JEFF Report 16

INTERCOMPARISON OF CALCULATIONS FOR GODIVA AND JEZEBEL

An intercomparison study organised by the JEFF Project,
with contributions from Britain, France, the Netherlands and Switzerland

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FOREWORD

Validation studies based on the analysis of discrepancies between calculated and measured reactor properties play a central role in the process leading to the improvement of reactor physics codes and their associated nuclear data libraries, as well as to the assessment of the accuracy of calculations. The nuclear data libraries can be adjusted to reduce the discrepancies. However, for the adjustments to be generally valid it is important to demonstrate that the numerical methods and physics models used in the codes provide an accurate treatment of all the complexities of the systems. Estimates of the uncertainties arising from approximations in the methods used in the different nuclear data processing and neutron transport codes can be obtained by intercomparing calculations made using different code systems. Calculations made for simple configurations using both deterministic and stochastic methods, with different degrees of refinement in the modelling, are intercompared using the same source of nuclear data. In this way, the accuracy of the different methods used at various stages, ranging from nuclear data processing systems to neutron transport calculations, can be assessed.

In a previous report (JEFF Report 15) the effect of methods approximations for the calculation of simple light water reactor configurations was addressed. In the present report, similar investigations are made for a completely different neutron spectrum, namely a fast spectrum. The well known Los Alamos critical assemblies GODIVA (highly enriched uranium) and JEZEBEL (plutonium) were considered. Both cores are unmoderated and unreflected. The simplified sphere models were retained.

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Introduction

The specifications adopted (see Annex 1) for these intercomparison calculations are those given in the CSEWG Benchmark Book, BNL 19302, ENDF 202. JEZEBEL is fast reactor benchmark number F1 (Revised 11-81) and GODIVA is benchmark F5 (Revised 11-81). JEZEBEL is a bare sphere of plutonium metal and GODIVA a bare sphere of highly enriched uranium. In addition to the values of k_{eff}, a three-group neutron balance was requested, with intermediate energy boundaries at 2.2313 MeV and 0.49787 MeV (these being boundaries of the half-lethargy scale based on 10 MeV).

The calculations have been made using different code systems with nuclear data derived from the JEF-2.2 library. Both deterministic and Monte Carlo methods have been used. The deterministic codes used are MICROX-2/ONEDANT (PSI), which uses a modified P_2 library in 93 energy groups, SCALE-4.2/XSDRNPM (IRI TU Delft, using the XMAS 172 energy group scheme in P_3 approximation), SHIVA/ECCO/ERANOS and SHIVA/ERANOS (Cadarache, which uses the SHIVA P_5 library in the XMAS 172 group scheme). The continuous energy (or hyperfine group) Monte Carlo codes used are MCNP-4A (Petten, Cadarache and Delft), MONK (Winfrith) and TRIPOLI-4 (Saclay and Cadarache). In addition, the multi-group Monte Carlo code KENO (in the SCALE-4 system) has been used at Delft. A comparison has also been made at Delft between KENO and MCNP (groupwise mode) using the SCALE-4.2 group cross-section data, in addition to MCNP-4A (continuous energy). The MCNP (groupwise) and KENO results are essentially in agreement with the S_n results.

The first aim of the intercomparison study has been to obtain information about the ranges of the values calculated using different methods but starting with the same nuclear data evaluation. The second aim has been to try to identify the sources of the discrepancies between the different methods.

Approximations in the methods

There are some significant discrepancies between the results obtained using different methods. Reaction rates have been edited in three energy groups so as to try to identify the sources of the differences.

There are approximations in the representation of some items of nuclear data in the continuous energy Monte Carlo codes. An approximation in the standard version of MCNP is the neglect of resonance shielding in unresolved resonance regions but the calculations made at Petten include a treatment of this. There are some approximations made in the hyperfine group representation of cross-sections in the MONK code. The representation is on a 1/128 lethargy group structure above 10 keV, together with a 2 element subgroup representation (within each fine group) to treat within fine group resonance structure for the uranium and plutonium isotopes in an approximate way. (Below this energy the group structure is much finer.) Also, both of these codes use only the prompt fission spectrum; the effect of this approximation is discussed in Annex 2. In TRIPOLI the total fission spectrum is used.

Some methods are still undergoing refinement, and approximations in the nuclear data libraries are being identified and corrected. A particular problem identified in earlier studies with plutonium solutions and investigated here as well is the ^{239}Pu fission spectrum used in the different codes. The total fission spectrum (MT=18 in the ENDF-6 nomenclature) in the JEF-2.2 file is the one which has been recommended for use by the evaluators. The standard procedure in NJOY, however, is to combine the partial fission reactions spectra (MT=19, 20, 21 and 38 in the ENDF-6 nomenclature) when these are available in the file. These are not consistent with the total spectrum in the ^{239}Pu file. There are also differences in the ^{239}Pu unresolved resonance region data (1-30 keV) in a version of the file used in France, where corrected data have been used.

Calculations with different numbers of energy groups and different weighting spectra have shown their effects to be very small in the group schemes used here, apart from the effect on the condensation of the fission spectrum matrix to a vector. The effect of approximations in the treatment of resonance shielding is also found to be negligible. Simplifications in the treatment of the incident neutron energy and isotope dependence of fission spectra could be a source of some of the differences between the results obtained using the multi-group methods (some methods only use the fission spectrum for the dominant fissile isotope but this is an acceptable approximation for GODIVA and JEZEBEL). These use a single fission spectrum vector rather than the incident neutron energy dependent fission spectrum matrix, and the method used to condense the matrix to obtain a fission spectrum vector can affect the results. Calculations have been made at PSI (MICROX-2) and at Delft (SCALE-4.2) by condensing the fission matrix using a previously calculated reactor spectrum, as well as investigations of other spectrum approximations. The dependence of the deterministic results on S_n order and P_n order, together with notes on other approximations in the methods, is discussed in Annex 1.

A problem which was found and corrected was the neglect of the anisotropic component of continuum inelastic scattering and (n,xn) neutrons in one of the calculation schemes. This had a significant effect on the GODIVA calculations, producing a value about 200 pcm higher. The continuum inelastic scattering and (n,xn) for ^{239}Pu in JEF-2.2 are isotropic, thus there was no corresponding effect for JEZEBEL. However, one should consider whether the continuum inelastic scattering of ^{239}Pu should be similarly anisotropic because this could have a comparable effect in the case of JEZEBEL.

