JEFF Report 15

LWR PIN CELL BENCHMARK INTERCOMPARISONS

An intercomparison study organised by the JEFF Project, with contributions from the UK, France, Germany, the Netherlands, Slovenia and the USA

September 1999

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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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 simplified reactor 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.

This report gives details of an investigation of the differences between results obtained using different codes for simple light water reactor pin cell models fuelled with uranium oxide or mixed uranium/plutonium oxide. In most of the cases studied the leakage has been assumed to be zero, but a cell with leakage treated by means of a buckling has also been analysed. Cases at different temperatures have been calculated so that temperature coefficient calculations could also be intercompared. Differences between square and cylindrical cell boundary conditions have been studied and shown to be important.

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Introduction

The intercomparisons have been carried out for:

- Light water reactor pin cells without leakage.
- The pin cells with axial and radial leakage represented in terms of a buckling.

Two types of pin cell have been studied, one fuelled with UO_2 (UOX), detailed in Appendix 1, and the other fuelled with $UPuO_2$, specified in Appendix 2, the latter in two versions with different plutonium isotopic compositions (MOX-1 and MOX-2). The effects of changes in temperature and water density have also been calculated in order to examine the consistency of temperature coefficient calculation methods. For the zero leakage UOX cell, four cases have been calculated: the reference case, a case with reduced water density, an isothermal temperature increase and a fuel temperature increase. For the two MOX cells the effect of an increase in fuel temperature has been calculated.

A feature of the pin cells is the large value of k_∞, about 1.4 for the UOX pin cell (at room temperature), 1.22 for the MOX pin cell with the degraded fuel (MOX-1) and 1.26 for the more conventional MOX fuel (MOX-2).

The calculations have been made using different code systems but with nuclear data in all cases derived from the JEF-2.2 library (although with differences of interpretation of ^{239}Pu fission spectra and differences in the ^{239}Pu unresolved resonance region data). Both deterministic and Monte Carlo methods have been used.

The first aim of this intercomparison exercise has been to get information about the ranges of calculated values. This is of relevance to the evaluation of the performance of the JEF data library and to the adjustment of the data. The second aim has been to try to establish reference solutions on the basis of continuous energy Monte Carlo calculations and to use these to evaluate the other methods. Reaction rates have been edited in three energy groups so as to try to identify the sources of the differences.

The computer codes which are intercompared

The deterministic cell codes used are APOLLO-2 (CEA Cadarache and Saclay), RESMOD (IKE Stuttgart), ECCO (Cadarache), SCALE-4.2/XSDRNPM S_{32} P_3 (IRI TU Delft), LWR-WIMS (AEA Technology Winfrith) and WIMSD-5A (ISJ Ljubljana). APOLLO-2, SCALE-4 and LWR-WIMS use the "XMAS" 172 energy group scheme but with different resonance shielding methods and different approaches to the treatment of fission spectra. WIMSD-5A uses the WIMS 69 group structure and a library generated using methods developed by the IAEA WIMS-D library update project. RESMOD uses a 292 group library (165 fast-epithermal/127 thermal groups) stored in AMPX-format, with a 26 000 group slowing down calculation between 3 eV and 2 keV. ECCO uses a library of 1 968 groups plus sub-groups. (Calculations have also been made using a hyperfine version of the ECCO library.) Two versions of the APOLLO-2 code have been used; the Saclay calculations use the most recent version, 4.1, and the Cadarache calculations use Version 2 (which has been used extensively in the past for integral data studies). More details of the methods are given in Appendix 3.

The continuous-energy (or hyperfine group) Monte Carlo codes used are MCNP-4A (Petten, Delft and Stuttgart), MCNP-4B (Cadarache), MONK-7 (Winfrith), VIM (ANL) and TRIPOLI-4 (Cadarache and Saclay). These could only be used for the pin cell cases with zero bucklings. In addition, the group energy Monte Carlo codes KENOVa (Delft) (in the SCALE-4 system) and

MORSE-K (Stuttgart) have been used. A comparison has also been made at Delft between KENOVa and MCNP (groupwise mode), using the SCALE-4 group cross-section data, and agreement obtained between these two broad group Monte Carlo methods.

VIM and TRIPOLI use the total fission spectrum whereas MCNP and MONK use the prompt fission spectrum only. Some other approximations are involved. For example, the Cadarache TRIPOLI-4 calculations for the UOX cells are at 300 K (instead of 293 K, whereas the Saclay TRIPOLI-4 calculations are at 293 K) and the MCNP and MONK calculations for the MOX cells are at 293 K, or 293.16 K, (instead of at 300 K). This difference of 7 K results in differences in k_∞ of about 50 pcm, the Cadarache TRIPOLI-4 calculations for the UOX cells being lower than for the specification and the MCNP and MONK calculations for the MOX cells being higher.

NJOY has been used to generate a large part of the data in the cross-section sets used in the different codes, supplemented in some cases by other codes to treat resonance shielding effects and to convert formats to those required by the codes. However, different versions of NJOY, and different options within NJOY, have been used, and these result in some differences.

