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# NUCLEAR DATA IMPROVEMENTS IN THE DECADE WITH SPECIAL EMPHASIS ON VERY RECENT DATA EVALUATIONS, AND THEIR APPLICATION TO THERMAL AND FAST REACTOR ANALYSIS

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Abstract

The present analysis describes mainly the application of JEF-2 and JENDL-3 to thermal and fast reactor systems. For thermal reactors the burnup behaviour of PWR-fuel up to about 30 GWd/to is investigated; nuclide concentrations are compared to experimental results from postirradiation analyses. For fast reactors, criticality for a variety of critical assemblies is evaluated and the results are compared, both among each other and to experiment.

The results with the new data sets are discussed in some detail. Some intercomparisons of group cross sections are presented, as those for inelastic scattering (U 238, Pu 239 to 241), fission and capture data for U 235 and Pu 239. Also some results from the ENDF/B-VI and BROND-2 files are included, as far as available at present.

## Introduction

The application of the European Joint Evaluated File JEF-1 to describe the physics behaviour of PWR power reactors [1] showed satisfactory agreement with experimental results of postirradiation analyses with the exception of the Cm 242 concentration at 30 GWd/t burnup. The good agreement of calculational results using JEF-1 data was also confirmed by an independent analysis on PWR-fuel cycle investigations at the University of Stuttgart [2]. No major surprises therefore are expected in using JEF-2 data for the analysis of PWRs, but expecting better results now for the Cm 242 concentration at 30 GWd/t burnup. For fast reactors, some calculations showed larger discrepancies with experimental results [3]: JEF-1 data could not have been used for fast reactor analysis without adjustments. The aim to develop the files JENDL-3 in Japan, of ENDF/B-VI in USA, JEF-2 in Europe and other files as BROND-2 in the USSR, was to calculate fast reactors with the basic group constant sets based on the various evaluated data files without major adjustments to experiments in critical facilities. The new versions of the data files have been distributed recently. This paper will concentrate on the application of JEF-2 and JENDL-3 to fast reactor systems to see whether the goal of using these unadjusted data sets for a reliable fast reactor analysis could be reached.

The processing of basic data to group constants, using the Karlsruhe version of NJOY, is carefully analysed to investigate whether major differences in C/E values for integral reactor quantities may result from the processing procedure. These investigations will be discussed in [7] and are not presented in this contribution.

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## Test of the Data Files JENDL-3 and JEF-2 on the Burnup Behaviour of Nuclide Concentrations in PWRs

There have been published already many results on the test of the JENDL-3 data file for PWR application [4]. These concern criticality for benchmark cores, for HCLWR cores of the PROTEUS experiments, including the voided configurations, and a burnup benchmark. The prediction of compositions for urania, transurania and fission products was felt to be in satisfactory agreement with the results from ORIGEN2. In this chapter, a comparison of the calculated isotopic compositions of JENDL-3 and JEF-2 as well as with experimental results from post-irradiation analyses will briefly be presented.

### Comparison of nuclide concentrations after irradiation of PWR-fuel, using JEF-2 and JENDL-3 data

In Table 1 the nuclide concentrations after about 30 GWd/tHM burnup in the Obrigheim power plant KWO are compared, using data sets derived from the JEF-1, JEF-2, and JENDL-3 data files. The irradiation history is simulated accurately. Only marginal differences can be observed between the results of the 3 data sets. The largest difference of about 9 % occurs for Np 237: JEF-2 gives a result lower by 9 % than JENDL-3. A similar deviation is observed for U236: The result, obtained on JEF-2 basis, is smaller by about 8 % than that using JENDL-3 (the JEF-1 result is in between JEF-2 and JENDL-3). For Pu 238 JEF-1 and JENDL-3 give identical results, JEF-2 is by about 6 % lower. All other results differ by no more than about 2 %.

### Comparison of calculated nuclide concentrations with experimental results

In [1] JEF-1 data had been applied for this analysis. It was observed that, with the exception of the Cm 242 concentration, all other actinide concentrations at about 30 MWd/tHM are in satisfactory agreement with experimental results, which are not of very high precision, but allow to reveal major discrepancies. The same agreement is found again with the JEF-2