Results of the calculations

The calculated values of the effective multiplication, k_{eff}, are presented in Table 1 and neutron balances are presented in Tables 2-5. Spectral indices are presented in Table 6. In the case of JEZEBEL, results are given for both partial fission reactions spectra and the total fission spectrum. The results have been grouped in the following way:

(a) Continuous energy and fine group Monte Carlo. TRIPOLI, MCNP and MONK. The three group neutron balances calculated using MCNP and MONK have been modified to include an approximate correction for the delayed neutron component of the fission spectrum. In the case of GODIVA the corrections are based on calculations made by Pelloni with and without the delayed neutron spectrum component of the fission spectrum (these calculations being given in the second section after Table 1). Refinements have been made in the representation and interpolation in the MONK fission spectra and continuum inelastic scattering secondary energy distributions (the standard representation being 32 equiprobable bin data) and this has resulted in a significantly improved agreement with MCNP.

(b) Multi-group methods using fission spectrum vectors obtained with an appropriate reactor weighting spectrum. These calculations were made using MICROX-2/ONEDANT and SCALE-4.2/(XSDRNPM and KENO). The data in these calculations were derived using NJOY-97.62.

(c) Multi-group methods using fission spectrum vectors obtained with other weighting spectra. These include the SHIVA/ECCO/ERANOS and SHIVA/ERANOS results.

It is the differences between the results of the codes in Groups (a) and (b) which are of special interest as a test of the accuracy of the processing and representation of the data in continuous energy or multi-group form.

Treatment of the fission spectrum and inelastic secondary energy and angular distributions

Concerning the results in Group (c), calculations made at Cadarache show that the value of k_{eff} increases by about 100 pcm when the incident neutron energy for which the fission spectrum is calculated increases from thermal to 1 MeV, the increase being approximately linear in incident neutron energy (the values being 94 pcm for GODIVA and 91 pcm for JEZEBEL, using the partial ^{239}Pu fission reactions spectra). In some methods only the fission spectrum of the dominant fissile isotope is used (an acceptable approximation in the case of GODIVA and JEZEBEL). In one of the first calculations performed the weighting spectrum used for deriving the single fission spectrum from the group dependent fission spectrum matrix was not well chosen, being the VITAMIN-J weighting spectrum, with its fusion peak. This had a significant effect on the derived fission spectra, reaction rate ratios and k_{eff} values (about 200 pcm).

Investigations have been made of certain aspects of the data representation in the MONK code, in particular the representation of the fission spectrum and the secondary energy and angular distributions of inelastic scattering to the continuum, (n,2n) etc. There are two approximations made in the case of ^{235}U: the coupled energy/angular distribution is replaced by separate energy and angular distributions calculated using the SIXPAK code. Secondly, in the standard treatment secondary energy and angular distributions are represented by 32 equiprobable bin data, the primary energy grid on which these are stored being the energies at which the data are stored in the JEF-2.2 files plus a ¼ lethargy grid.

The effect of the separation of the continuum inelastic scattering secondary energy and angular distributions in the case of GODIVA has been investigated by Pelloni and the effect on k_{eff} is found to be very small, about 13 pcm.

An investigation of the effect of using 32 bins to represent the fission spectrum and continuum inelastic scattering secondary energy and angular distributions has been made at Winfrith. This was done by using both a 950 equiprobable bin representation and by using an improved method of interpolation in both the primary energy representation and the secondary 32 bin data and the 950 bin data. The effects on the k_{eff} value of GODIVA and on the three group spectra are found to be significant.

The GODIVA results are taken from calculations using the special MONK DICE library with 950 bins for the secondary energy/angle distributions for ^{235}U. It was found that there was a difference between results obtained with the 950 bin data and results obtained using 32 bins with the improved interpolation. The JEZEBEL results are taken from calculations using ^{239}Pu data with the fine incident energy grid. Interpolation was used in addition to this. The calculations used 32 bins, with the SQRT(E) interpolation method in the lowest energy bin for the fission spectrum.

In the standard MONK treatment of secondary energy distributions there is a test of the consistency of the energy of a scattered neutron with the Q value. In the case of the ^{235}U continuum inelastic scattering distributions there is an inconsistency which is significant near the threshold. P.G. Young has explained this as a consequence of the energy bins used in the nuclear reaction theory code, GNASH. He plans to correct this inconsistency in the next version of the ^{235}U evaluation. MONK calculations have been made both with and without this Q value test. In the case of GODIVA the difference is significant and the two sets of results are presented in the tables, MONKQ denoting the results including the Q test. The TRIPOLI and MCNP results for GODIVA are somewhat more consistent with the results obtained without the Q test.

In the representation of the anisotropy for elastic scattering TRIPOLI-4 uses as many equiprobable cosine bins as necessary to achieve an internal criterion of precision in the approximation of the Legendre polynomial expansion of angular distributions. Moreover there is linear interpolation of density within each bin. At the energies of interest in the present benchmarks there are only 32 cosine bins but the interpolation still exists in each bin, which is perhaps a source of difference with MCNP in the leakage treatment.

GODIVA

Range of k_{eff} values

There is a difference of 114 (±14) pcm between the TRIPOLI continuous energy and the KENO multi-group k_{eff} values, these being the lowest and highest values in Groups (a) and (b). The Petten and Cadarache MCNP results are consistent with the TRIPOLI result whereas the MONK result, including the Q test, is closer to the MICROX and SCALE results. The difference between the TRIPOLI and MCNP Monte Carlo results and the Group (b) multi-group methods (MICROX-2 and SCALE-4.2) appears to be significant.

Neutron balances

The neutron balances have been normalised to the fission neutron production, the sum of the absorption and leakage then being equal to $1/k_{eff}$. The three group neutron balances are within about 50 pcm of each other for the Monte Carlo calculations, corrected for the contribution of delayed neutrons to the fission spectrum, and the MICROX-2 and SCALE-4.2 multi-group results. The ratios of leakage to absorption (see Table 3.3) are also about the same for all these codes.

