuclear data evaluations.

The release of a frozen version of the JEF library during 1992 (JEF2.2) enabled code-specific libraries to be produced for benchmarking in the major application areas. Work leading to the production of an initial JEF2.2-based MONK library was performed during 1992-94 and this was followed by further library development work to improve the resonance representation, thermal cross-section data, and the plutonium fission spectrum. The resulting MONK nuclear data library is known as DICE96J2V4[1] and includes cross-sections stored in a 13,193 energy group scheme (compared with 8,220 groups for the UKNDL-based library). This paper summarises work performed during the period 1996 to 1999 supported by BNFL and British Energy which has resulted in the acceptance of the MONK JEF2.2-based library for criticality applications in the UK. The results of MONK calculations using the JEF2.2 library are summarised and some general conclusions are drawn on the predictive capability of the MONK/JEF2.2 package.

Use of Validation Data

In order to help assess criticality safety or a particular situation, the k-effective calculated by MONK can be used in a criterion of the form $k_{MONK} + E_{PD} + E_{SM} + E_R + E_{MC} < 1\text{-}X$
where:

- E_{PD} is an allowance for the systematic bias of the MONK code and data library and may be positive or negative if sufficient justification can be made
- E_{SM} is the total random error made up from random errors in the preparation and execution of the MONK calculation
- E_R is the bias to allow for operational or accidental changes causing increases in reactivity
- E_{MC} is a function of the statistical uncertainty of the Monte Carlo method.
- X is a sub-critical allowance depending on operational and/or regulatory requirements

It is the value of the systematic bias (E_{PD}) that is of direct relevance here as it is chosen to allow for apparent errors/uncertainties in the nuclear data and their representation in the code based on the validation calculations. In fact E_{PD} can be split into two components:

- E_{PD1} arising from the agreement observed between calculation and experiment
- E_{PD2} arising from any interpolation/extrapolation required to move from experiment to intended application

[1] DICE is the name of the module of both MONK and MCBEND (a Monte Carlo shielding code) that performs neutron collision modelling; 96 is the year the library was produced; J2 means JEF2; V4 means version 4 of the DICE JEF2.2-based library

Where the criticality analyst has at his/her disposal 'exact' experimental matches (in terms of nuclides, geometry, neutron spectrum, leakage etc.) for the intended application, E_{PD2} would be zero and the value of E_{PD} would depend solely on how the code results agreed with the experimental measurements (E_{PD1}), with suitable allowance for experimental uncertainties. Unfortunately exact matches are rare, although adequate basic similarity is more common.

In the absence of suitable levels of similarity, the interpolation/extrapolation uncertainty (E_{PD2}) must be dealt with and here sensitivity analysis comes into play. One of the benefits of the Monte Carlo method, and the use of physically realistic interaction modelling in particular, is the confidence with which interpolation (and limited extrapolation) of the validation data can be performed. This is especially true when using an unadjusted nuclear data library such as the MONK JEF2.2-based library being benchmarked here. However, extrapolation in the absence of experimental data should be treated with extreme caution, and the range of applicability of derived E_{PD1} and E_{PD2} values must be clearly defined.

Summary of Results

The summary of MONK/JEF2.2 results given below is broken down under six broad system types. The experiments studied have been taken from various international laboratory programmes, with the majority of the experimental descriptions being taken from the handbook of the International Criticality Safety Benchmark Evaluation Project [2]. Comparisons are made both with experimental values and with MONK calculations using the well-established UKNDL-based library that has been in use with MONK since 1987.

Uranium Oxide Lattice Systems

For low-enriched UO_2 lattice systems there is strong evidence to suggest that the JEF2.2-based library with MONK can calculate k-effective close to the level of the experimental uncertainties. Good agreement between calculation and experiment is observed for uranium lattices for a range of systems (enrichment, moderator ratio, absorbers) from different international laboratories. The JEF results are consistently better than those using the UKNDL library (particularly for the under-moderated lattices where MONK/UKNDL can over-predict by up to 1%) and are generally within two experimental standard deviations of unity.