A comprehensive set of calculations was made at ECN Petten using MCNP-4A and several effects were investigated, including square versus cylindrical boundary conditions for the pin cells and the importance of the unresolved resonance region. The difference in k_∞ values between the square (reflected) and cylinder (with isotropic reflection), calculated using continuous energy Monte Carlo, is about 0.0025 in the case of the UO_2 pin cell ($k_\infty \sim 1.4$) (see Table 1B) but is calculated to be much larger for the MOX pin cells, about 0.008 for fuel MOX-1 ($k_\infty \sim 1.22$) (see Table 9). Similar results have been found using other code systems, and these are discussed below.

The differences between the results for the pin cell case with leakage treated by means of a buckling are particularly large, about 1 600 pcm (see Table 7). SCALE-4 gave an even larger difference, the value depending on the option used to derive the diffusion coefficient for the different regions of the cell, or for the cell as a whole. In this case there is no reference continuous-energy Monte Carlo calculation because the available methods cannot treat a cell with an applied buckling (although this can be done using the group plus sub-group Monte Carlo method MONK-5W). For this reason alternative whole reactor benchmarks have been proposed to study leakage effects.

Some calculation methods are still undergoing refinement, and approximations in the nuclear data used in the codes are being identified and corrected. Also, in some cases there is an element of ambiguity concerning the pin cell boundary condition, square or cylindrical (different approximations being involved in the resonance shielding treatment and the broad group flux calculation). The intercomparisons have resulted in corrections being made to some code systems and some features of the methods are now better understood.

UOX pin cell results

The results of the calculations for the four cases of the zero leakage UOX pin cell model are given in Table 1 and the differences between the different cases are shown in Table 2.

Treatment of (n,2n) reactions

In making the comparisons a difficulty is encountered associated with the treatment of (n,xn) reactions. In the case of LWR-WIMS these reactions are treated as negative absorptions; in APOLLO

and ECCO the (n,xn) source neutrons are included with the scattered neutrons and the net production of neutrons in scattering is subtracted from the total removal in calculating k_∞ and k_{eff}. If the alternative approach is used of adding the (n,xn) cross-sections to the absorption cross-sections and adding the neutrons produced in (n,xn) to the neutrons produced in fission the resulting values of k_∞ are about 100×10^{-5} lower for the UOX cell (this being the difference between 1.39/(1-0.0013) and (1.39 + 0.0026)/(1 + .0013). (The two methods give essentially the same result when k_∞, or k_{eff}, is equal to unity, the difference in the above case being a consequence of the large departure of k_∞ from unity.)

Treatment of resonance shielding in the zirconium clad

The treatment of resonance shielding in the zirconium cladding is a source of difference between the methods. When the shielding is not treated, as in the case of the Delft SCALE-4 calculations, the value of k_∞ is about 125×10^{-5} lower for the UOX cell Case 1, as is shown by the WIMS calculations made with and without zirconium resonance shielding (see Table 6). In some code schemes the resonance shielding treatment is restricted to the fuel isotopes, with the zirconium shielding being calculated outside the code and the shielded cross-section being input to the cross-section set used by the code. Another method used is to calculate an equivalence to a homogeneous medium, but the equivalence methods which are incorporated in some codes have been developed to treat fuel isotopes in a central cylindrical pin, and may not be accurate for resonant materials in other regions. (This is the case for the earlier version of APOLLO-2, Version 2.) An improved treatment of this effect has been included in the later version, APOLLO-2.4.1. Methods using hyperfine groups, or sub-groups, such as ECCO and the continuous energy Monte Carlo codes, MCNP and MONK, should treat the effect correctly.

The range of values of k_∞ for the reference case (calculated in cylindrical geometry) is 478×10^{-5}, with the WIMS-D (Ljubljana) value deviating most from the MCNP (Petten) value (363×10^{-5}) and the SCALE-4.2 XSD (Delft) value the next (248×10^{-5}). Note, however, that the resonance shielding in zirconium is not treated in this case and the treatment of the (n,2n) term could also affect the comparison.

The ranges of values for the effects of changes in water density and changes in temperature (excluding the MCNP and TRIPOLI results) are:

	Range
Water density reduction	5.2%
Isothermal temperature change to 550 K	5.9%
Fuel temperature from 550 K to 900 K	6.1%
Total temperature change	3.4%

The MCNP and TRIPOLI values for the differences are in broad agreement with the results of the deterministic calculations (within about 2 s.d.) although the values for the changes relative to the intermediate temperature (550 K) appear to be outside the ranges of the deterministic results.

Three-group neutron balances

Table 4 presents a three-group neutron balance comparison of the MCNP calculations for the cylindrical and square cell representations. It shows that the difference between the square and cylindrical cell results for MCNP is due primarily to a reduction in ^{238}U resonance region capture

(by about 1.4%) and an increase in hydrogen capture at thermal energies (by about 2%) for the square cell case.

