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An overview of JEF2.2 qualification for criticality calculations

(Preliminary draft)

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CONTENT

I. Introduction

This report summarises several benchmarking studies in the field of criticality-safety performed using different calculational codes. The common denominator between them is the utilisation of applications libraries based on the JEF2.2 evaluation. The studies reported here are originated from independent national programs in France and UK that are synthesised in paragraphs III and IV and from common work performed in the frame of the JEF working group through inter-comparison exercises, with contributions from AEAT-Winfrith, CEA-Saclay, CEA-Fontenay-aux-Roses, ECN-Petten and TUI-Delft (paragraph V). Sensitivity analysis are described in paragraph VI followed by general conclusions and perspectives.

II. Codes used

In UK, a continuing effort for the validation of JEF2.2 has been produced[1,2]. The code used is MONK7 which is a Monte-Carlo code employing hyperfine group cross sections (13,193 groups) and a continuous energy/angle treatment. The MONK library uses unadjusted JEF2.2 nuclear data as issued by the NEA data bank processed using NJOY in conjunction with a MONK-specific processing package.

In France a new criticality package, named CRISTAL, is being developed and extensively benchmarked; the calculation of more than 300 experimental configuration will be available in mid '98. This package is based on the three main codes: APOLLO2 (172 energy groups assembly and core code utilising Pij and Sn methods), MORET4 (multigroup Monte-Carlo code) and TRIPOLI4 (pointwise Monte-Carlo code) all these codes using application libraries based on the JEF2.2 evaluation. Thus, this work will bring additional information about the quality of JEF2.2 for criticality applications. Since this work is in progress, we will also refer to earlier published studies[3-6] with JEF2.2 where the following codes were used: APOLLO1 (99 energy groups assembly code utilising the Pij methods for flux calculation and specific self-shielding treatments), MORET3 (multigroup Monte-Carlo code using pre homogenised and self-shielded cross sections calculated with APOLLO1), TRIMARAN2 (multigroup Monte-Carlo code using pre homogenised and self-shielded cross sections calculated with APOLLO2).

MCNP4A was used[7] in inter-comparison studies. This codes uses a pointwise cross section library derived from JEF2.2 and a continuous energy/angle treatment.

KENOVa was also used[8] in the inter-comparison studies. This codes uses an application library derived form JEF2.2 (172-group structure). Specific modules from the SCALE system were also used.

III. Experimental programs investigated

Homogeneous Uranium media

There are three sub-classes of media in this category.

Low-enriched uranium solutions (more than 40 experiments): the experiments studied are:

- cylinders and spheres of UO_2F_2 solution, reflected by water (Valduc, 40 experiments),

- bare annular cylinder of UO_2F_2 solution (Sheba, 1 experiment),
- bare spheres of UO_2F_2 solution (ORNL, 3 experiments)

The uranium concentration range covered extends from 450 to 1080 g/l.

High-enriched uranium solutions (more than 30 experiments): the experiments studied are:

- cylinders of uranyl nitrate solutions reflected by concrete or plastic (Rocky Flats - 12 configurations)
- spheres of uranyl nitrate solution, unreflected, some with boron poisoning (CSWEG benchmarks - 5 configurations)
- spheres of water-reflected uranyl oxyfluoride solution (Oak Ridge - 11 configurations)
- cylinders of nitrate solutions (Valduc)

The overall U concentration range covered extends from 15 to 700 g/l.

Uranium Powder Systems (14 experimental configurations). The experiments studied are:

- homogeneous damp low-enriched uranium oxide powders (Springfields - 4 configurations)
- arrays of cans containing homogeneous damp low-enriched uranium oxide powder, with interstitial moderating and absorbing plates, reflected by plastic (Rocky Flats - 10 configurations)
- arrays of cans containing homogeneous damp low-enriched uranium oxide powder, with H :U ratio of 2 or 3, reflected by polythene (Valduc - in preparation)

Arrays of UO_2 pins

Different lattices of water moderated and partially or totally reflected, low enriched UO_2 pins were considered. The uranium enrichment varies from 2.6 % to 7 %. Square and triangular lattices with pitches from 1.26 cm to 1.80 cm were calculated including configurations with soluble (B, Gd) and solid poison (Hf, Cd, boral and steel) and with different reflector materials (water, concrete, lead). Experiments originated from B&W, PNL, Valduc and Winfrith.