For eight of the nine experiments studied (71 configurations in total, excluding the apparently anomalous lead-reflected experiment 32 in Table 1), the mean k-effective is 0.9994 $\pm$0.0004, compared with 1.0083$\pm$0.0006 for MONK with its standard UKNDL library; thus adoption of the JEF library would produce more accurate predictions for uranium lattices and also remove the long-standing more significant over-prediction of MONK for under-moderated systems. The MONK/JEF2.2 results for Experiment 32 are significantly higher than both those for MONK/UKNDL and the measurements, even though the fuel rods involved are the same as those used in Experiments 2 and 40 where good agreement between MONK/JEF2.2 and experiment is observed (and the MONK/JEF2.2 results are lower than the MONK/UKNDL values). This suggests that there are errors/uncertainties in the JEF2.2 lead data, particularly as similar discrepancies have been reported by other analysts. This data problem needs to be investigated further, although based on the experiment studied, the effect is conservative from a criticality safety point of view.

The mean calculated results by moderation level for all the uranium oxide experiments are plotted in Figure 1 (note that the $H:U_{fissile}$ values are pin-cell averages). This graph also shows the results for very under-moderated powder experiments for which the agreement between calculation and experiment is comparable with that for the lattices. A summary of the uranium oxide lattice experiments studied is given in Table 1 (for each experiment several cases have been calculated).

MONK Exp. No.	Description	Reference
1	2.35 Wt% U^{235} enriched UO_2 pins in water with various absorbers	LEU-COMP-THERM-016
2	4.75 Wt% U^{235} enriched UO_2 pins in water with various pitches	LEU-COMP-THERM-007
3	4.31 Wt% U^{235} enriched UO_2 pins in water with various absorbers	LEU-COMP-THERM-009
7	2.46 Wt% U^{235} enriched UO_2 pins in water with various absorbers	BAW-1484-7 [3]
25	4.46 Wt% U^{235} damp U_3O_8 powder in cubic aluminium cans	NUREG/CR-0674 [4]
27	7 Wt% U^{235} enriched UO_2 pins in water	LEU-COMP-THERM-018
32	4.75 Wt% U^{235} enriched UO_2 pins in water with lead reflector	LEU-COMP-THERM-027
40	4.75 Wt% U^{235} enriched UO_2 pins in water with hafnium reflector	LEU-COMP-THERM-029
42	Low-enriched damp powder reflected by polythene	MARACAS [5]
45	Up to 10 Wt% U^{235} enriched UO_2 pins in water	LEU-COMP-THERM-022.
50	Low-enriched uranium lattices (VVER fuel)	LEU-COMP-THERM-015