The accuracy of the TRIPOLI, MONK and MCNP calculations is high (~10 to 15 pcm) but the correction applied to the MCNP and MONK results for the effect of the delayed neutron spectrum is only approximate. A higher accuracy is needed to give a clear indication of the sources of the differences. The ν value in TRIPOLI appears to be about 0.1% low and the leakage fractions in MONKQ, MICROX-2 and SCALE-4.2 appear to be slightly lower than in TRIPOLI and MCNP.

Spectral indices

The spectral index calculations [Table 6(a)] made using TRIPOLI, the deterministic codes and the other Monte Carlo codes (corrected to take into account the delayed neutron component in the fission spectrum) agree to within 0.07% for the fission ratios, ^{239}Pu/^{235}U and ^{233}U/^{235}U. For the threshold fission rate ratios, ^{238}U/^{235}U and ^{237}Np/^{235}U, the differences are larger and the MCNP results (with delayed neutron spectrum correction) are in less good agreement with the other Group (a) and (b) results. Excluding the MCNP results and the Group (c) deterministic results the ranges for TRIPOLI, MONK results (with delayed neutron spectrum correction) and the MICROX and XSD results are 0.26% for the ^{238}U/^{235}U fission ratio and 0.20% for the ^{237}Np/^{235}U ratio. For the ^{197}Au capture ratio there is again good agreement between TRIPOLI, MONK (with delayed neutron spectrum correction) and the Group (b) deterministic calculations, a range of 0.18%. The MCNP result (with delayed neutron spectrum correction) for the threshold fission reaction ^{238}U/^{235}U is about 1% higher than the values given by the other methods and the results for the other ratios also show larger differences, but within the estimated statistical uncertainty of 1%.

JEZEBEL

Effect of the choice of fission spectrum, total or partial fission reactions spectra

The calculations for JEZEBEL were made using the two different fission spectra for ^{239}Pu as well as different methods for treating the incident neutron energy dependence and different options in NJOY. The standard NJOY processing uses the spectra for the partial fission reactions (first chance, second chance, etc.) to produce the fission spectrum matrix, whereas the recommended fission spectrum is the one tabulated for the total fission cross-section. At PSI Pelloni has made calculations using both spectra. Using the spectrum associated with the total fission cross-section gives a value of k_{eff} which is 183 pcm higher than the value calculated using the sum of the partial fission cross-section spectra. The ^{238}U fission rate at the core centre (relative to the ^{235}U fission rate) is calculated to be 3.3% higher in the PSI calculation using the total fission spectrum, in much better agreement with the measured value. There are similar changes for the ^{237}Np fission rate (+2%) and the gold capture (-2.7%). Different fission spectra are compared in Table 7. Calculations have also been made at Cadarache of the effect of choice of fission spectrum on the value of k_{eff}.

Ranges of k_{eff} values

For the partial fission reactions spectra there is the Petten MCNP continuous energy Monte Carlo result and the Group (b) MICROX-2 result (using the appropriately incident neutron energy averaged fission spectrum). The difference between the two k_{eff} values is 62 (±10) pcm. The fission spectrum in the SHIVA/ECCO/ERANOS calculation is closely similar to that in the MICROX-2 calculation and the k_{eff} value is close to the MCNP result. However, the SHIVA/ERANOS value is about 200 pcm lower.

The k_{eff} values obtained using the total fission spectrum are higher than for those obtained using partial fission reactions spectra. The different Group (a) and (b) results lie within a range of 75 pcm, the MCNP value being 75 (±11) pcm higher than the TRIPOLI value, with the MICROX-2 multi-group value being close to TRIPOLI and the SCALE-4.2 multi-group value intermediate between the two. The MONK results are also intermediate between the TRIPOLI and MCNP values.

Neutron balances

The neutron balances show a tendency for the MICROX-2 results to have a smaller Group 1 leakage fraction and a larger Group 2 fraction, but the differences for some of the other codes are of the same order. The components of the neutron balances calculated using TRIPOLI, MCNP, MONK, MICROX-2, SCALE-4.2 and SHIVA/ECCO/ERANOS agree to better than 100 pcm.

Spectral indices

There is similar good agreement between the results for the deterministic S_n codes and those found for GODIVA [Table 8(b)]. The TRIPOLI and MONK results are consistent with these to within the estimated uncertainties. Including a delayed neutron spectrum correction into the MONK results would improve the agreement.

The use of the total fission spectrum improves the C/E values for the $^{238}U/^{235}U$ and $^{237}Np/^{235}U$ fission ratios. When this spectrum is used there is a similar pattern of C/E values for JEZEBEL to those obtained for GODIVA.

Conclusions

We take as the primary solutions (a) the continuous energy, or fine group, Monte Carlo results obtained using TRIPOLI, MONK and MCNP, and (b) the multi-group S_n solutions calculated using fission spectrum vectors derived by means of appropriate reactor weighting spectra (PSI MICROX-2 and Delft SCALE-4.2). It has been found that the multi-group solutions are very sensitive to the way in which the fission spectrum vector is derived. Those multi-group codes using other fission spectra have been separated in the comparisons [Group (c)]. The MCNP and MONK neutron balances have been modified to make an approximate allowance for the delayed neutron component of the fission spectra (which has not been treated in the versions of MCNP and MONK used in the calculations described here).

There are some significant differences between the different solutions. The TRIPOLI and MCNP k_{eff} results for JEZEBEL (total fission spectrum) appear to be significantly different (75 ±11 pcm), with the MONK and the multi-group results being intermediate between the two*. The multi-group k_{eff} results for GODIVA appear to be significantly higher (about 70 pcm) than the TRIPOLI and MCNP Monte Carlo results. There are some significant differences between the MICROX-2 and SCALE-4.2 three-group neutron balance components, suggesting some small spectrum calculation approximations.

The results relating to the effect of the difference between the use of the total fission spectrum for ^{239}Pu, rather than the partial fissions spectra, and for the incident neutron energy dependence of both the ^{235}U and ^{239}Pu fission spectra, show how important the choice is.

The JEF-2.2 data give values of k_{eff} which are about 420-520 pcm low for GODIVA and about 350 pcm low for JEZEBEL (total fission spectrum). The C/E values for the spectral indices are consistent between GODIVA and JEZEBEL when the ^{239}Pu total fission spectrum is used. The $^{239}Pu/^{235}U$ fission ratio is about 1% low, the $^{233}U/^{235}U$, $^{238}U/^{235}U$ and the $^{237}Np/^{235}U$ fission ratios are about 3% low, and the ^{197}Au capture/^{235}U fission ratio is about 5% low.