Plutonium solutions:

The experiments studied (more than 120) are:

- numerous experiments (wide range of Pu concentrations) with water reflected plutonium nitrate solutions with ~4wt% Pu240 (PNL - 56 configurations)
- water-reflected and bare plutonium nitrate solutions (cuboidal and annular geometry) with ~19wt% Pu240 (Valduc - 32 configurations)
- water reflected plutonium nitrate solutions with ~43% Pu240 (PNL - 9 configurations)
- water-reflected plutonium nitrate solutions with ~19% Pu240, some poisoned with Hf plates (Valduc - 19 configurations)

The overall Pu concentration range covered extends from 13 to 268 g/l.

Homogeneous mixed (U+Pu) solutions

The experiments studied (more than 60) are:

- water and polythene-reflected cylinders of Pu/U nitrate solution with Pu/(U+Pu) ~ 0.25 (Aldermaston - 10 configurations)

water-reflected cylinders of Pu/U nitrate solution with Pu/(U+Pu) ~ 0.25 (PNL - 13 configurations)
- water, polythene and concrete-reflected annular cylinders of Pu/U nitrate solution poisoned by B with Pu/(U+Pu) ~ 0.22 and 0.97 (PNL - 13 configurations)
- water-reflected cylinders of Pu/U nitrate solution with Pu/(U+Pu) ~ 0.23 and 0.52 (PNL - 3 configurations)
- water-reflected cylinders of Pu/U nitrate solution poisoned by Gd and B with Pu/(U+Pu) ~ 0.25 (PNL - 19 configurations)
- water reflected solutions of Pu/depleted uranium with Pu/(U+Pu) ~ 0.30 (Valduc - 4 configurations)

The overall Pu concentration range covered extends from 11 to 195 g/l and the U concentration range extends from 3 to 380 g/l.

Mixed oxide pins

The experiments studied (more than 60) are:
- mixed U/Pu water-reflected lattices (~20% Pu) at various moderation levels, with and without absorbing plates and pins (PNL - 39 configurations)
- mixed U/Pu water-reflected lattices (~4% Pu) at various moderation levels (PNL - 7 configurations)
- mixed U/Pu (same composition as an UO_2 fuel, initial enrichment of 4.75 %, irradiated in a LWR to 37.5 GWd/t) water reflected square lattices (~1% Pu) at various moderation levels (Valduc - HTC program, 11 experiments)

Metal Systems

The experiments studied (27) are:
- bare and reflected uranium metal sphere (Los Alamos - 2 configurations)
- high-enriched uranium metal spheres with various reflectors (Russia - 5 configurations)
- intermediate-enriched uranium metal spheres with various reflectors (Russia - 4 configurations)
- bare and reflected uranium metal sphere (Los Alamos - 3 configurations)
- plutonium metal plates interspersed with various other materials (Winfrith - 7 configurations, including one oxide case)
- plutonium metal spheres with various reflectors (Russia - 6 configurations)

IV. Results

Homogeneous Uranium media

Low-enriched uranium solutions: the three experimental programs give inconsistent information. In fact, the calculated k-effective values for Valduc experiments (U concentration from 550 to 1080 g/l) are about 2000 pcm high, for the Sheba experiment (U concentration: 978 g/l) the calculated k-effective is about 1000 pcm high while reasonable good agreements with experiments are found for the ORNL experiments (U concentration from 452 to 491 g/l). This situation clearly indicate that problems do exist in some of the experimental programs investigated and it is difficult to conclude at this stage about the ability of JEF2.2-based calculations to reproduce the experimental values.

High-enriched uranium solutions: the calculated k-effective values show reasonable agreement with experiment (taking into account an experimental uncertainty of up to 500 pcm) and generally lie within ±500 pcm of the experimental values. Some exceptions exist for the Rocky Flats experiments but the larger over-predictions observed there are also seen for other code/data combinations reported in the ICSBEP handbook and, as there are no significant differences between the experiments in terms of nuclear data sensitivities, could be due to systematic experiment uncertainties.

Uranium Powder Systems: the calculated k-effective values for the Rocky Flats experiments are in reasonable agreement with experimental values, with most configurations within ±400 pcm of unity (although a couple of configurations under-predict by up to 1200 pcm. For the Springfields experiments however, under-predictions of up to ~5000 pcm are observed which seem hard to believe even though the spectrum for these cases is significantly harder than the Rocky Flats cases. Analysis of the MARACAS experiments is proceeding as an aid to further understand this discrepancy.