Table 1 - Summary of Uranium Oxide Experiments

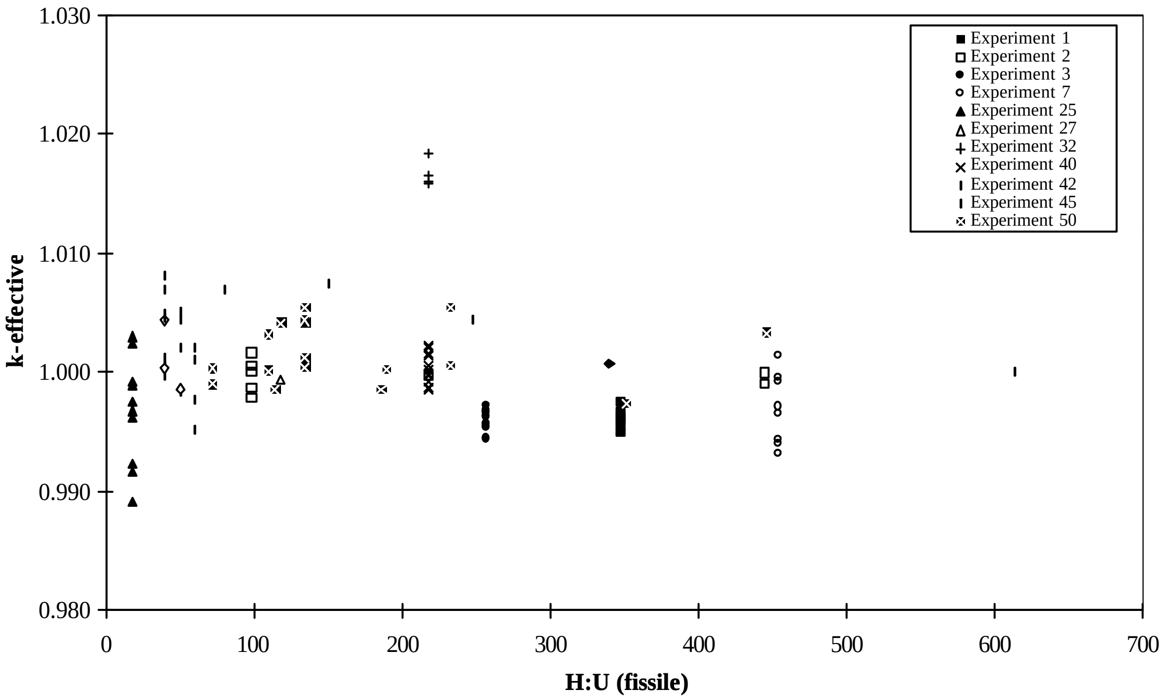

Figure 1 - Plot of MONK/JEF2.2 Calculated k-effective against $H:U_{fissile}$ atom ratio - Uranium Oxide

Mixed Uranium-Plutonium Oxide Lattice Systems

Good agreement is also obtained for mixed oxide lattice experiments, with MONK/JEF2.2 results generally better than those for the UKNDL library. Six systems have now been studied with four different plutonium compositions in the fuel. For these experiments (63 configurations in total), the mean k-effective is 0.9962±0.0004, compared with 0.9922±0.0005 for MONK with the UKNDL library. Therefore adoption of the JEF library would significantly reduce the under-prediction present in the UKNDL MONK library.

The mean calculated results by moderation level for all the mixed oxide experiments are plotted in Figure 2 (note that the H:$(Pu+U)_{fissile}$ values are pin-cell averages). This shows the general good agreement over a wide moderation range but also shows that for MONK/JEF2.2 calculations, the consistent under-prediction observed for MONK/UKNDL has only been reduced, not eliminated. A summary of the mixed uranium-plutonium oxide experiments studied is given in Table 2.

MONK Exp. No.	Description	Reference
6	Homogeneous PuO_2/UO_2/polystyrene with H:(Pu+U) ratio = 51.85	NT Vol. 26 [6]
11	Mixed PuO_2/UO_2 pins in water (19.84wt% Pu, 11% Pu^{240})	MIX-COMP-THERM-001
16	Mixed PuO_2/UO_2 pins in water (19.84wt% Pu, 11% Pu^{240}) with boral	PNL-3313 [7]
19	Mixed PuO_2/UO_2 pins in water (4.0wt% Pu, 18% Pu^{240})	MIX-COMP-THERM-005
39	Mixed PuO_2/UO_2 pins in water (19.84wt% Pu, 11% Pu^{240}) with Gd	PNL-3313 [7]
44	Mixed PuO_2/UO_2 pins in water (3.0wt% Pu, 22% Pu^{240})	MIX-COMP-THERM-004
48	Mixed PuO_2/UO_2 pins in water (6.6wt% Pu, 8% Pu^{240})	MIX-COMP-THERM-003