Further calculations would be helpful in refining the comparisons.

- The fission spectra used in MCNP and MONK should be modified to include the delayed neutron component.

- It is only in the Delft SCALE-4.2 multi-group calculations that the reactor spectra have been used to obtain both the group averaged cross-sections and the fission spectrum vector (the PSI calculations treat just the fission spectrum effect). It would be helpful to have a second calculation to determine the magnitude of the effect for the group cross-sections.

- Calculations made using multi-group cross-sections derived from the cross-section data as it is used in TRIPOLI, MCNP and MONK would be interesting in helping to see if there are differences between the data processing and representation.

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* The ^{239}Pu evaluation used in the TRIPOLI and SHIVA libraries differs from the standard JEF-2.2 file in the unresolved resonance range 1-30 keV. However, the effect of this difference is expected to be very small in the calculations for JEZEBEL.

Annex 1

Some Notes on Approximations in the Methods

S_n order extrapolation

Increasing the S_n order increases the leakage fraction and thus decreases the value of k_{eff}. The differences will depend on the particular angular quadrature set used but, in fact, they are approximately the same for all the deterministic calculations.

Cadarache studies of dependence on S_n order

In the Cadarache SHIVA/ERANOS study the extrapolation to infinite S_n order was made using the following formula in terms of reactivity, ρ:

$$\rho(inf) = 2*\rho(2n) - \rho(n)$$

The calculations were performed up to order 32. Consistent results were obtained with the orders 32, 16 and 8 showing that there is linearity.

Special attention was given to the spatial mesh so that the results of direct and adjoint calculation were identical (within 0.6 pcm maximum). The spatial mesh was 0.1 mm.

In the SHIVA/ECCO/ERANOS study the S_{16} values for GODIVA and JEZEBEL were extrapolated using the following formula in terms of k_{eff}:

$$k(inf) = [4*k(2n) - k(n)]/3$$

resulting in a reduction of the S_{16} values by 67 pcm and 100 pcm, respectively, to extrapolate to S_∞. This extrapolation is different from that used in the SHIVA/ERANOS study.

PSI studies of dependence on S_n order

The variation, with S_n order, of the value of k_{eff}, and of the three group values of the leakage fraction of the neutron balance, is calculated to be as in the following table:

GODIVA

S_n order	k_{eff}	Leakage (Group 1)	Leakage (Group 2)	Leakage (Group 3)	Leakage (total)
32	0.99582	0.1437	0.2880	0.1442	0.5760
96	0.99566	0.1438	0.2881	0.1442	0.5762

k_{eff} (extrapolated) = 0.99565

The k_{eff} decrease between the S_{32} and S_{96} value is 16 pcm, the suggested decrease from the S_{32} to the S_∞ value of 17 pcm being appropriate. Results from an earlier study (high k_{eff}):

S_n order	4	8	16	32	∞ (extrapolated)
k_{eff}	1.00889	1.00251	1.00075	1.00025	1.00008
F49/F25	0.99302	0.99317	0.99320	0.99321	0.99321
F28/F25	0.97250	0.97476	0.97529	0.97542	0.97546
F37/F25	0.96727	0.96832	0.96855	0.96862	0.96864
F23/F25	0.96677	0.96666	0.96663	0.96662	0.96662
C197/F25	0.93993	0.93909	0.93891	0.93886	0.93884

In the earlier study the difference between the S_{16} and S_{32} values was found to be 50 pcm. These values are consistent with the Cadarache SHIVA/ECCO/ERANOS extrapolation from S_{16} to S_∞ of 67 pcm.

JEZEBEL (sum of the partial fissions spectra)

S_n order	k_{eff}	Leakage (Group 1)	Leakage (Group 2)	Leakage (Group 3)	Leakage (total)
16	0.99558	0.2083	0.3281	0.1340	0.6705
32	0.99484	0.2086	0.3285	0.1341	0.6712
96	0.99461	0.2087	0.3286	0.1341	0.6715

k_{eff} (extrapolated) = 0.99458

The k_{eff} decrease between the S_{16} and S_{32} value is 74 pcm and between the S_{16} and S_{96} value is 97 pcm. The S_∞ extrapolated value is 100 pcm lower than the S_{16} value, as in the Cadarache SHIVA/ECCO/ERANOS study.

JEZEBEL (total fission spectrum)

S_n order	k_{eff}	Leakage (Group 1)	Leakage (Group 2)	Leakage (Group 3)	Leakage (total)
16	0.99741	0.2154	0.3275	0.1265	0.6694
32	0.99676	0.2156	0.3279	0.1266	0.6701
96	0.99644	0.2157	0.3280	0.1266	0.6701

k_{eff} (extrapolated) = 0.99641

The k_{eff} decrease between the S_{16} and S_{32} value is 65 pcm and between the S_{16} and S_{92} value is 97 pcm. The extrapolated value is again taken to be 100 pcm lower than the S_{16} value and 35 pcm lower than the S_{32} value.

Delft studies of the effect on k_{eff} of varying the S_n order

k_{eff} values versus S_n order

S_n	32	128	256	Difference between S_{32} and S_{256}
GODIVA	0.99591	0.99574	0.99573	-18 pcm
JEZEBEL	0.99698	0.99673	0.99671	-27 pcm

The weighting spectrum used in NJOY to condense cross-sections is IWT=1, a previously calculated reactor spectrum.

Studies of the effect of varying the order of the P_n treatment

The Cadarache SHIVA studies used P_5, the Delft SCALE-4.2 studies used P_3 and the PSI MICROX-2 studies used a modified P_2.

PSI studies showed that increasing the order from P_2 modified to P_4 modified had very little effect.

Multi-group weighting spectra

The PSI and Delft calculations used NJOY 97-62.

In the PSI calculations the cross-sections were derived using the weighting spectrum IWT=4 with the fission spectrum boundary at 820.3 keV. For the Group (b) results the fission spectrum vectors were derived using the weighting spectrum IWT=1 and pre-calculated reactor spectra.