Arrays of UO_2 pins

The calculated k-effective values show general good agreement with experiments (at the level of the total calculation/experimental uncertainty) for cases describing simple lattices reflected by water; for the PNL and B&W cases, the calculated results tend to be low compared with unity (~300 pcm) whereas for the Valduc (without lead) and Winfrith experiments the calculated results are within the Monte Carlo uncertainty of the measured values (±100 pcm). Lead-reflected and concrete-reflected cases exhibit over-predictions of more than 1000 pcm, as the lattices are the same as the other Valduc experiment where good agreement is observed, this discrepancy would appear to be related to the lead cross-sections and to concrete composition (water content...). Hf and Cd poisoned cases also show high k-effective values.

Plutonium solutions

The calculated k-effective values show reasonable agreement with experiment (taking into account an experimental uncertainty of up to 500 pcm) and generally lie within 700 pcm above the experimental values; the highest calculation-experiment discrepancy being observed for very low Pu concentrations (~1000 pcm). The one exception is the set of experiments including those poisoned by Hf plates where over-predictions of ~1800 pcm are observed. As the solution properties are similar to other experiments where much better agreement with experiment is obtained, this would suggest systematic experimental uncertainties (problems with the JEF2.2 data for hafnium are not likely to be a significant contributor as this experiment includes unpoisoned cases that produce similarly high calculated results).

Homogeneous mixed (U+Pu) solutions

For the higher fissile concentration cases, the calculated k-effective values generally follow the trend of the mixed oxide lattices and show an under-prediction at the 300-400 pcm level. For the more dilute systems however, agreement with experiment improves such that

calculated results are within one standard deviation of unity. For low (U+Pu) concentrations the results are similar to those of Pu solutions; an over-prediction of about 1000 pcm is observed. The exception is for the Aldermaston experiments where larger over-predictions are observed (~1400 pcm). As these solutions have similar properties to those in the other sets of experiments, it is possible that systematic experimental uncertainties are the cause of this additional discrepancy.

Mixed oxide pins

The calculated k-effective values show reasonable agreement with experiment: the Valduc experiments give very good agreements (discrepancies are within the combined experimental and calculation uncertainties); a tendency towards under-prediction at the 300-400 pcm level is observed for the other experiments and in a small number of cases the under-prediction is about 1000 pcm although there appears to be no experimental difference for these systems. A further experiment (from JAERI) is being studied to try to add laboratory independence to the conclusions.

Metal Systems

For both the uranium and plutonium metal cases, agreement with experiment is generally within ±400 pcm.

V. Inter-code comparisons

Introduction

An early JEF inter-comparison exercise involving UO_2 lattice systems provided useful feedback both on the nuclear data and reactor physics calculation methods, particularly on the differences between Monte Carlo and deterministic methods[9]. This study also considered bare fast uranium and plutonium systems. Subsequently, two criticality code inter-comparison exercises for homogeneous systems have been performed within the framework of the JEF Working Group[7,8,10-13].

For these homogeneous exercises, the comparison has largely concentrated on the use of Monte Carlo methods. The two comparisons selected are in areas of significant interest for criticality assessors: plutonium nitrate and uranyl fluoride solutions. To avoid different interpretations of the experiments, the inter-code specifications have been taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook.

Plutonium Nitrate Solutions

The plutonium nitrate solution inter-comparison exercise comprised six configurations selected from two experimental programmes. The first three configurations were selected from programmes performed at the Pacific Northwest Laboratory (PNL). The Pu240 content varies from 3wt% to 5wt% and the plutonium concentration ranged from 27 to 119 g/l. These configurations were water reflected spheres. The second three configurations were selected from a programme performed at Valduc comprising plutonium nitrate solution (~19% Pu240)

n a large cubic tank reflected by water. The plutonium concentration ranged from 13.2 to 105 g/l.