Table 2 - Summary of Mixed Uranium-Plutonium Oxide Experiments

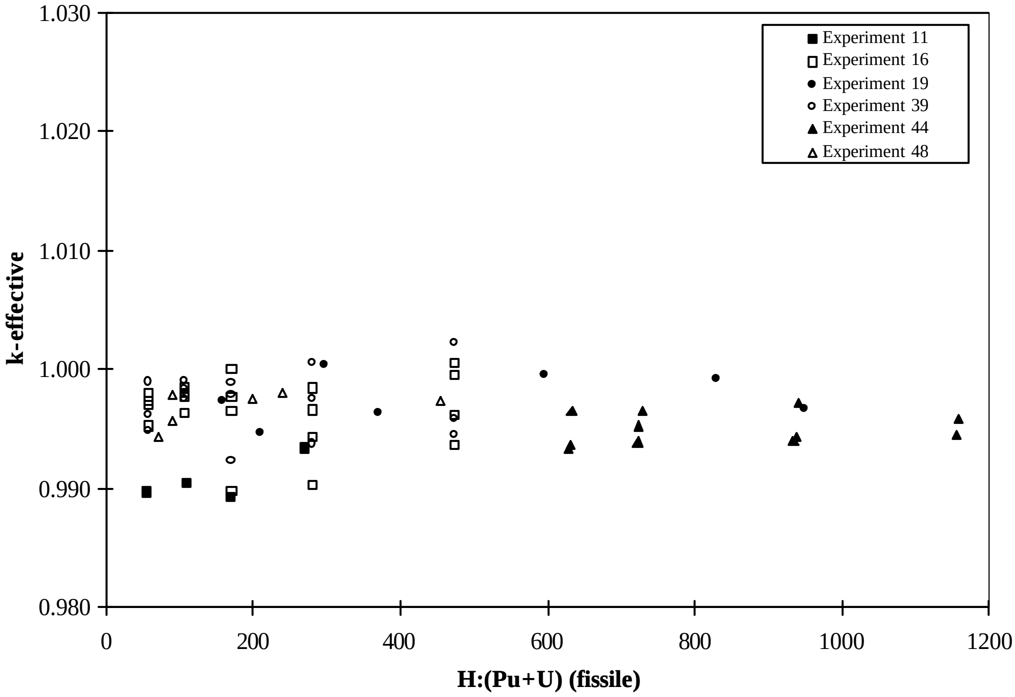

Figure 2 - Plot of MONK/JEF2.2 Calculated k-effective against H:$(Pu+U)_{fissile}$ atom - Mixed Oxide

Uranium Solution Systems

Six uranium solution systems have been studied, involving both low and high-enriched uranium. These result in a mean over-prediction at about the two experimental standard deviation level for the harder spectrum case (experiment 13) but generally better agreement for the other experiments. Experiment 52 shows a trend in calculated k-effective with respect to Gadolinium concentration.

This trend is also seen for other code/data combinations reported in the benchmark specification document [2]. The overall mean calculated value (excluding experiment 52) from the 50 configurations is 1.0017±0.0009 and the results are shown in Figure 3. In all cases the results are lower than those for the UKNDL data but there is some evidence of a possible correlation between the calculated values and $H:U_{fissile}$ ratio. However, it should be noted that the over-prediction observed for experiment 13 is also displayed for results using KENO (ENDF/B-IV data) and MCNP (ENDF/B-V data) reported in the ICSBEP handbook, possibly indicating systematic experimental uncertainties; removal of Experiment 13 from the figure would go some way towards removing the suggestion of a correlation effect. However, given the experimental uncertainties present, a decision to discard one of the experiments will not be taken until additional supporting data are available.