In the Delft calculations the cross-sections and the fission spectrum vector were derived using the same weighting spectrum, IWT=1 and pre-calculated reactor spectra for the results given in Group (b). Results have also been obtained using IWT=4 and fission spectrum boundaries at 830.3 keV, 1 keV and 1 eV.

TRIPOLI and MCNP results

Results have been provided by different contributors and to different accuracies and it is only the results with the smallest standard deviations which are included in the tables. To obtain the different components of the TRIPOLI calculations – one group neutron balance, three group neutron balance and spectral index calculations – separate TRIPOLI calculations were made. However, it is understood that the results are not independent but that the same random number sequences are used in each calculation. The values which were obtained in the three group neutron balances at Cadarache have been included in Table 1.

Annex 2

Calculations made for GODIVA of the Effect of Including the Delayed Neutron Component of the Fission Spectrum

Calculations made by S. Pelloni, PSI

Neutron balances

	Fission	Capture	(n,2n)	Leakage	Total	k_{eff}
Incl. dn χ	0.38613	0.04571	-0.00240	0.57255	1.00199	0.99802
No dn χ	0.38601	0.04546	-0.00241	0.57306	1.00212	0.99789
Difference	-0.00012	-0.00025	-0.00001	0.00051	0.00013	-0.00013
Difference (%)	-0.03	-0.55	-0.42	0.09	0.01	-0.01

Three-group neutron balances

	Absorption			Leakage		
	Group 1	**Group 2**	**Group 3**	**Group 1**	**Group 2**	**Group 3**
Energy boundary (in MeV)	>2.2313	>0.49787	<0.49787			
Incl. dn χ	0.08584	0.19474	0.15125	0.13898	0.28850	0.14507
No dn χ	0.08642	0.19521	0.14984	0.13993	0.28922	0.14391
Difference	0.00058	0.00047	-0.00141	0.00095	0.00072	-0.00116
Difference (%)	0.68	0.24	-0.93	0.68	0.25	-0.80

Ratio of leakage to absorption

	Group 1	Group 2	Group 3
Incl. dn χ	1.61906	1.48146	0.95914
No dn χ	1.61919	1.48158	0.96042
Difference	0.00013	0.00012	0.00128
Difference (%)	0.01	0.01	0.13

Notes: Incl. dn χ = Delayed neutron component of the fission spectrum included

No dn χ = Delayed neutron component of the fission spectrum not included

Difference = (NOT INCLUDED - INCLUDED)

Difference (%) = (NOT INCLUDED - INCLUDED)/INCLUDED (%)

The group averaging is not the same as that used in the reference PSI calculations, but the differences are considered to be a valid estimate of the effect of omitting the delayed component.

Values of (C/E - 1)% for the central reaction rate ratios

	F49/F25	F28/F25	F37/F25	F23/F25	C197/F25
Incl. dn χ	-0.81	-4.53	-3.94	-3.26	-4.94
No dn χ	-0.70	-3.87	-3.49	-3.27	-5.44
Difference	0.11	0.66	0.45	-0.01	-0.50

Notes: Incl. dn χ = Delayed neutron component of the fission spectrum included
No dn χ = Delayed neutron component of the fission spectrum not included
Difference = (NOT INCLUDED - INCLUDED)

Table 1. k_{eff} results for GODIVA and JEZEBEL

Laboratory and method	**GODIVA**	**JEZEBEL**	
Choice of ^{239}Pu fission spectrum for JEZEBEL		Partial fissions spectra	Total fission spectrum
Continuous energy and hyperfine group Monte Carlo methods			
Cadarache TRIPOLI-4 (continuous energy)	0.99476 **L** ±0.00010		0.99636 **L** ±0.00010
ECN Petten MCNP 4A (continuous energy, dn fission spectrum component not treated)	0.9951 ±0.00010	0.9952 **H** ±0.0001	
Cadarache MCNP 4A (continuous energy, dn fission spectrum component not treated)	0.99487 ±0.00030		0.99711 **H** ±0.00005
Winfrith MONK (including Qcheck, dn fission spectrum component not treated)	0.9958 ±0.00015		0.9968 ±0.00015
Winfrith MONK (no Qcheck, dn fission spectrum component not treated)	0.9953 ±0.00015		0.9966 ±0.00015
Multi-group methods using fission spectrum vectors derived for the particular system			
PSI MICROX-2 (P_2 mod. S_{32} extrapolated S_∞)	0.99565	0.99458 **L**	0.99641
Delft SCALE 4.2 XSD (P_3 S_{32} extrapolated S_{128})	0.99573		0.99671
Delft SCALE 4.2/KENO (172 group)	0.9959 **H** ±0.00010		0.9966 ±0.00010
Range (in pcm)	114 (±14)	62 (±10)	75 (±11)
Multi-group methods using fission spectrum vectors derived using other weighting methods			
Delft SCALE 4.2 XSD (IWT=4 standard thermal)	0.99431		0.99491
Delft KENO (multi-group) (IWT=4 standard thermal)	0.9941 ±0.00010		0.9949 ±0.00010
Delft SCALE 4.2 XSD (IWT=4 fission spec. > 1 keV)	0.99599		0.99671
Delft KENO (multi-group) (IWT=4 fission spec. > 1 keV)	0.9958 ±0.00010		0.9967 ±0.00010
Cadarache SHIVA/ECCO/ERANOS (P_5; S_{16} extrapolated S_∞)	0.99618	0.99520	
Cadarache SHIVA/ERANOS (P_5; S_{32} extrapolated S_∞)	0.99483	0.99321	

Notes: **H** and **L** denote the highest and lowest values

dn fission spectrum component not treated = denotes that the fission spectrum is the prompt neutron fission spectrum only, the delayed neutron component not being included

including Qcheck = denotes that in the MONK calculation the secondary energy distributions have been modified to be consistent with the Q values

no Qcheck = denotes that in the MONK calculation no modification has been made to the secondary energy distributions so as to make them consistent with the Q values

IWT=4 standard thermal = denotes that the weighting spectrum used to treat group averaging in NJOY is the standard (thermal maxwellian; 1/E; fission spectrum) weighting

IWT=4 fission spec. > 1 keV = denotes that the boundary between the 1/E and fission spectrum part of the weighting spectrum has been lowered to an energy of 1 keV