In each case, in addition to the benchmark description provided in the ICSBEP handbook, infinite media calculations were performed and bare sphere calculations using a derived 'approximately critical' radius. The purpose for defining three models is as follows:
infinite media - this model aims to compare the main characteristics of the codes: cross-sections, slowing down models and self-shielding treatment. These features do not depend on the geometry, leakage and anisotropy treatment.
bare sphere - this model aims to compare the leakage calculation in the various codes. In order to consider near-critical systems, the spherical radii have been obtained by buckling conversions where the material bucklings have been calculated using the APOLLO1 code.
benchmark model - this model is used to compare calculations with experimental measurements.

Participants in the inter-comparison exercise were invited to provide results for k-effective together with fluxes, reaction rates and, where appropriate, leakage in both two and fifteen energy groups.

Early results in this inter-comparison showed a significant difference between the MONK results and those for WIMS, TRIPOLI and APOLLO. Investigation of the reaction rate results indicated that these differences were largely as a result of discrepancies in the thermal range (below 0.53 eV) with compensating differences being present in the lowest two groups of the fifteen energy group scheme used for the comparison. This difference was tracked down to an unnecessary approximation in the weighting function used in the processing codes employed to produce the MONK JEF library. When this was removed, the agreement was improved although there now appeared to be two sets of results with MONK and MCNP showing good agreement but both producing results inconsistent with the remaining set of codes. There was also some system dependency of the difference between the two code sets with the larger differences existing for the more concentrated and smaller systems.

The difference this time was eventually tracked down to an inconsistency in the JEF data library itself in the Pu239 file[14]. The JEF2.2 tabulation for Pu239 includes nuclear data for both total fission and for the individual partial fission reactions ((n,f), (n,nf),....). The processor of application libraries can choose which to employ, although the default option for the ACER module (part of NJOY-based processing route used for the MONK and MCNP JEF2.2-based libraries) is to utilise the partial reactions as they are assumed to be (slightly) more accurate.

The cross-section data in the JEF2.2 Pu239 evaluation are self-consistent (total fission equals the sum of the partial fission data and this is checked by the library compilers) but it transpires that the energy distribution for secondary neutrons from fission are not. In fact the total fission has modern (and recommended) data tabulated whereas the partial fission secondary energy data have not been similarly updated. For comparisons, the Pu239 evaluation in ENDF/B-VI (revision 3) has the modern Madland (1988) fission spectrum allocated to the total fission reaction and this is the same spectrum used for total fission in JEF2.2. There are no spectra allocated to partial fission reactions in the ENDF/B-VI evaluation and it now seem likely that these have been removed to prevent the problem now seen in processing the JEF2.2

evaluation (comments in the ENDF/B-VI evaluation confirm that Madland's work includes the effect of all forms of neutron induced fission). Therefore choosing the recommended partial fission data results in utilising superseded secondary energy distribution data and upon investigation it was found that this could have an effect of up to 1% in k-effective for some systems. The MONK and MCNP Pu239 files were therefore updated and the results and further discussion relate to these 'final' libraries.

The calculated k-effective values for the various contributors are summarised in Tables I, II and III. It is important to recall that the discrepancies observed in the initial phase of this inter-code comparison were up to 1500 pcm. After removing the two inconsistencies described above, the updated results are fairly consistent. In fact, very good agreement is obtained for infinite media cases with the results for Monte Carlo codes lying within two standard deviations of each other. For deterministic calculations, differences between results are relatively small though they can reach 250 pcm. For bare spheres the agreement is also good between the different Monte Carlo codes. The maximum discrepancy for each configuration is within two or three combined standard deviations. For experimental configurations the agreement is only slightly less good, generally within two standard deviations but with some results differing by up to three combined standard deviations. The consistency of the results obtained indicate that clear code-independent feedback can now be provided about the ability of the JEF2.2 data to compute plutonium nitrate solution systems.

Code	No. of groups	P1	P2	P3	P4	P5	P6
MONK7	Hyperfine	1.6803± 0.0005	1.6627± 0.0005	1.5076± 0.0004	1.0946± 0.0005	1.4985± 0.0005	1.4767± 0.0005
WIMS7	69	1.6812	1.6645	1.5079	1.0946	1.4991	1.4766
WIMS7	172	1.6806	1.6642	1.5081	1.0951	1.4997	1.4771
TRIPOLI4	Point	1.6804± 0.0012	1.6628± 0.0012	1.5096± 0.0010	1.0951± 0.0009	1.4966± 0.0010	1.4764± 0.0011
APOLLO1	99	1.6805	1.6638	1.5085	1.0976	1.4997	1.4775
APOLLO2	99	1.6793	1.6618	1.5082	1.0948	1.5004	1.4782
APOLLO2	172	1.6778	1.6609	1.5077	1.0943	1.4989	1.4772