MONK Exp. No.	Description	Reference
13	High-enriched Uranyl Nitrate Solutions at various H:U ratios (93.17wt% U^{235})	HEU-SOL-THERM-002
23	Uranyl Nitrate Solution (~95% enriched)	HEU-SOL-THERM-013
35	High-enriched Uranyl Nitrate Solutions (U concentration from 20-700 g/l)	HEU-SOL-THERM-009/012
43	Low-enriched uranyl nitrate solutions	LEU-SOL-THERM-002
51	Low-enriched uranium solutions (new STACY experiments)	LEU-SOL-THERM-004
52	High-enriched uranyl nitrate solution with dissolved Gd poison	HEU-SOL-THERM-018

Table 3 - Summary of Uranium Solution Experiments

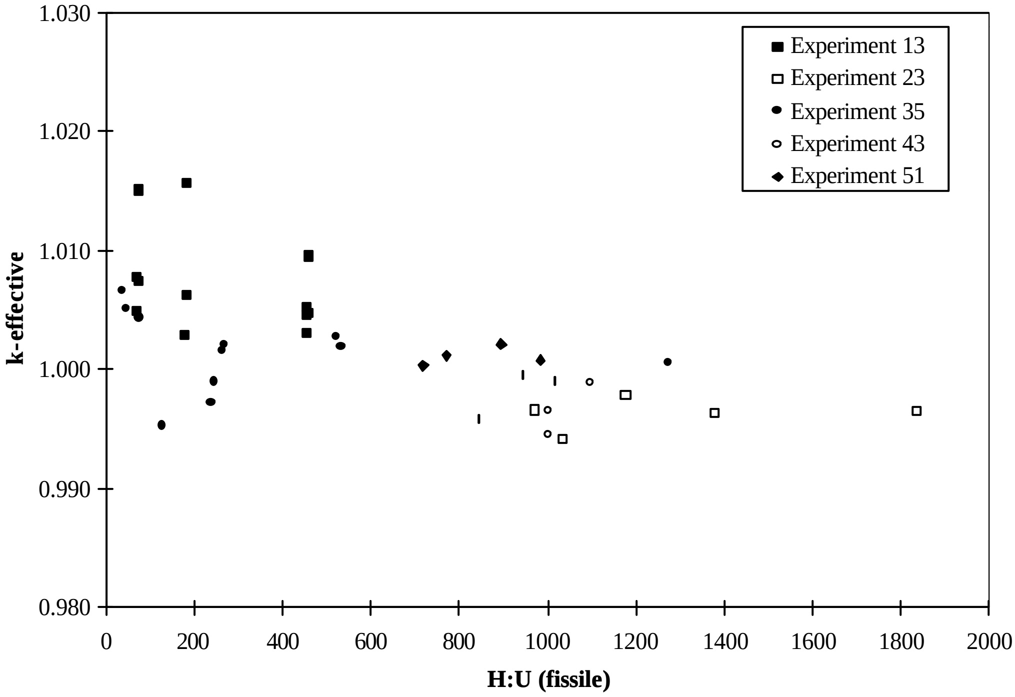

Figure 3 - Plot of MONK/JEF2.2 Calculated k-effective against $H:U_{fissile}$ atom ratio - Uranium Solutions

Plutonium Solution Systems

For plutonium nitrate solution experiments there is strong evidence to suggest that the JEF2.2-based library with MONK over-predicts the value of k-effective by about 0.5% (see Figure 4). This evidence is based on eleven independent experiments (involving over one hundred configurations) performed at two experimental facilities over a wide range of moderation. The overall mean calculated value of k-effective is 1.0069±0.0007. If Experiment 38 is excluded (which shows anomalous over-predictions of almost 2%), the mean value reduces to 1.0046±0.0004. Thus on average MONK/JEF will calculate plutonium solution systems approximately 0.5% higher than MONK/UKNDL, where excellent agreement with experiments is generally observed.

The over-prediction by MONK/JEF2.2 is reasonably consistent across the full range of $H:Pu_{fissile}$ ratio, although there is some evidence of a slightly higher over-prediction for the experiments with higher Pu240 contents (experiments 12, 14 and 22 have much higher Pu240 content that the others) - the mean values are 1.0032±0.0006 and 1.0067±0.0004 for high and low Pu240 cases respectively.