Tables 5 and 6 compare the three group neutron balances for some of the deterministic codes with the MCNP data. The most significant differences are summarised in Tables 3(a), 3(b) and 3(c). We note that the resonance shielding treatment in LWR-WIMS and WIMS-D is based on a square cell equivalence method. Some conclusions from the intercomparisons are:

- *Group 1*. The older version of APOLLO-2 (Version 2) and LWR-WIMS give ^{238}U fission rates about 1.8% higher than MCNP (cyl.), ECCO, SCALE and the improved APOLLO-2.4.1, whereas WIMS-D gives a value 1.3% lower. However, different approximations are made in the treatment of fission spectra (for example, the 1 MeV ^{235}U fission spectrum is used in LWR-WIMS for all isotopes and incident neutron energies). The 1 MeV fission spectra were used in the earlier APOLLO-2.2 cross-section library whereas a reactor spectrum average of the fission spectrum matrix was used when deriving the later APOLLO-2.4.1 library. The delayed neutron component of the fission spectrum is not included in the MCNP and MONK calculations and this could result in an overestimation of the ^{238}U fission rate by perhaps several tenths of a per cent, implying that the APOLLO-2.4.1 and ECCO values are close to the correct values. The delayed neutron component is treated by TRIPOLI, and we see agreement between APOLLO-2.4.1 and TRIPOLI for the square cell calculations.

- *Group 2*. There is a range in ^{238}U capture of about ±0.5%, relative to MCNP. There are differences of 4% (for WIMS-D) and 2% (for APOLLO-2), for the ratio of ^{235}U capture to fission, and differences of up to 2.4% in ^{235}U fission relative to ^{238}U capture. We note that this latter ratio has improved in the more recent APOLLO-2.4.1 calculations.

- *Group 3*. In the thermal energy range it is the relative values which are important. The differences from the MCNP values are less than about 0.4%.

Pin cells with an applied buckling

The results for the cases with leakage (see Table 7) show large discrepancies. The results obtained using the SCALE code have been omitted at present because of the very large differences (the value calculated using the flux × volume averaged transport cross-section is 1.00734). We see that the range of values for the reference case, Case 5, is 1 593 pcm, with the LWR-WIMS value being much lower than the others. This difference corresponds to about 10% in the leakage fraction. The problem possibly arises from the method used to treat the shielding of the total cross-sections of the fuel isotopes in the resonance region (flux or current averaging) and of producing the cell averaged value. The ranges of values for the differences between the different cases (reduced water density and elevated temperatures) are also shown, these being similar to the values for the zero leakage cases.

A reference calculation method is required. There are Monte Carlo methods which treat heterogeneous problems with imposed bucklings. MONK 5W, for example, is a group Monte Carlo method which can treat problems with applied bucklings, and the WDSN-ST code treats an axial buckling explicitly, but these are broad group methods. These methods use the Bn approximation, and this is the recommended method for this benchmark intercomparison.

Because of this problem of providing a reference calculation for cases with leakage a simple geometry reactor assembly, the Winfrith DIMPLE SO1A assembly, has been adopted as a benchmark. This can be calculated using Monte Carlo methods. However, the deterministic calculations become

more complicated. The Studsvik KRITZ cores have also been calculated. The advantage of these assemblies is that the k_{eff} values have been measured and bucklings have also been derived from measurements. Thus an intermediate level of comparison can be made using cell models with the measured bucklings.

The calculations made for the KRITZ cores at two temperatures (in XY geometry with an axial buckling) using APOLLO-2, CASMO (Studsvik), the SCALE-4 system and LWR-WIMS give results in reasonably good agreement with each other and with experiment both for k_{eff} and the change in k_{eff} with temperature. This is in contrast to the above results for the pin cell. Some pin cell calculations for these cores have also been made.

MOX pin cells

The results for these cells are presented in Tables 8(a) to 8(c). The cylindrical geometry cases in Table 8(a) show a wide variation of 500 to 700×10^{-5}. The differences between the calculations for the two temperatures are given in Table 8(b). In the case of the LWR-WIMS results the large deviation is probably due to the limited treatment of temperature dependence of fuel isotope cross-sections and resonance shielding at thermal energies (that is, below 4 eV). We should note that ECCO, TRIPOLI, APOLLO-2 and MCNP (Cadarache) use a different version of the ^{239}Pu fission spectrum (the MT=18 fission spectrum) whereas the other deterministic codes use the MT=19, etc. spectra. These CEA codes also use different unresolved resonance region data for ^{239}Pu. This might account for some differences between the values although there is no consistent trend to be found when the square cell results are also taken into account. The MCNP (Petten) and VIM results are consistent, as are the MCNP (Cadarache) and TRIPOLI results. *(The Petten MCNP (cylindrical geometry) value for the hot case for fuel 1, and possibly also for fuel 2, appears to be anomalous.)*

For the square cell calculations there is agreement to within about 200 pcm between the six continuous energy Monte Carlo calculations, MCNP (Petten, Cadarache and Stuttgart), TRIPOLI, MONK and VIM. The ECCO results are once again high.