Table I - Summary of K-effective Results for the Plutonium Nitrate Solution Comparison (Infinite Media)

Code	No. of groups	P1	P2	P3	P4	P5	P6
MONK7	Hyperfine	1.0005± 0.0010	0.9960± 0.0010	0.9987± 0.0009	0.9990± 0.0005	1.0048± 0.0009	1.0009± 0.0009
TRIPOLI4	Point	0.9992± 0.0009	0.9986± 0.0010	1.0001± 0.0009	0.9982± 0.0010	1.0023± 0.0010	1.0034± 0.0009
APOLLO2-TRIMARAN	99	1.0006± 0.0010	0.9966± 0.0010	1.0001± 0.0010	1.0004± 0.0010	1.0036± 0.0010	1.0027± 0.0010
APOLLO1-MORET3	99	0.9990± 0.0010	0.9979± 0.0010	1.0000± 0.0010	0.9981± 0.0010	1.0011± 0.0010	1.0016± 0.0010
MCNP	Point	1.0014 ± 0.0030	0.9956± 0.0010	0.9976± 0.0008	0.9967± 0.0008	1.0029± 0.0032	0.9997± 0.0008

Table II - Summary of K-effective Results for the Plutonium Nitrate Solution Comparison (Bare Spheres)

Code	No. of groups	P1	P2	P3	P4	P5	P6
MONK7	Hyperfine	1.0068± 0.0008	1.0031± 0.0008	1.0017± 0.0008	1.0108± 0.0008	1.0059± 0.0008	1.0054± 0.0008
TRIPOLI4	Point	1.0066 ± 0.0009	1.0030± 0.0009	1.0018± 0.0009	1.0100± 0.0009	1.0085± 0.0010	1.0080± 0.0010
APOLLO1-MORET3	99	1.0031± 0.0010	0.9988± 0.0010	0.9998± 0.0010	1.0143± 0.0010	1.0082± 0.0010	1.0086± 0.0010
MCNP	Point	1.0060 ± 0.0007	1.0024± 0.0009	0.9998± 0.0008	1.0091± 0.0005	1.0072± 0.0010	1.0042± 0.0008

Table III - Summary of K-effective Results for the Plutonium Nitrate Solution Comparison (Benchmark Models)

Uranyl Fluoride Solutions

The uranyl fluoride solution inter-comparison exercise comprised six configurations selected from a single experimental programme. These configurations were selected from a programme performed at the Oak Ridge National Laboratory (ORNL). The U235 enrichment is 93.2wt% in each case and the uranium concentration ranges from 20 to almost 700 g/l. These configurations were all water reflected spheres. The same sets of calculations were performed as for the plutonium nitrate inter-comparison exercise.

To date, there are five sets of results available for this inter-comparison exercise. Tables IV, V and VI show the calculated k-effective obtained by MONK7, TRIPOLI4, APOLLO1-MORET3, APOLLO2-MORET4 and KENO-Va. For the infinite media cases, agreement between MONK7 and TRIPOLI4 is generally within two standard deviations and always within three standard deviations (and similar to the level of agreement observed for the plutonium solution cases); it is noted however that in each case the MONK result is higher than the TRIPOLI value. Agreement between MONK, TRIPOLI and APOLLO is also good with the APOLLO result consistently closer (and slightly higher) than the MONK value. The KENO-Va results are generally higher although within two standard deviations of the MONK values. For the bare sphere cases, good agreement is again observed between MONK and TRIPOLI (with one exception the agreement is within two standard deviations). For APOLLO-MORET (both versions) and KENO-Va the results are generally significantly different than the MONK/TRIPOLI values with several differences in excess of 400 pcm. The MONK and TRIPOLI values continue to line up well for the experimental configurations (maximum discrepancy is ~200 pcm and all within two standard deviations). The APOLLO2-MORET4 results agree better with MONK/TRIPOLI for these water-reflected cases, generally within two standard deviations except for Case 5. The KENO-Va results are generally significantly higher than the other codes, with differences of the order of 500 pcm. The general consistency of the results obtained from MONK, TRIPOLI and APOLLO-MORET for the water-reflected cases indicate that code-independent feedback can now be provided about the ability of the JEF2.2 data to compute uranium oxyfluoride solution systems.