MONK Exp. No.	Description	Reference
5	Plutonium Nitrate Solutions (4.6 wt% Pu^{240}, Pu: 24.4 - 172.3 g/l), various reflectors	PNL-2700 [8]
12	Plutonium Nitrate Solutions (42.9 wt% Pu^{240}, Pu: 40.6 - 140.0 g/l)	NS&E Volume 52 [9]
14	Plutonium Nitrate Solutions (18.9 wt% Pu^{240}, Pu: 28.7 - 152.0 g/l)	PU-SOL-THERM-022
18	Plutonium Nitrate Solutions (4.67 wt% Pu^{240}, Pu: 73.0 - 268.7 g/l)	PU-SOL-THERM-001
20	Plutonium Nitrate Solutions (4.05 to 4.40 wt% Pu^{240}, Pu: 29 - 41 g/l)	PU-SOL-THERM-005
21	Plutonium Nitrate Solutions (3.12 wt% Pu^{240}, Pu: 25 - 27 g/l)	PU-SOL-THERM-006
22	Plutonium Nitrate Solutions (19.0 wt% Pu^{240}, Pu: 13 - 105 g/l)	PU-SOL-THERM-012
26	Plutonium Nitrate Solutions (3.12 wt% Pu^{240}, Pu: 50 - 77 g/l)	PU-SOL-THERM-002
28	Plutonium Nitrate Solutions (1.76 to 3.12 wt% Pu^{240}, Pu: 33 - 44 g/l)	PU-SOL-THERM-003
29	Plutonium Nitrate Solutions (0.54 to 3.43 wt% Pu^{240}, Pu: 26 - 40 g/l)	PU-SOL-THERM-004
38	Plutonium Nitrate Solutions (19.0 wt% Pu^{240}) with Hf plates	SEESNC No. 129 [10]
49	Interacting cylinders of Plutonium Nitrate Solution in air	PU-SOL-THERM-013