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Table 1: Comparison of Nuclide Concentrations at 30 GWd/tHM burnup for PWR fuel (KWO), calculated with different data sets

units: at. $b^{-1}cm^{-1}$ = $10^{24}$ at./$cm^3$

| Data Sets / Nuclide | JEF-1 | JEF-2 | JENDL-3 |
|---|---|---|---|
| Pu 239 | 5.14 E-3 *) | 5.13 E-3 | 5.14 E-3 |
| Pu 240 | 2.00 E-3 | 2.02 E-3 | 2.01 E-3 |
| Pu 241 | 1.07 E-3 | 1.08 E-3 | 1.07 E-3 |
| Pu 242 | 3.87 E-4 | 3.91 E-4 | 3.89 E-4 |
| U 234 | 2.97 E-6 | 2.92 E-6 | 2.99 E-6 |
| U 235 | 8.63 E-3 | 8.67 E-3 | 8.53 E-3 |
| U 236 | 3.78 E-3 | 3.66 E-3 | 3.94 E-3 |
| U 238 | 9.47 E-1 | 9.47 E-1 | 9.47 E-1 |
| U 233 | 3.16 E-9 | 3.15 E-9 | 3.15 E-9 |
| Np 237 | 4.02 E-4 | 3.74 E-4 | 4.07 E-4 |
| Pu 238 | 1.35 E-4 | 1.27 E-4 | 1.35 E-4 |
| Am 241 | 9.75 E-5 | 9.84 E-5 | 9.94 E-5 |
| Am 243 | 6.02 E-5 | 6.11 E-5 | 6.02 E-5 |
| Cm 242 | 3.69 E-6 | 3.73 E-6 | 3.60 E-6 |
| Cm 244 | 1.50 E-5 | 1.53 E-5 | 1.53 E-5 |

*) E-n always means $10^{-n}$

and the JENDL-3 data bases. The Cm 242 concentrations for all three data files are overpredicted by about a factor of 2 compared to experimental results. Already in [1] it was suspected that very probably the experimental results, which are difficult to obtain because of the very short half-life of Cm 242 ($T_{1/2}$ = 163 days), are in error. This aspect is still under investigation.

## Check on Fission Product Nuclear Data

Fission product nuclear data have not been changed from JEF-1 to JEF-2. Tests of JEF-1 fission product data have been reported in [5] and, for JENDL-3, in [4]. Results with JEF-1 data are within the experimental error bars of 10 %. JENDL-3 gives a satisfactory good prediction for Sb-125 and Eu 154 concentrations.

## Test of Recently Established Nuclear Data Files for Fast Reactor Applications

The fast energy range up to now was not appropriately described with cross sections for the unresolved resonance region, the capture and fission data especially for U 238 and Pu 239, and inelastic scattering for almost all heavy nuclides. Therefore, design calculations for fast reactors very frequently were performed by using adjusted data sets or using bias or "fudge factors" to integral quantities. Both schemes are unsatisfactory from the point of view of describing the important physical features of fast reactor systems of very different designs which are under discussion presently, i.e. with different fuel (oxide, metal, nitride), of special actinide burner reactors to reduce the long term hazard of nuclear waste, of modular and heterogeneous cores, and of other futuristic characteristica. The neutron spectrum usually varies from relative soft to relative hard spectrum systems. Therefore, a check of the quality of a modern data set should cover the whole range of neutron spectra above about 100 eV up to some MeV.

Table 2: $k_{eff}$ for Several Fast Critical Assemblies

| Assembly | Fiss Fuel | Spectrum | $k_{eff}$ | | Comments |
|---|---|---|---|---|---|
| | | | JEF-2 | JENDL-3 | |
| GODIVA | U | Hard | 1.0025 | 1.0124 | 1-dim. $S_{16}$ Transp. Appr. |
| JEZEBEL | Pu | Hard | 0.9960 | 1.0014 | 1-dim. $S_{16}$ Transp. Appr. |
| ZPR III-10 | U | ↓ | 1.0062 | 1.0033 | 2-dim. Diff. +Corr.*) |
| ZPR III-25 | U | Softening | 1.0025 | 0.9935 | 2-dim. Diff. +Corr.*) |
| SNEAK-3A1 | U | ↓ | 1.0010 | 0.9888 | 2-dim. Diff. +Corr.*) |
| SNEAK-3A2 | U | Soft | 1.0014 | 0.9865 | 2-dim. Diff. +Corr.*) |
| ZPR III-48 | Pu | FBR Prot. | 0.9899 | 0.9972 | 2-dim. Diff. +Corr.*) |
| ZEBRA-6A | Pu | FBR Prot. | 0.9819 | 0.9903 | 2-dim. Diff. +Corr.*) |

*)The corrections are assumed to be the same as those derived originally for the KFKINR set; they include mainly transport and heterogeneity.