Cell boundary effects

An important effect studied in the Petten MCNP calculations is the difference between the cylindrical cell (with an isotropic, or white boundary condition) and the square reflected cell. For the MOX fuel cells the effect has also been calculated using continuous energy Monte Carlo methods at Cadarache (using MCNP and TRIPOLI) and at ANL (using VIM) (see Table 9). All these calculations have confirmed the effect for the MOX Fuel 1 as being a difference of about 750×10^{-5} in a k_∞ value of about 1.22. Calculations made using the deterministic codes ECCO and APOLLO-2 and using SCALE-2 (XSD/KENO, using the same broad group data, and resonance shielding data, in the two calculations) give differences of a similar magnitude, while MORSE-RESMOD gives an effect about half as large. In Tables 10 and 11 the components of the difference are analysed using the Petten MCNP data. The largest effect on going from the cylindrical boundary to the square boundary is the 1.7% reduction in resonance absorption, predominantly by ^{238}U. This results in an increase in the thermal flux, at which energy fission in ^{239}Pu predominates. The effect is partly offset by a 4.6% increase in capture in water at thermal energies.

For the UOX pin cell reference case (Case 1) the difference in k_∞ value between the cylindrical and square cell has now been calculated using several code schemes, in addition to the Petten MCNP. Calculations have been made at Cadarache using MCNP and at Saclay using TRIPOLI, and these are

in agreement with the Petten calculations, giving an effect of about 250 pcm in a k_∞ value of about 1.39. Calculations have been made using APOLLO-2 at Cadarache and Saclay, the values being in broad agreement with the MCNP results. For the codes in the SCALE-4 system (XSD – deterministic and KENO – group Monte Carlo) which calculate the resonance shielding treating the cell as cylindrical, the difference is smaller, 104 $(\pm 10) \times 10^{-5}$. Components of the difference calculated using Petten MCNP are given in Table 4(a) and using APOLLO-2.4.1 in Table 4(b). Again the main difference is seen to be a reduction in resonance absorption in ^{238}U and the consequent increase in the thermal flux, with the balance of events at thermal energies between the fuel and the water being altered (an increase in hydrogen absorption).

An interesting result obtained using ECCO is that if an isotropic boundary condition is assumed for the square boundary the result goes in the opposite direction, giving a reduction of 429×10^{-5} relative to the cylindrical geometry result, instead of an increase of 665×10^{-5} (for MOX Fuel 1).

Concluding remarks

Calculations made for simple pin cell benchmarks have shown that the differences between the results obtained using different code schemes are quite significant and should be taken into account in assessing the quality of the nuclear data library and in cross-section adjustment studies. The discrepancies are particularly large for cases with leakage treated via a buckling.

For accurate calculations cylindricalisation of the cell boundary is not an acceptable approximation.

There are approximations in the data libraries used in the neutronics codes which are perhaps not always taken into account when comparing calculations with experiment. Examples are the use of the prompt fission spectrum (rather than the total fission spectrum) in MCNP and MONK. The fission spectrum approximations can be greater in some deterministic codes, in particular the limitation to the use of the spectrum for one incident neutron energy, and possibly to the spectrum for one isotope (LWR-WIMS). There is also the difference between the vector fission spectrum data derived using different options in NJOY.

More detailed studies are needed to understand the reasons for some of the remaining differences. However, there are discrepancies which can be seen to be due to specific approximations in the methods used in the codes, as described, for example, in section entitled *Three-group neutron balances*. The Monte Carlo codes show a satisfactory degree of convergence, bearing in mind the fission spectrum approximations and temperature differences in some cases, and these can be used to provide reference results in these cases.

TABLES

Table 1(a). UOX cylindrical geometry pin-cell (zero leakage) k_∞ values

Case 1	Case 2	Case 3	Case 4
Isothermal (293 K)	Reduced H_2O density	Fuel at (900 K)	Isothermal (550 K)

Continuous energy Monte Carlo results

** Denotes a calculation made using the prompt fission spectrum, rather than the total fission spectrum.*

MCNP-4A (Petten)*	1.38774	1.33452	1.30309	1.31492
(Unres. region shielded)	(±0.00040)	(±0.00040)	(±0.00040)	(±0.00040)
MCNP-4B (Cadarache)*	1.38731			
	(±0.00007)			
TRIPOLI-4 (Saclay)	1.38805	1.33585	1.30246	1.31539
	(±0.00046)	(±0.00092)	(±0.00091)	(±0.00087)

Deterministic results

Δk_∞ values are relative to the Petten MCNP cylindrical cell result, in units of 10^{-5}.

RESMOD (Stuttgart)	1.38884	1.33685	1.30476	1.31985
Δk_∞	110			
ECCO (Cad.) (Hyperfine)	1.38889	1.33661		
Δk_∞	115*H			
ECCO (Cadarache)	1.38750	1.33515	1.30265	1.31770
Δk_∞	-24			
APOLLO-2.4.1 (Saclay)	1.38735	1.33452	1.30224	1.31696
Δk_∞	-39			
(APOLLO-2.2,Cadarache)	(1.38981)	(1.33775)	(1.30604)	(1.32086)
Δk_∞	(207)			
LWR-WIMS (Winfrith)	1.38797	1.33783	1.30519	1.32014
Δk_∞	23			
WIMS-D (Ljubljana)	1.38411	1.33166	1.29828	1.31362
Δk_∞	-363 *L			
SCALE-4.2 XSD (Delft)	1.38526	1.33366	1.30059	1.31623
(Zr unshielded). Δk_∞	-248			
(with est. Zr correction)	1.38628	*see Table 6*		
Δk_∞	-146			

k_∞ RANGE for Case 1: 478×10^{-5}

Notes: H denotes the highest and L the lowest value.