However further work is required to understand the cause of the larger differences between hyperfine/point libraries and broad group libraries for the unreflected cases. The cause of the significantly discrepant results from KENO-Va has not been investigated.

Code	No. of groups	U1	U2	U3	U4	U5	U6
MONK7	Hyperfine	1.8530± 0.0003	1.8706± 0.0003	1.8868± 0.0003	1.8761± 0.0003	1.6230± 0.0003	1.2598± 0.0003
TRIPOLI4	Point	1.8496± 0.0010	1.8691± 0.0010	1.8858± 0.0010	1.8749± 0.0010	1.6203± 0.0010	1.2588± 0.0010
APOLLO1	99	1.8534	1.8711	1.8875	1.8773	1.6247	1.2613
APOLLO2	172	1.8531	1.8708	1.8867	1.8770	1.6242	1.2610
KENO-Va	172	1.8567± 0.0010	1.8736± 0.0010	1.8887± 0.0010	1.8775± 0.0010	1.6234± 0.0010	1.2597± 0.0010

Table IV - Summary of K-effective Results for the Uranyl Fluoride Solution Comparison (Infinite Media)

Code	No. of groups	U1	U2	U3	U4	U5	U6
MONK7	Hyperfine	1.0001± 0.0007	0.9992± 0.0007	1.0014± 0.0007	1.0041± 0.0007	1.0234± 0.0007	1.0194± 0.0007
TRIPOLI4	Point	0.9999± 0.0010	1.0007± 0.0010	1.0025± 0.0010	1.0073± 0.0010	1.0249± 0.0010	1.0209± 0.0010
APOLLO1-MORET3	99	0.9974± 0.0010	0.9948± 0.0010	0.9994± 0.0010	1.0028± 0.0010	1.0201± 0.0010	1.0224± 0.0010
APOLLO2-MORET4	99	0.9958± 0.0010	0.9950± 0.0010	0.9980± 0.0010	1.0050± 0.0010	1.0211± 0.0010	1.0185± 0.0010
KENO-Va	172	1.0044± 0.0010	1.0040± 0.0010	1.0051± 0.0010	1.0092± 0.0010	1.0249± 0.0010	1.0213± 0.0010

Table V - Summary of K-effective Results for the Uranyl Fluoride Solution Comparison (Bare Spheres)

Code	No. of groups	U1	U2	U3	U4	U5	U6
MONK7	Hyperfine	1.0070± 0.0007	1.0068± 0.0007	1.0039± 0.0007	0.9974± 0.0007	1.0028± 0.0007	1.0007± 0.0007
TRIPOLI4	Point	1.0077± 0.0010	1.0078± 0.0010	1.0042± 0.0010	0.9991± 0.0010	1.0050± 0.0010	1.0019± 0.0010
APOLLO1-MORET	99	1.0001± 0.0010	1.0010± 0.0010	0.9983± 0.0010	0.9905± 0.0010	1.0022± 0.0010	1.0003± 0..0010
APOLLO1-MORET3	99	1.0075± 0.0010	1.0064± 0.0010	1.0044± 0.0010	0.9974± 0.0010	1.0078± 0.0010	1.0018± 0.0010
KENO-Va	172	1.0123± 0.0010	1.0114± 0.0010	1.0087± 0.0010	1.0017± 0.0010	1.0078± 0.0010	1.0021± 0.0010

Table VI - Summary of K-effective Results for the Uranyl Fluoride Solution Comparison (Benchmark Models)

VI. Sensitivity analysis

Introduction

In the previous section we have shown the contribution that inter-code comparisons can make to reducing calculation inaccuracy. If such work is pursued for other types of material we can reach a situation where benchmarking results are almost code independent and where calculation-experiment discrepancies reflect the imperfect quality of input data (by which we mean geometry and composition description data and microscopic nuclear data). As in both cases measurements are the main source of data, uncertainty calculations are needed to determine the reactivity worth of experimental uncertainties.

Concerning integral experiments, an important effort has been devoted in the framework of ICSBEP to calculate the effect of experimental uncertainties on integral parameters. However, it is important to note the difficulty of estimating possible systematic errors related to experimental techniques which may concern a whole experimental program. This means that experimental programs performed in different laboratories are to be considered in benchmarking studies for the same class of problem whenever possible.