Table 4 - Summary of Plutonium Solution Experiments

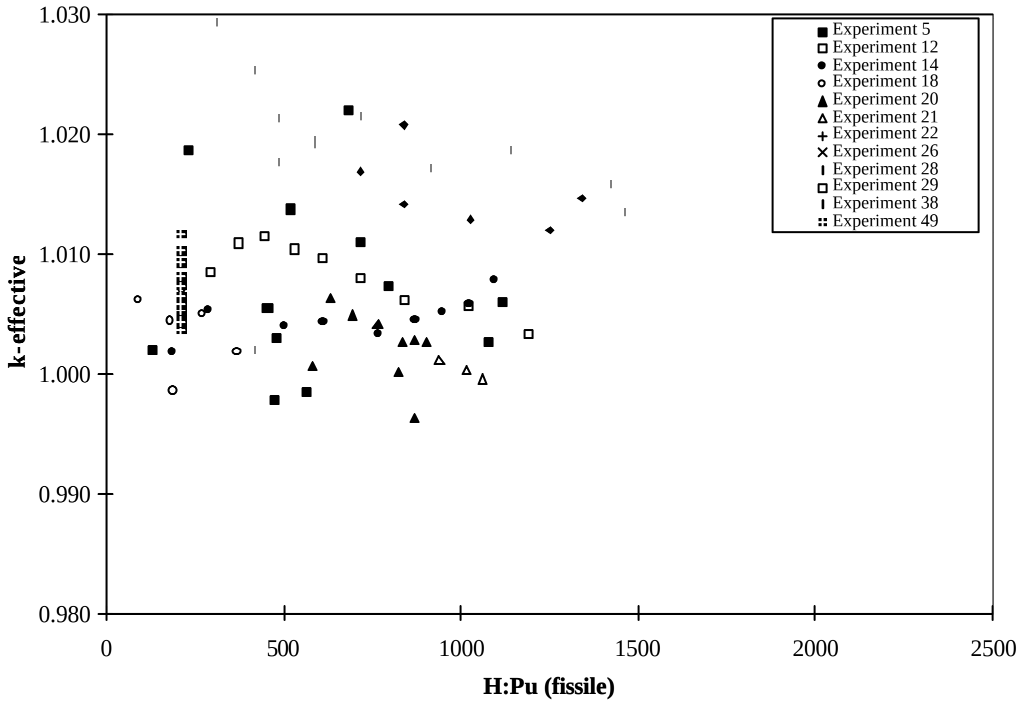

Figure 4 - Plot of MONK/JEF2.2 Calculated k-effective against $H:Pu_{fissile}$ atom ratio - Plutonium Solutions

Mixed Uranium-Plutonium Solution Systems

For mixed nitrate solution systems there is reasonable agreement between MONK/JEF2.2 and experiment, particularly for the higher moderation levels (see Figure 5). At lower moderation levels, the agreement is more in line with the mixed oxide lattice experiments, where a small under-prediction is observed (together with generally better agreement with experiment than MONK/UKNDL).

The mean value overall for MONK/JEF from the 58 configurations is 1.0001±0.0011 but there remains some evidence of a correlation between calculated k-effective and H:(Pu+U).

MONK Exp. No.	Description	Reference
10	Water reflected cylinders of Pu/U nitrate (58 - 330 g (Pu+U)/l, 0.4 Pu/(Pu+U))	MIX-SOL-THERM-003
17	Water reflected cylinders of Pu/U nitrate (42 - 300 g (Pu+U)/l, 0.3 Pu/(Pu+U))	NT Volume 26 [11]
24	Water reflected cylinders of Pu/U nitrate (61 - 489 g (Pu+U)/l, 0.22 & 0.97 Pu/(Pu+U))	MIX-SOL-THERM-001
30	Mixed Pu/U nitrate poisoned by Gd and B (~250 g (Pu+U)/l, 0.3 Pu/(Pu+U))	NS&E Volume 62 [12]
33	Water reflected cylinders of Pu/U nitrate (23 - 53 g (Pu+U)/l, 0.23 & 0.52 Pu/(Pu+U))	MIX-SOL-THERM-002