The older APOLLO-2.2 values have been included (in brackets). They are of interest because many integral data studies were made using the version.

LWR WIMS has calculated resonance shielding for a square geometry cell, in this case.

The estimated result for SCALE-4.2 XSD including a correction for resonance shielding in Zr is based on the LWR WIMS calculations with and without this correction (see Table 6).

Table 1(b). UOX square cell geometry pin cell (zero leakage) k_∞ values

Case 1	Case 2	Case 3	Case 4
Isothermal (293 K)	Reduced density	Fuel at (900 K)	Isothermal (550 K)

Continuous energy Monte Carlo results

** Denotes a calculation made using the prompt fission spectrum, rather than the total fission spectrum.*

MCNP-4A (Petten)* (Unres. region shielded)	1.39011 (±0.00040)			
MCNP-4B (Cadarache)*	1.38979 (±0.00007)			
MCNP-4A (Stuttgart)*	1.38994 (±0.00060)	1.33827 (±0.00060)	1.30678 (±0.00060)	
MONK-7 (Winfrith)*	1.38910 (±0.00010)			
TRIPOLI-4 (Cadarache)	1.38849 (±0.00018)			
TRIPOLI-4 (Saclay)	1.38997 (±0.00027)			

Deterministic results. With Δk_∞ values relative to MCNP Petten, in units of 10^{-5}.

APOLLO-2.4.1	1.39087	1.33912	1.30755	1.32190
Δk_∞	76			
(APOLLO-2.2)	(1.39205)			
Δk_∞	(194)			

Group Monte Carlo results *(cylindrical geometry res. shielding, square cell group fluxes)*

SCALE4 KENOV (Delft)	1.38630 (±0.00010)	1.3352 (±0.00010)	1.3026 (±0.00010)	1.3183 (±0.00010)

Difference in k (in units of 10^{-5}) between the square cell boundary condition and the cylindrical boundary for Case 1

MCNP-4A (Petten)	$\Delta k_\infty = 237 \pm 56$
MCNP-4B (Cadarache)	$\Delta k_\infty = 248 \pm 10$
TRIPOLI (Saclay)	$\Delta k_\infty = 192 \pm 53$
APOLLO-2.4.1	$\Delta k_\infty = 352$
(APOLLO-2.2)	($\Delta k_\infty = 224$)
SCALE-4 (Delft)	$\Delta k_\infty = 104$

Note: The SCALE-4 resonance shielding has been calculated using the same method for both square (KENOV) and cylindrical (XSD) boundary conditions and this probably explains the smaller effect.

Table 2. Differences between the k_∞ values of the different cases, in units of 10^{-5}

Cylindrical cell results

	Cases 1-2	**Cases 2-4**	**Cases 4-3**	**Cases 2-3**	**Cases 1-3**
	Change in H_2O density	293-550 K	Fuel temp. to 900 K	Total temp. change	Total change
MCNP (Petten)	5 322 (±60)	1 960 (±60)	1 183 (±60)	3 143 (±60)	8 465 (±60)
TRIPOLI-4 (Saclay)	5 220 (±100)	2 046 (±130)	1 293 (±130)	3 339 (±130)	8 559 (±100)
RESMOD (Stuttgart)	5 199	1 700 L	1 509	3 209	8 408
ECCO (Cad.) (hyperfine)	5 228				
ECCO (Cadarache)	5 235	1 745	1 505	3 250	8 485
APOLLO-2.4.1 (Saclay)	5 283 H	1 756	1 472 L	3 228 L	8 511
(APOLLO-2.2) (Cadarache)	(5 206)	(1 689)	(1 482)	(3 171)	(8 377)
LWR-WIMS (Winfrith)	5 014 L	1 769	1 495	3 264	8 278 L
WIMS-D (Ljubljana)	5 245	1 804 H	1 534	3 338 H	8 583 H
SCALE-4.2 (Delft)	5160 (Zr unshielded)	1 739	1 564 H	3 307	8 467

Notes: L *denotes the lowest value,* H *the highest value (excluding MCNP and TRIPOLI-4).*
LWR WIMS has square geometry resonance shielding.

RANGE excluding the Monte Carlo results

MID VAL.	5 148	1 752	1 518	3 283	8 430
RANGE	269	104	92	110	305
RANGE (%)	5.2%	5.9%	6.1%	3.4%	3.6%

Square cell results

MCNP-4A (Stuttgart)	5 167 (±90)			3 149 (±90)	8 316 (±90)
KENOV (Delft)	5 110 (±14)	1 690 (±14)	1 570 (±14)	3 260 (±14)	8 370 (±14)
APOLLO-2.4.1	5 175	1 722	1 435	3 157	8 332

Notes: SCALE-4/KENOV has cylindrical geometry resonance shielding.
The Petten MCNP result for the fuel temperature rise from 550 to 900 K appears discrepant.