Turning our attention to nuclear data, for some neutronic applications (reactor physics for instance), the microscopic data are often not known to sufficient accuracy to give the overall target accuracy in calculated integral parameters. Furthermore, criticality benchmarking studies show that the experiment-calculation discrepancies are higher in specific media of interest to criticality safety than those obtained in reactor physics applications. Thus, it is important to know to what extent nuclear data uncertainties contribute to the overall discrepancies.

Nuclear Data Uncertainty Propagation

One way of answering this question is to determine the effect of microscopic data uncertainties on the calculation of integral parameters. This can be done 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-effective 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 $cov(x_i,x_j)$ 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 (P0 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[16] and used for the adjustment of the JEF2.2 based application library ERALIB-1 for fast neutron reactors.

The a priori uncertainty u on k-effective 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.

Results

The results are reported in Table VII. The effect of nuclear data uncertainties on calculated integral parameters ranges from about 500 pcm up to 1400 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 under-estimate 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:

$$\begin{aligned} \mathrm{cov}(x_i, x_i) &= 1 \\ \mathrm{cov}(x_i, x_{i+1}) &= 0.66, \\ \mathrm{cov}(x_i, x_{i+2}) &= 0.33 \end{aligned}$$

$\mathrm{cov}(x_i, x_j) = 0$ 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 cross sections - both capture (from 200 pcm to 1400 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 1000 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).

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 - 1400	700 - 900	800 - 1200	650	1000	550 - 700
u without correlation terms (in pcm)	500 - 1300	500 - 750	700 - 1200	540	700	400 - 600

Table VII: Reactivity effect of nuclear data uncertainties

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.

VII. Conclusions and recommendations

It was the aim of this paper to summarise on-going activities for the benchmarking of JEF2.2 for criticality applications. Results from national programs in UK and France as well as joint studies performed in the framework of the JEF working group were presented. Individual code comparisons with experimental systems are already good, in most cases superior to those with previous data libraries. The results could be summarised as follows:

- the situation of low-enriched uranium solutions needs further investigations particularly to review experimental data investigated and to understand the origin of the inconsistency in the information derived from these experiments,

- for low-enriched uranium powders the calculation of Rocky Flats and Maracas experiments (work in progress and may lead to inter-code comparison exercise) gave better agreements and thus increased the confidence on the JEF2.2 data; it is now believed that the large under-prediction observed with the Springfields experiments are likely to be originated in the experimental data,

- for high-enriched uranium solutions reasonably good agreements were found, the discrepancies being within the combined experimental/calculation uncertainties

- Pu solutions is the field were real improvements where made and the current situation is quite satisfactory compared to few years ago: the agreements are reasonably good whereas an over-prediction of about 1000 pcm is observed for very low Pu concentrations; in particular, it has been shown that the fission spectra of the partial (n,xnf) reactions were not accurate enough and that the recommendation for JEF2.2 users is to describe the fission process as one reaction,

- the same conclusions applies for mixed (U+Pu) solutions where an over-prediction of about 1000 pcm is observed for very low uranium and plutonium concentrations,

- simple uranium lattices are well calculated with JEF2.2; less satisfactory results are obtained when the array is reflected by lead or concrete (more than 1000 pcm over-prediction) and when Hf or Cd plates are used; further studies are needed as the assessment of improvements with lead cross-sections originating from the EFF-2 file,

- reasonable good agreements were seen for mixed oxide lattices,

- uranium and plutonium fast metal systems are well calculated with JEF2.2.

Future work

Future work will obviously focus on the areas, described above, were the situation needs further investigations. The ongoing work in France in the framework of the CRISTAL project as well as the effort planned to extend the MONK validation database will bring additional results and more inter-comparisons between pointwise cross sections based codes and multigroup based ones. The preliminary sensitivity analysis presented in this paper showed that criticality calculations is an application area where a great variety of sensitivity profiles are encountered and that in many cases the discrepancies between calculations and experiments are comparable to the reactivity effect of nuclear data uncertainties. The generalisation of the work performed in the frame of reactor physics (see for instance reference 16) to include feedback to nuclear data from well established criticality benchmarks and well validated calculations will be beneficial to criticality assessor and to nuclear data community.

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