Table 2. Neutron balances for GODIVA

Balances normalised to 1 fission neutron production
The absorption + leakage values have been normalised to the quoted values of 1/k_{eff}

	Fission	Capture	(n,2n)	Leakage	Total	Derived k_{eff}	Quoted k_{eff}
TRIPOLI	0.3859	0.0453	-0.0027	0.5768	1.0053		0.9947
Petten MCNP	0.3854	0.0450	-0.0027	0.5773	1.0050	0.9950	0.9951
MCNP (dn mod.)	0.3855	0.0453	-0.0027	0.5768	1.0049	0.9951	
MONKQ	0.3854	0.0451	-0.0027	0.5763	1.0041	0.9959	0.9958
MONKQ (dn mod.)	0.3855	0.0454	-0.0027	0.5758	1.0040	0.9960	
MONK	0.3854	0.0449	-0.0027	0.5770	1.0046	0.9954	0.9953
MONK (dn mod.)	0.3855	0.0452	-0.0027	0.5765	1.0045	0.9955	
MICROX (PSI)	0.3856	0.0453	-0.0027	0.5762	1.0044		0.9957
Delft (IWT=1)	0.3855	0.0452	-0.0027	0.5764*	1.0044		0.9957*
Delft (thermal)	0.3861	0.0458	-0.0024				0.9946
Delft (X > 1 keV)	0.3853	0.0451	-0.0027		1.0040		
SHIVA/ECCO	0.3854	0.0451	-0.0027	0.5760**	1.0038		0.9962**

Table 2.1. Differences relative to TRIPOLI ($\times 10^{-4}$)

	Fission	Capture	(n,2n)	Leakage	Total
MCNP (dn mod.)	-4	–	–	–	-4
MONKQ (dn mod.)	-4	1	–	-10	-13
MONK (dn mod.)	-4	-1	–	-3	-8
MICROX	-3	–	–	-6	-9
Delft XSD (IWT=1)	-4	-1	–	-4	-9
SHIVA/ECCO	-5	-2	–	-8	-15

Notes: *(dn mod.) indicates that the corrections calculated by Pelloni have been applied for the effect of including the delayed neutron component of the fission spectrum.*

** Delft result for S_{32} extrapolated using the data of Pelloni.*

*** Cadarache S_{16} result for SHIVA/ECCO/ERANOS extrapolated.*

Table 3. Three group neutron balances for GODIVA

	Absorption			Leakage		
	Group 1	Group 2	Group 3	Group 1	Group 2	Group 3
Energy boundary (MeV)	>2.2313	>0.49787				
TRIPOLI	0.0881	0.1933	0.1499	0.1441	0.2882	0.1444
MCNP	0.0886	0.1939	0.1480	0.1449	0.2893	0.1431
MCNP (dn mod.)	0.0880	0.1934	0.1494	0.1439	0.2886	0.1443
MONKQ	0.0885	0.1936	0.1487	0.1446	0.2884	0.1433
MONKQ (dn mod.)	0.0879	0.1931	0.1501	0.1436	0.2877	0.1445
MONK	0.0886	0.1937	0.1482	0.1449	0.2890	0.1432
MONK (dn mod.)	0.0880	0.1932	0.1496	0.1439	0.2883	0.1444
MICROX	0.0880	0.1931	0.1498	0.1438	0.2881	0.1442
Delft XSD	0.0882	0.1930	0.1495	0.1442*	0.2879*	0.1443*
Delft (X > 1 keV)	0.0887	0.1927	0.1490			
SHIVA/EC	0.0885	0.1930	0.1490	0.1444**	0.2877**	0.1439**

Table 3.1. Differences relative to TRIPOLI ($\times 10^{-4}$)

	Absorption				Leakage			
	Group 1	Group 2	Group 3	Total	Group 1	Group 2	Group 3	Total
MCNP (dn mod.)	-1	1	-5	-5	-2	4	-1	1
MONKQ (dn mod.)	-2	-2	2	-2	-5	-5	1	-9
MONK (dn mod.)	-1	-1	-3	-5	-2	1	–	-1
MICROX	-1	-2	-1	-4	-3	-1	-2	-6
Delft XSD	1	-3	-4	-6	1*	-3*	-1*	-3*
Delft (X > 1 keV)	6	-6	-9	-9				
SHIVA/ECCO	4	-3	-9	-8	3**	-5**	-5**	-7**

Table 3.2. Ratio of leakage to absorption

	Group 1	Group 2	Group 3
MCNP	1.635	1.492	0.967 (-0.001 for dn)
TRIPOLI	1.636	1.491	0.963
MONKQ	1.635	1.490	0.964 (-0.001 for dn)
MONK	1.635	1.492	0.966 (-0.001 for dn)
MICROX	1.634	1.492	0.963
Delft XSD	1.635	1.492	0.965
SHIVA/ECCO	1.632**	1.491**	0.966**

Notes: *(dn mod.) indicates that the corrections calculated by Pelloni have been applied for the effect of including the delayed neutron component of the fission spectrum.*

** Delft result for S_{32} extrapolated to S_{96}.*

*** Cadarache result for SHIVA/ECCO/ERANOS S_{16} with an approximate extrapolation.*

Table 4. Neutron balances for JEZEBEL

	Fission	Capture	(n,2n)	Leakage	Total	Derived k_{eff}	Quoted k_{eff}
Partial fission reactions spectra							
Petten MCNP	0.3186	0.0159	-0.0007	0.6711	1.0049	0.9951	0.9952
MCNP (dn mod.)	0.3186	0.0159	-0.0007	0.6711	1.0049		
PSI MICROX	0.3188	0.0160	-0.0007	0.6715	1.0056		0.99461
SHIVA/ECCO	0.3187	0.0159	-0.0008	0.6709*	1.0047		0.99520
Total fission spectrum							
Cadarache TRIPOLI	0.3185	0.0153	-0.0006	0.6705	1.0037		0.9963
Cadarache MCNP	0.3184	0.0153	-0.0006	0.6698	1.0029		0.9971
MCNP (dn mod.)	0.3184	0.0153	-0.0006	0.6698	1.0029		
Winfrith MONKQ	0.3182	0.0153	-0.0006	0.6700	1.0031		0.9968
MONKQ (dn mod.)	0.3182	0.0153	-0.0006	0.6700	1.0031		
PSI MICROX	0.3185	0.0154	-0.0006	0.6703	1.0036		0.99644
Delft XSD	0.3184	0.0153	-0.0006	0.6701**	1.0032		0.9967
Delft (standard thermal spec)	0.3190	0.0156	-0.0006				0.9952