Table 3(a). Comparisons of components of the neutron balance and percentage differences from the Petten MCNP (cylindrical geometry) values

	F(^{238}U)/F(^{235}U)		**^{238}U res capture**		**Group 2 ^{238}U cap/total A**	
Cylindrical geometry		% diff.		% diff.		% diff.
MCNP (Petten)*	0.05175		0.1648		0.15452	
ECCO	0.05165	-0.2%	0.1650	+0.1%	0.15471	+0.1%
APOLLO-2.4.1	0.05152	-0.5%	0.1649	+0.1%	0.15467	+0.1%
(APOLLO-2.2)	(0.05261)	(+1.7%)	(0.1640)	(-0.5%)	(0.15370)	(-0.5%)
LWR-WIMS sq.shield	0.05274	+1.9%	0.1647		0.15428	-0.2%
WIMS-D (Ljubljana)	0.05106	-1.3%	–		0.15544	+0.6%
SCALE (Delft)	0.05185	+0.2%	0.1657	+0.5%	0.15538	+0.6%
Square geometry						
MCNP (Petten)*	0.05199	+0.5%	0.1626	-1.3%	0.15237	-1.4%
TRIPOLI-4	0.05139	-0.7%			0.15240	-1.4%
MONK*	0.05169	-0.1%	0.1633	-0.9%	0.15287	-1.1%
APOLLO-2.4.1	0.05128	-0.9%	0.1622	-1.6%	0.15213	-1.5%

** Denotes a calculation made using the prompt fission spectrum, rather than the total fission spectrum.*

^{238}U res capture = Fraction of neutrons slowed down to the resonance group captured in ^{238}U in Group 2.

Group 2 ^{238}U cap/total A = Capture in ^{238}U in Group 2 divided by the total absorptions.

The ^{238}U/^{235}U fission ratio calculated using the more recent APOLLO-2.4.1 data library, with the improved fission spectra, is in better agreement with TRIPOLI4 than was APOLLO-2.2. Neglect of the delayed neutron component of the fission spectrum in MCNP and MONK gives a ratio which is higher by about 0.5 to 1.0%.

LWR WIMS has used the square geometry resonance shielding option but, in fact, the ^{238}U Group 2 capture result is in better agreement with the cylindrical geometry calculations.

Table 3(b). Comparisons of components of the neutron balance and percentage differences from the Petten MCNP (cylindrical geometry) values

Group 2 ratios

	Group 2 (F5/C8)		Group 2 (C5/F5)		Group 2 (Zr/C8)	
Cylindrical geometry		% diff.		% diff.		% diff.
MCNP (Petten)*	0.2678		0.5476		0.0183	
ECCO (Cadarache)	0.2662	-0.6%	0.5477	–	0.0185	+1%
APOLLO-2.4.1	0.2676	-0.1%	0.5581	+1.9%	0.0185	+1%
(APOLLO-2.2)	(0.2699)	(+0.8%)	(0.5586)	(+2.0%)	(0.0176)	(-4%)
LWR-WIMS (Winfrith) sq. shield	0.2643	-1.3%	0.5537	+1.1%	0.0185	+1%
WIMS-D (Ljubljana)	0.2615	-2.4%	0.5704	+4.2%		
SCALE (Delft)	0.2639	-1.5%	0.5536	+1.1%	0.0231	+26%
Square geometry						
MCNP (Petten)*	0.2702	+0.9%	0.5468	-0.1%	0.0185	+1%
TRIPOLI-4	0.2698	+0.7%	0.5464	-0.2%	0.0184	+1%
MONK*	0.2698	+0.7%	0.5472	-0.1%	0.0182	-1%
APOLLO-2.4.1	0.2710	+1.2%	0.5578	+1.9%	0.0188	+3%

** Denotes a calculation made using the prompt fission spectrum, rather than the total fission spectrum. This should not affect the Group 2 ratios and thermal values.*

Table 3(c). Averages in the thermal region

	α5	C8/F5	$(H_2O + O)$/F5
Cylindrical geometry			
MCNP (Petten)	0.1744	0.1689	0.1114
TRIPOLI-4	0.1744	0.1690	
ECCO	0.1744	0.1688	0.1113
APOLLO-2.4.1	0.1745	0.1684	0.1114
(APOLLO-2.2)	(0.1745)	(0.1683)	(0.1110)
LWR-WIMS	0.1744	0.1687	0.1119
WIMS-D (Ljubljana)	0.1743	0.1692	
SCALE (Delft)	0.1744	0.1687	0.1117
Square geometry			
MCNP (Petten)	0.1743	0.1689	0.1132
TRIPOLI-4	0.1744	0.1690	
MONK (Winfrith)	0.1742 (±.0002)	0.1687 (±.0002)	0.1131 (±.0002)
APOLLO-2.4.1	0.1747	0.1686	0.1122