## Observations from Tests of Data Sets based on JEF-2 and JENDL-3 for Fast Assemblies

Only a selection of the obtained results can be presented here. A full documentation of all investigations will be published as a KfK-report [7]. Table 2 shows the results for $k_{eff}$ for a variety of fast reactor critical assemblies with uranium and plutonium fuel, based on the JEF-2 and JENDL-3 nuclear data libraries. The spectra of these systems range from very hard (GODIVA, JEZEBEL) to fairly soft neutron spectra. For the high leakage systems a high transport - $S_{16}$ - approximation was used, the follow-up assemblies were calculated in 2-dimensional diffusion theory with transport corrections and corrections for heterogeneity and improved neutron slowing down.

In general, both data sets describe fairly well the criticality of both uranium and plutonium assemblies: With JEF-2 only for the assembly ZEBRA-6A (characteristic for a prototype fast reactor) $k_{eff}$ is underpredicted by about 2 %.

This first assessment with non-adjusted data sets is encouraging, especially for the JEF-2 basis. The results were carefully analysed and lead to following more detailed conclusions. The criticality values given in Table 2 for GODIVA and JEZEBEL may be slightly overpredicted due to the application of the transport approximation; using instead the higher moments of the scattering matrices up to $P_3$ may lead to a reduction by about 0.3%. However, both data sets underestimate the criticality of JEZEBEL by about 1% relative to that derived for GODIVA. In addition, JENDL-3 gives higher criticality values by 0.9% for GODIVA and 0.5% for JEZEBEL. A better agreement would be obtained if $\nu\sigma_f$ would be slightly increased for Pu 239 in JEF-2 (which is confirmed by the fact that $k_\infty$ for pure

Pu 239 is 1% lower for JEF-2 relative to JENDL-3), and slightly reduced for U 235 in JENDL-3 (assuming that $\sigma_t$ of both isotopes is known reasonably well).

With increasing spectrum softness (the assemblies in Table 2 are arranged in that order) the criticality of U-fueled assemblies tends to an underprediction with JENDL-3 whereas it remains practically unchanged with JEF-2. This favorable tendency which gives confidence in the neutron production cross section of JEF-2, does, unfortunately, not continue when going to assemblies with even softer spectra. There exists a tendency to an overprediction as we found when considering e.g. the so-called steam density coefficient as measured in the SNEAK-3A series of experiments where the hydrogen concentration was increased stepwise. In this case $\Delta k(\Delta H)$ was in much better agreement with experiment when using JENDL-3 instead of JEF-2. This leads to the conclusion that in JENDL-3 the energy dependence of $\nu\sigma_f(E)$ and/or of $\alpha(E)$ for U 235 in the epithermal range up to a few keV may be more suitable than that of JEF-2 (having in mind that $\sigma_c$ for U 238 of both files is in rather good agreement).

The already mentioned underprediction of criticality for the Pu-fueled critical JEZEBEL by JEF-2 becomes even more significant for the assemblies ZPR III-48 and ZEBRA-6A with softer neutron spectra (JENDL-3 shows a similar but slightly less pronounced tendency). A discrepancy of about 0.7% in $k_{eff}$ resulting between both files is not very encouraging because both assemblies are considered to be representative benchmarks for medium-sized prototypes of LMFBR power reactors.

Our intercomparisons clearly demonstrate that for hard spectrum $k_\infty$ experiments ,which are sensitive to the U238 inelastic scattering, such as ZEBRA-8H, SNEAK-8, ZPR IX-25, which have U-fuel, JEF-2 may lead to an underprediction by about 1%, but this underprediction increases considerably (to more than 2%) with JENDL-3 which clearly indicates that the energy loss caused by neutron inelastic scattering on U 238 is too large in JENDL-3 and should probably also be slightly reduced in JEF-2. For the Pu-fueled $k_\infty$-experiment ZPR III-55 the difference between JEF-2 and JENDL-3 exceeds 1%, but both $k_{eff}$-values seem acceptable with no clear preference for one of the two files.

A rather striking discrepancy between both datasets was observed when comparing $k_{eff}$ for similar compositions but differing in the fissile material. A typical example is ZPR-6-6A and ZPR-6-7 or other combinations, like SNEAK-2A-R1 and SNEAK-6A-Z1 or the inner core configurations of SNEAK 9A0 and SNEAK-9B. In all these cases we observed that $k_{eff}$ (JENDL-3) - $k_{eff}$ (JEF2) was roughly +1% for Pu-fueled compositions and -1% for U-fueled ones. In our opinion this surprising feature deserves further investigations, although the $k_{eff}$-values will probably stay in a ±1% uncertainty range, but in our opinion advanced nuclear data files should lead to better results because uncertainty bands of that amount were typical of adjusted group constant sets one or two decades ago.