Table 4.1. Differences relative to MCNP (dn mod.) for cases using partial fissions spectra ($\times 10^{-4}$)

	Fission	Capture	(n,2n)	Leakage	Total
MICROX	2	1	–	4	7
SHIVA/ECCO	1	–	-1	-2	-2

Table 4.2. Differences relative to TRIPOLI for total fission spectrum cases

	Fission	Capture	(n,2n)	Leakage	Total
MCNP	-1	0	0	-7	-8
MONKQ	-3	0	0	-5	-7
MICROX	0	1	0	-2	-1
Delft XSD	-1	0	0	-4	-5

Table 4.3. Differences for MCNP between partial fissions and total fission spectra ($\times 10^{-4}$)

MCNP	2	6	-1	13	20

Notes: *(dn mod.) indicates that the corrections calculated by Pelloni have been applied for the effect of including the delayed neutron component of the fission spectrum.*

The dn mod. has been estimated on the basis of the ^{239}Pu delayed neutron yield, a smaller effect than for ^{235}U.

** Cadarache SHIVA/ECCO extrapolated from S_{16} to S_{96} using the data of Pelloni.*

*** Delft XSD extrapolated from S_{32} to S_{96} using the data of Pelloni.*

Table 5. Three-group neutron balances for JEZEBEL

	Absorption			Leakage		
	Group 1	Group 2	Group 3	Group 1	Group 2	Group 3
(MeV)	>2.2313	>0.49787				
Partial fission reactions spectra						
Petten MCNP	0.0991	0.1654	0.0701	0.2095	0.3285	0.1331
MCNP (dn mod.)	0.0989	0.1651	0.0706	0.2091	0.3279	0.1341
PSI MICROX	0.0988	0.1653	0.0706	0.2087	0.3286	0.1341
Cadarache SHIVA	0.0990	0.1652	0.0704	0.2090*	0.3279*	0.1338*
Total fission spectrum						
Cadarache TRIPOLI	0.1022	0.1651	0.0665	0.2163	0.3274	0.1267
Cadarache MCNP	0.1023	0.1654	0.0660	0.2164	0.3278	0.1256
MCNP (dn mod.)	0.1021	0.1651	0.0665	0.2160	0.3272	0.1266
Winfrith MONKQ	0.1026	0.1650	0.0657	0.2170	0.3274	0.1256
MONKQ (dn mod.)	0.1024	0.1647	0.0662	0.2166	0.3268	0.1266
PSI MICROX	0.1021	0.1652	0.0665	0.2157	0.3280	0.1266
Delft XSD	0.1023	0.1650	0.0664	0.2164**	0.3273**	0.1264**

Table 5.1. Differences relative to Petten MCNP (dn mod.) for cases using partial fissions spectra

	Absorption			Leakage		
	Group 1	Group 2	Group 3	Group 1	Group 2	Group 3
MICROX	-1	2	–	-4	7	–
SHIVA/ECCO	1	1	-2	-1	0	-3

Table 5.2. Differences relative to TRIPOLI for total fission spectrum cases

	Absorption			Leakage		
	Group 1	Group 2	Group 3	Group 1	Group 2	Group 3
MCNP (dn mod.)	-1	–	–	-3	-2	-1
MONKQ (dn mod.)	2	-4	-3	3	-6	-1
PSI MICROX	-1	1	–	-6	6	-1
Delft XSD	1	-1	-1	1	-1	-3

Notes: (dn mod.) indicates that the corrections calculated by Pelloni have been applied for the effect of including the delayed neutron component of the fission spectrum.

** Cadarache SHIVA/ECCO extrapolated from S_{16} to S_{96} using the data of Pelloni.*

*** Delft XSD extrapolated from S_{32} to S_{96} using the data of Pelloni.*

Table 5.3. Ratio of leakage to absorption

	Group 1	Group 2	Group 3
Partial fission reactions spectra			
MCNP	2.114	1.986	1.899
PSI MICROX	2.112	1.988	1.899
SHIVA/ECCO	2.111	1.985	1.901
Total fission spectrum			
TRIPOLI	2.117	1.983	1.905
MCNP	2.115	1.982	1.903
MONKQ	2.114	1.984	1.911
PSI MICROX	2.113	1.985	1.904
Delft XSD	2.115	1.984	1.904

Table 5.4. Differences for MCNP of using partial fission reactions spectra instead of total fission spectrum ($\times 10^{-4}$)

MCNP	-32	0	41	-69	7	75

Table 5.5. Per cent differences between MCNP partial fission reactions spectra and total fission spectrum cases

MCNP	-3.1%	–	6.2%	-3.2%	0.2%	6.0%

Table 6(a). Values of (C/E - 1)% for the central reaction rate ratios – GODIVA

	F49/F25	F28/F25	F37/F25	F23/F25	C197/F25
TRIPOLI (Cadarache)	-0.80 (±0.13)	-3.00 (±0.8)	-3.41 (±0.16)	-3.31 (±0.13)	-5.6 (±1.3)
MCNP (Petten)	-0.66 (±1.0)	-3.18 (±1.0)	-3.26 (±1.0)	-3.28 (±1.0)	-6.42 (±1.0)
MCNP (dn mod.)	-0.77	-3.84	-3.71	-3.27	-5.92
MONKQ (Winfrith)	-0.67	-2.08	-3.13	-3.35	-6.01
MONKQ (dn mod.)	-0.78	-2.74	-3.58	-3.34	-5.51
MONK (Winfrith)	-0.64	-2.10	-3.02	-3.34	-6.10
MONK (dn mod.)	-0.75	-2.76	-3.47	-3.33	-5.60
MICROX (S_n)	-0.76	-2.94	-3.50	-3.33	-5.52
Delft XSD (S_n)	-0.74	-2.78	-3.38	-3.33	-5.69
Range excluding the Monte Carlo results	0.02	0.16	0.12	0	0.17
Range including TRIPOLI and MONK (dn mod.), excluding MCNP (dn mod.)	0.06	0.26	0.20	0.03	0.18
SHIVA/ERANOS(S_n)	-0.74	-2.49	-3.14	-3.33	-6.03

Notes: (dn mod.) indicates that the corrections calculated by Pelloni have been applied for the effect of including the delayed neutron component of the fission spectrum.