Table 4(a). Three-group neutron balance comparison for Case 1

Differences between the Petten MCNP cylindrical and square boundary values

Neutron absorption normalised to 100 000

	Cylinder	Square	Difference
$H_2O + O_2$ capture			
Group 1	466	469	3
Group 2	187	188	1
Group 3	5 448	5 547	99
Total	**6 101**	**6 204**	**103**
Zr capture			
Group 1*	67	67	–
Group 2	283	282	-1
Group 3	300	301	1
Total	**650**	**650**	**–**
^{235}U fission			
Group 1	685	687	2
Group 2	4 138	4 117	-21
Group 3	48 899	48 996	97
Total ^{235}U fission	**53 722**	**53 800**	**78**
^{235}U capture			
Group 1*	110	110	–
Group 2	2 266	2 251	-15
Group 3	8 526	8 540	14
Total ^{235}U capture	**10 902**	**10 901**	**-1**
Total ^{235}U absorption	**64 624**	**64 701**	**77**
^{238}U fission			
Group 1	2 779	2 796	17
Group 2	1	1	–
^{238}U capture			
Group 1*	2 131	2 134	3
Group 2	15 452	15 237	-215
Group 3	8 261	8 276	15
Total ^{238}U absorption	**28 624**	**28 444**	**-180**
Total absorption	**99 999**	**99 999**	**–**

** Denotes that the (n,xn) production has been subtracted from the capture in Group 1.*

Table 4(a). Three-group neutron balance comparison for Case 1 (*continued*)

Differences between the Petten MCNP cylindrical and square boundary values

Neutron production

	Cylinder	**Square**	**Difference**
^{235}U			
Group 1	1 752	1 759	7
Group 2	10 068	10 019	-49
Group 3	119 195	119 389	294
Total ^{235}U production	**131 015**	**131 167**	**252**
^{238}U			
Group 1	7 753	7 802	49
Group 2	3	3	–
Total ^{238}U production	**7 756**	**7 805**	**49**
Total production	**138 771**	**138 972**	**301**

Table 4(b). Three-group neutron balance comparison for Case 1

Differences between the APOLLO-2.4.1 cylindrical and square boundary values

Neutron absorption normalised to 100 000

	Cylinder	Square	Difference
$H_2O + O_2$ capture			
Group 1	460	459	-1
Group 2	186	187	1
Group 3	5 446	5 503	57
Total	**6 092**	**6 149**	**57**
Zr capture			
Group 1*	67	67	–
Group 2	286	285	-1
Group 3	300	303	3
Total	**653**	**655**	**2**
^{235}U fission			
Group 1	683	684	1
Group 2	4 139	4 127	-12
Group 3	48 889	49 051	162
Total ^{235}U fission	**53 711**	**53 862**	**151**
^{235}U capture			
Group 1*	109	111	2
Group 2	2 310	2 300	-10
Group 3	8 530	8 558	28
Total ^{235}U capture	**10 949**	**10 969**	**20**
Total ^{235}U absorption	**64 660**	**64 831**	**171**
^{238}U fission			
Group 1	2767	2762	-5
Group 2	1	1	–
^{238}U capture			
Group 1*	2 125	2 131	6
Group 2	15 467	15 213	-254
Group 3	8 233	8 259	26
Total ^{238}U absorption	**28 593**	**28 366**	**-227**
Total absorption	**99 998**	**100 001**	**3**

** Denotes that the (n,xn) production has been subtracted from the capture in Group 1.*

Table 4(b). Three-group neutron balance comparison for Case 1 (*continued*)

Differences between the APOLLO-2.4.1 cylindrical and square boundary values

Neutron production

	Cylinder	**Square**	**Difference**
^{235}U			
Group 1	1 745	1 748	3
Group 2	10 072	10 041	-31
Group 3	119 200	119 590	390
Total ^{235}U production	**131 017**	**131 379**	**362**
^{238}U			
Group 1	7 718	7 704	-14
Group 2	3	3	–
Total ^{238}U production	**7 721**	**7 707**	**-14**
Total production	**138 738**	**139 086**	**348**

Components of the difference between square and cylindrical geometry calculations (production/absorption)

	MCNP	**APOLLO-2.4.1**
(H_2O + O_2)	-103	-57
Zr	–	-2
^{235}U fission	174	211
^{235}U capture	1	-20
^{238}U fission	32	-9
^{238}U capture	197	222
Abs. normalisation	–	3
Total	**301**	**348**