Table 5 - Summary of Mixed Uranium-Plutonium Solution Experiments

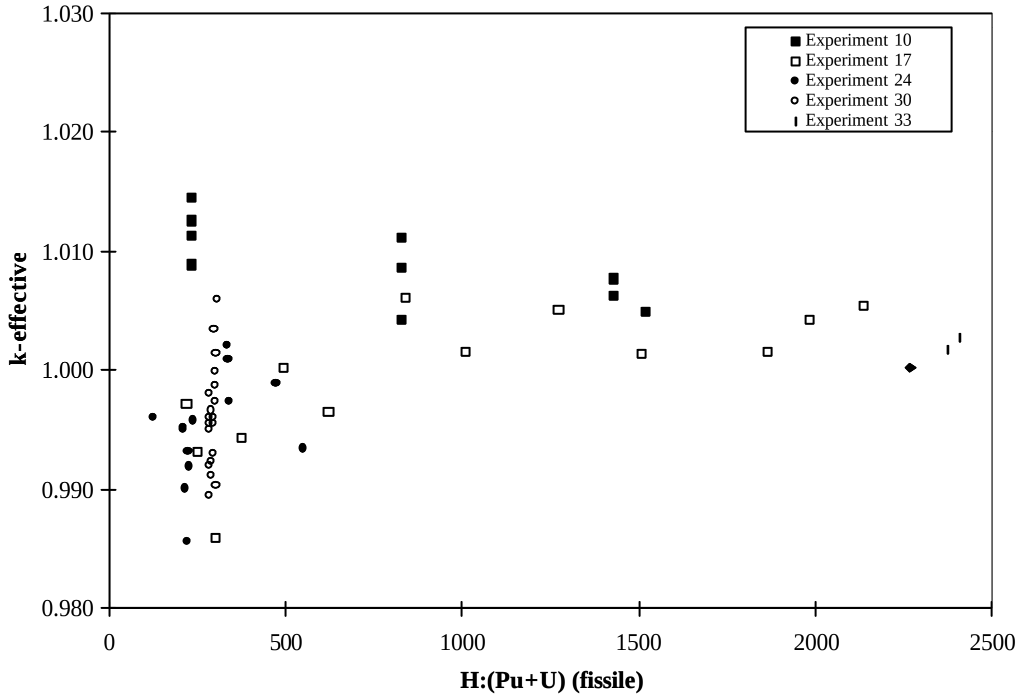

Figure 5 - Plot of MONK/JEF2.2 Calculated k-effective against H:$(Pu+U)_{fissile}$ atom ratio

Metal Systems

Uranium metal systems studied include bare and reflected metal spheres of both high and intermediate enrichment (>90% and ~36% respectively). The MONK/JEF2.2 results agree well with experimental values and there is a useful improvement in the agreement compared with MONK/UKNDL results. The mean value for the high enriched cases is 1.0037±0.0011 for MONK/JEF2.2 (compared with 1.0051±0.0010 for MONK/UKNDL) and that for the intermediate cases is 1.0061±0.0024 (compared with 1.0089±0.0018 for MONK/UKNDL).

Plutonium metal systems studied include bare and reflected metal spheres (1.5-20% Pu240) and the more intermediate energy metal plate assemblies. The MONK/JEF2.2 results agree well with experimental values and as for the uranium metal cases there is a useful improvement in the agreement compared with MONK/UKNDL results for the spherical cases. The mean value for the spherical cases (all Pu240 contents) is 0.9984±0.0012 for MONK/JEF2.2 (compared with 1.0064±0.0020 for MONK/UKNDL). For the more intermediate energy plate assemblies the improvement is much larger (up to several percent in k-effective), demonstrating the significant nuclear data improvements available in the JEF2.2 library over this energy range. For the seven plate assemblies, all but one of the MONK/JEF2.2 cases agrees with the measured value (not all are critical cases) within 1%, and the discrepant one only differs by 1.2%; for MONK/UKNDL, only one of the seven cases is within 1% of the measured value and the average difference is ~3%.

MONK Exp. No.	Description	Reference
9	Bare and natural uranium reflected uranium metal sphere	HEU-MET-FAST-001
36	High-enriched uranium metal spheres with various reflectors	HEU-MET-FAST-018
37	Intermediate-enriched uranium metal spheres with various reflectors	IEU-MET-FAST-003
46	High-enriched uranium metal plates in water	HEU-MET-THERM-006
47	High-enriched uranium metal/polythene stacks of cylinders	HEU-MET-FAST-034
8	Bare and natural uranium reflected plutonium metal sphere	PU-MET-FAST-001
31	Plutonium metal plates interspersed with plates of various other materials	MIX-MET-FAST-008
41	Plutonium metal spheres with various reflectors	PU-MET-FAST-030

Table 6 - Summary of Metal Experiments

Conclusions

This report has summarised the results of an extensive programme of benchmarking for MONK with a JEF2.2-based nuclear data library. The main conclusions of the programme are:

- Agreement between calculation and experiment for MONK/JEF2.2 is generally good taking into account both calculation and experimental uncertainties (i.e. generally within two standard deviations and often within one standard deviation)
- Agreement between calculation and experiment for MONK/JEF2.2 is generally better than for MONK/UKNDL - the main exception to this conclusion is for plutonium nitrate solutions where the MONK/JEF2.2 package tends to over-predict by about 0.5%
- Based on the generally improved agreement between calculation and experiment for the experiments studied to date and the pedigree of the JEF2.2 data, it has been proposed to the UK nuclear industry that the MONK JEF2.2 library should be adopted for criticality analysis

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