## Intercomparison of Important Nuclear Data from Different Modern Data Files

In this contribution it is possible to give only some selected examples for present day differences in the fundamental data files. In the high energy range the inelastic scattering of neutrons on heavy nuclides is of high importance. Fig. 1 shows a comparison between JEF-2 data and those from the adjusted KFKINR set for U 238. The data differ appreciably; although adjustment not necessarily improves the cross sections themselves, it might be concluded that JEF-2 data might be changed into the direction of JEF-1 data, which almost coincide with those of KFKINR. JENDL-3 data also differ from JEF-2 data. This is more pronounced for Pu 239 (Fig. 2) where a difference of up to 40% around 100 keV is seen. In Fig. 3 the inelastic scattering cross section for Pu241 is depicted for the data files JEF-2, JENDL-3, ENDF/B-VI and BROND-2: This situation, although not so important as for U 238, is highly unsatisfactory. Moreover, for JEF-2 and JENDL-3 the differences in the scattering matrices are remarkable for all heavy nuclides: Here the recently created international Task Force for re-evaluation of the inelastic scattering processes might bring some clarification. Fig. 4 shows the differences in the capture cross section of U 235 between JEF 2 and JENDL-3. The diffeences in the range from 100 eV to 1keV were already mentioned before. Special emphasis should be given to the energy dependence of $\sigma_c$ in this range. Fig. 5 shows the comparison of the fission cross section of Pu 240 between JEF-2 and ENDF/B-VI. These large differences (up to about 80%) should be investigated. Fig. 6 gives the differences of the capture cross section for Pu 241 between the BROND-2 and JEF-2 libraries. Again, these differences should be clarified and removed.

## Conclusion

In a first assessment, the recently evaluated data files JEF-2 and JENDL-3 have been tested for thermal reactors (PWR's) and for a some fast critical assemblies with uranium and plutonium fuel of varying neutron spectra (from very hard to soft). For PWR's nuclide concentrations after a burnup of about 30 GWd/t agree well with experimental results with the exception of Cm 242. For fast critical assemblies criticality values obtained with JEF-2 data are mostly very near to experimental ones. The discussion of these results show that further improvement seems to be necessary, especially for inelastic scattering of neutrons on heavy materials, the values of $\sigma_f(E)$ in the fast energy range, $\alpha(E)$ values for U 235 in the resonance range and the fisison cross section of Pu 240 and also of Am 243, and Cu 244, which are not discussed in this contribution.

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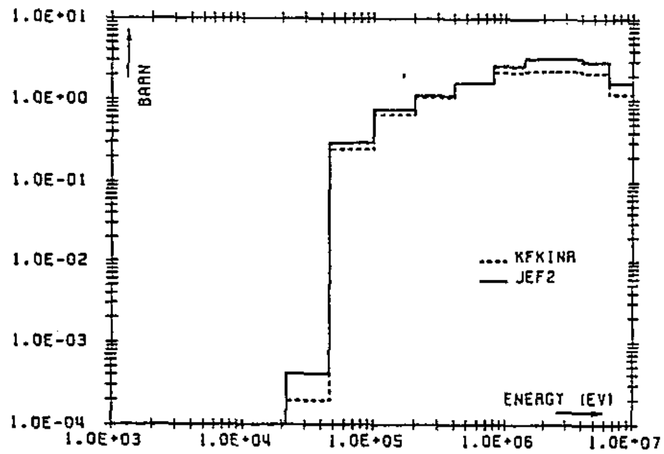