There is consistency between TRIPOLI, MONK (dn mod.), MICROX and Delft XSD.

Table 6(b). Values of (C/E - 1)% for the central reaction rate ratios – JEZEBEL

	F49/F25	F28/F25	F37/F25	F23/F25	C197/F25
Partial fission reactions spectra results					
MCNP (Petten)	-1.45 (±1.0)	-6.28 (±1.0)	-4.84 (±1.0)	-3.44 (±1.0)	-2.60 (±1.0)
MICROX (S_n)	-1.58	-6.51	-5.39	-3.41	-1.76
SHIVA/ERANOS(S_n)	-1.60	-6.41	-5.27	-3.42	-1.99
SHIVA/ECCO/ERAN	-1.59	-6.41	-5.30	-3.42	-2.41
Range excluding the MCNP results	0.02	0.10	0.12	0.01	0.65
Total fission spectrum results					
TRIPOLI (Cadarache)	-1.07 (±0.11)	-3.04 (±0.5)	-3.31 (±0.12)	-3.50 (±0.11)	-4.7 (±1.2)
MONKQ (Winfrith)	-1.04	-2.70	-3.19	-3.53	-4.25
MICROX (S_n)	-1.05	-3.19	-3.38	-3.50	-4.45
Delft XSD (S_n)	-1.04	-3.08	-3.32	-3.52	-4.60
Range excluding the Monte Carlo results	0.01	0.11	0.06	0.02	0.15
Range including the Monte Carlo results	0.03	0.49	0.19	0.03	0.45

Notes: In the case of JEZEBEL estimates of the delayed neutron correction to the fission spectrum have not been made and this affects the MCNP and MONK results. The effects are smaller than for GODIVA. Including a delayed neutron correction in the MONK results would improve the agreement and reduce the ranges for the ratios $^{238}U/^{235}U$, $^{237}Np/^{235}U$ and $^{197}Au(n,\gamma)/^{235}U$.

There is an improvement in the threshold fission rates, F28/F25 and F37/F25, resulting from the use of the recommended fission spectrum (total fission spectrum, MT=18).

Table 7. Comparison of JEZEBEL fission spectra

	Total fission spectrum				Partial fissions spectra	
Energy group (MeV)	**Thermal Prompt[a]**	**1 MeV Prompt[b]**	**MICROX (PSI)[c]**	**SCALE-4.2 (Delft)[c]**	**MICROX (PSI)[c]**	**^{239}Pu (SHIVA) Fast[d]**
20-10	148	163	193	198	277	286
10-6.0653	2 671	2 820	3 016	3 053	3 296	3 314
6.0653-3.6788	11 996	12 277	12 596	12 653	12 224	12 258
3.6788-2.2313	22 147	22 258	22 372	22 378	21 042	21 060
2.2313-1.3534	23 174	23 057	22 967	22 929	22 159	22 150
1.3534-0.82085	17 171	17 007	16 859	16 824	17 155	17 134
0.82085-0.49787	10 562	10 438	10 321	10 304	10 975	10 956
0.49787-0.30197	5 891	5 817	5 726	5 719	6 252	6 239
0.30197-0	6 241	6 161	5 950	5 942	6 621	6 604
Fraction above 1.3534 MeV	**60 135**	**60 577**	**61 144**	**61 211**	**58 998**	**59 068**

Notes: [a] *Thermal neutrons induced fission; spectrum of prompt emitted neutrons.*

[b] *1 MeV neutrons induced fission; spectrum of prompt emitted neutrons.*

[c] *At PSI and Delft the fission spectra have been incident neutron energy averaged using a pre-calculated JEZEBEL flux to condense from the fission spectrum matrix to a single fission spectrum.*

[d] *At CEA Cadarache the SHIVA spectrum is a fast reactor averaged fission spectrum. However, it is similar to the PSI spectrum.*

Annex 3

Model Descriptions for GODIVA and JEZEBEL

CSEWG Benchmark Book, BNL 19302, ENDF 202, Revised 11-81

Fast reactor benchmark no. 5: GODIVA

- A homogeneous bare sphere of enriched uranium, measured eigenvalue = 1.000 ± 0.001

Radius

- 8.741 cm

Composition

Isotope	Density (nuclei/b-cm)
^{235}U	0.04500
^{238}U	0.002498
^{234}U	0.000492

Spectral indices

- Central fission ratios (relative to ^{235}U fission):

$F(^{238}U)/F(^{235}U)$	0.1647 ± 0.0018
$F(^{233}U)/F(^{235}U)$	1.59 ± 0.03
$F(^{237}Np)/F(^{235}U)$	0.837 ± 0.013
$F(^{239}Pu)/F(^{235}U)$	1.402 ± 0.025

- Ratio of capture in ^{197}Au to ^{235}U fission (relative to thermal $^{197}Au(n,g)$ of 98.8 ± 0.3):

$C(^{197}Au)/F(^{235}U)$	0.100 ± 0.002

Fast reactor benchmark no. 1: JEZEBEL

- A homogeneous bare sphere of plutonium metal, measured eigenvalue = 1.000 ± 0.002.

Radius

- 6.385 cm.

Composition

Isotope	Density (nuclei/b-cm)
^{239}Pu	0.03705
^{240}Pu	0.001751
^{241}Pu	0.000117
Ga	0.001375

Spectral indices

- Central fission ratios (relative to ^{235}U fission):

F(^{238}U)/F(^{235}U)	0.2137 ± 0.0023
F(^{233}U)/F(^{235}U)	1.578 ± 0.027
F(^{237}Np)/F(^{235}U)	0.962 ± 0.016
F(^{239}Pu)/F(^{235}U)	1.448 ± 0.029

- Ratio of capture in ^{197}Au to ^{235}U fission (relative to thermal ^{197}Au(n,g) of 98.8 ± 0.3):

C(^{297}Au)/F(^{235}U)	0.083 ± 0.002