Fig. 1. Comparison of $\sigma_{inel}$ for U 238

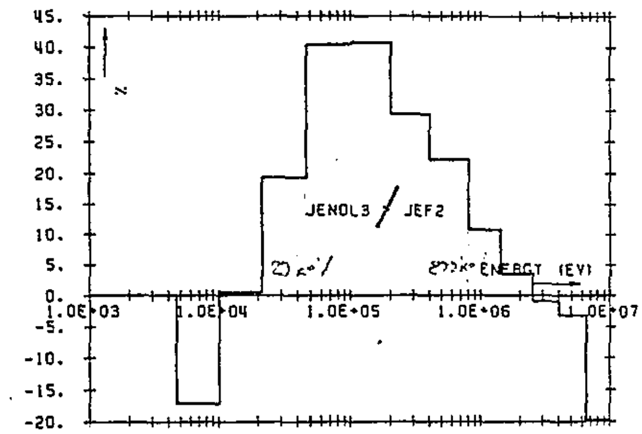


Fig. 2. Difference in % for $\sigma_{inel}$ of Pu 239

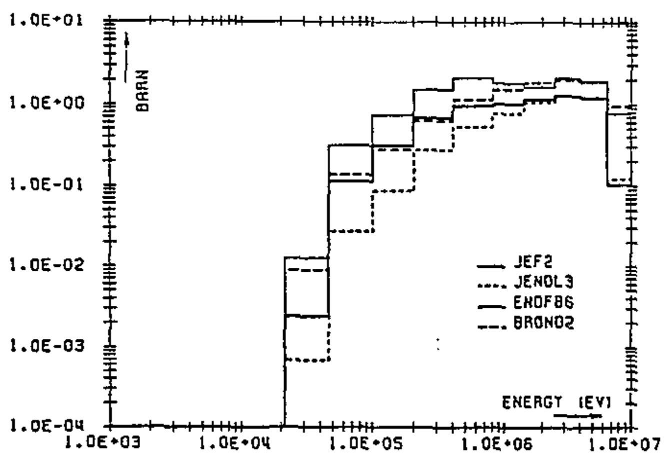


Fig. 3. Comparison of $\sigma_{inel}$ for Pu 241

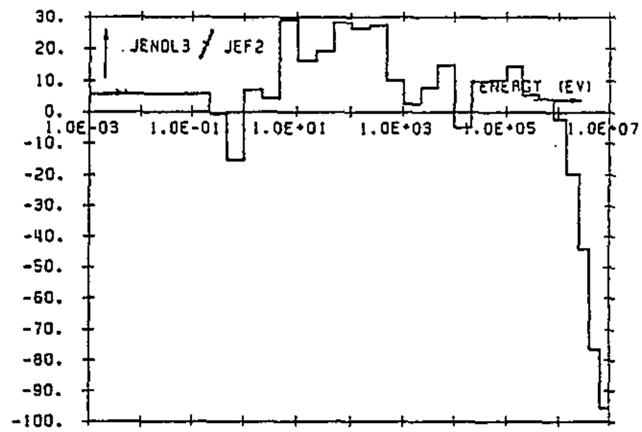


Fig. 4. Difference in % for $\sigma_c$ of U 235

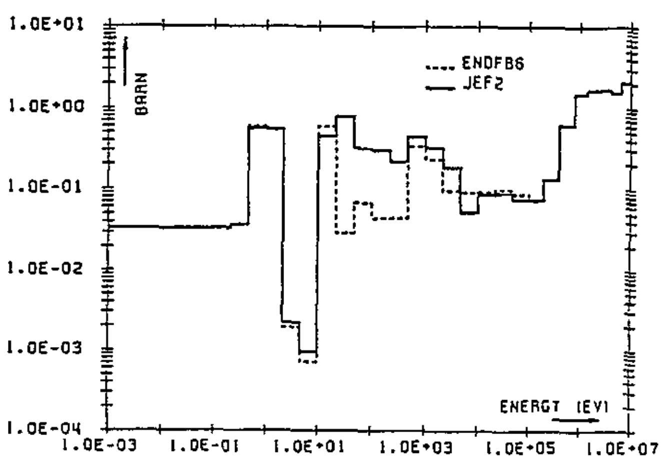


Fig. 5. Comparison of $\sigma_f$ for Pu 240

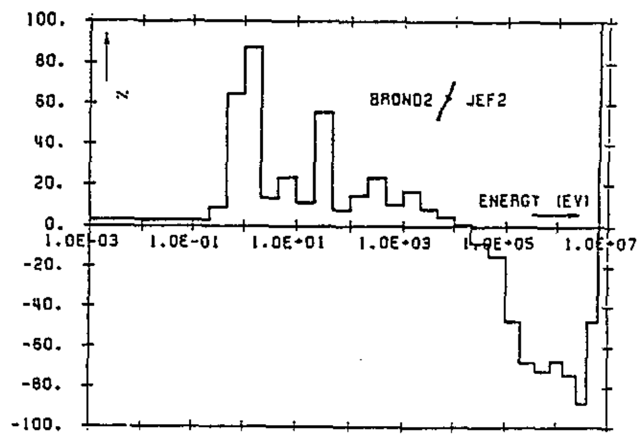


Fig. 6. Difference in % for $\sigma_c$ of Pu 241