Table 5. Three-group neutron balance comparison for Case 1

Differences relative to the Petten MCNP (cylindrical boundary) values

Neutron absorption normalised to 100 000

	MCNP	ECCO		LWR-WIMS		APOLLO-2.4.1	
		Difference		Difference		Difference	
$H_2O + O_2$							
Group 1	466	472	6	483	17	460	-6
Group 2	187	186	-1	187	–	186	-1
Group 3	5 448	5 447	-1	5 471	23	5 446	-2
Total	**6 101**	**6 105**	**4**	**6 141**	**40**	**6 092**	**-9**
Zr							
Group 1*	67	59	-8	58	-9	67	–
Group 2	283	286	3	286	3	286	3
Group 3	300	302	2	300	–	300	–
Total	**650**	**647**	**-3**	**644**	**-6**	**653**	**3**
Subtotal	**6 751**	**6 752**	**1**	**6 785**	**34**	**6 745**	**-6**
^{235}U fission							
Group 1	685	684	-1	687	2	683	-2
Group 2	4 138	4 119	-19	4 078	-60	4 139	1
Group 3	48 899	48 924	25	48 895	-4	48 889	-10
Total	**53 722**	**53 727**	**5**	**53 660**	**-62**	**53 711**	**-11**
^{235}U capture							
Group 1*	110	110	–	110	–	109	-1
Group 2	2 266	2 256	-10	2 258	-8	2 310	44
Group 3	8 526	8 530	4	8 527	1	8 530	4
Total	**10 902**	**10 896**	**-6**	**10 895**	**-7**	**10 949**	**47**
Total ^{235}U absorption	**64 624**	**64 623**	**-1**	**64 555**	**-69**	**64 660**	**36**
^{238}U fission							
Group 1	2 779	2 773	-6	2 829	50	2 767	-12
Group 2	1	2	1	1	–	1	–
^{238}U capture							
Group 1*	2 131	2 123	-8	2 152	21	2 125	-6
Group 2	15 452	15 471	19	15 428	-24	15 467	15
Group 3	8 261	8 257	-4	8 249	-12	8 233	-28
Total ^{238}U absorption	**28 624**	**28 626**	**2**	**28 659**	**35**	**28 593**	**-31**
Total abs.	**99 999**	**100 001**	**2**	**99 999**	**–**	**99 998**	**-1**

** Denotes that the (n,xn) production has been subtracted from the capture in Group 1.*

Table 5. Three-group neutron balance comparison for Case 1 (*continued*)

Differences relative to the Petten MCNP (cylindrical boundary) values

Neutron production

	MCNP	ECCO		LWR-WIMS		APOLLO-2.4.1	
			Difference		Difference		Difference
^{235}U							
Group 1	1 752	1 749	-3	1 757	5	1 745	-7
Group 2	10 068	10 022	-46	9 923	-145	10 072	+4
Group 3	119 195	119 280	85	119 210	15	119 200	+5
Total	**131 015**	**131 051**	**36**	**130 890**	**-125**	**131 017**	**+2**
^{238}U							
Group 1	7 753	7 741	-12	7 906	153	7 718	-35
Group 2	3	6	3	3	–	3	–
Total	**7 756**	**7 747**	**-9**	**7 909**	**153**	**7 721**	**-35**
Total production	**138 771**	**138 798**	**27**	**138 799**	**28**	**138 738**	**-33**

Components of the difference (production/absorption)

	ECCO	LWR-WIMS (ZR shielded)	APOLLO-2.4.1
($H_2O + O_2$)	-4	-40	9
Zr	3	6	-3
^{235}U fission	31	-63	13
^{235}U capture	6	7	-47
^{238}U fission	-4	103	-23
^{238}U capture	-7	15	19
Abs. normalisation	2	–	-1
Total	**27**	**28**	**33**

Table 6. Three group neutron balance comparison for Case 1

Cases with Zr unshielded

Differences relative to the Petten MCNP (cylindrical boundary, Zr shielded) values

The (n,2n) contribution to the SCALE neutron balance is estimated using APOLLO-2.2 results, the value (in Group 1) and the resulting sums being given in brackets.

	MCNP	WIMS (Zr shielded)		WIMS (Zr unshielded)		SCALE (Zr unshielded)	
			Difference		Difference		Difference
$H_2O + O_2$							
Group 1	466	483	17	484	18	462	-4
Group 2	187	187	–	186	-1	186	-1
Group 3	5 448	5 471	23	5 466	18	5 466	18
Total	**6 101**	**6 141**	**40**	**6 136**	**35**	**6 114**	**13**
Zr							
Group 1*	67	58	-9	67	–	74 (-7)*	(–)
Group 2	283	286	3	359	76	359	76
Group 3	300	300	–	300	–	299	-1
Total	**650**	**644**	**-6**	**726**	**76**	**(725)**	**(75)**
Subtotal	**6 751**	**6 785**	**34**	**6862**	**111**	**(6 839)**	**(88)**
^{235}U fission							
Group 1	685	687	2	687	2	684	-1
Group 2	4 138	4 078	-60	4 074	-64	4 100	-38
Group 3	48 899	48 895	-4	48 847	-52	48 811	-88
Total	**53 722**	**53 660**	**-62**	**53 608**	**-114**	**53 595**	**-127**
^{235}U capture							
Group 1*	110	110	–	110	–	113 (-4)*	(-1)
Group 2	2 266	2 258	-8	2 257	-9	2 270	4
Group 3	8 526	8 527	1	8 519	-7	8 515	-11
Total	**10 902**	**10 895**	**-7**	**10 886**	**-16**	**(10 894)**	**(-8)**
Total ^{235}U absorption	**64 624**	**64 555**	**-69**	**64 494**	**-130**	**(64 489)**	**(-135)**
^{238}U fission							
Group 1	2 779	2 829	50	2 831	52	2 778	-1
Group 2	1	1	–	1	–	1	–
^{238}U capture							
Group 1*	2 131	2 152	21	2 151	20	2 233 (-111)*	(-9)
Group 2	15 452	15 428	-24	15 420	-32	15 538	86
Group 3	8 261	8 249	-12	8 240	-21	8 235	-26
Total absorption							
Total ^{238}U	**28 624**	**28 659**	**35**	**28 643**	**19**	**(28 674)**	**(50)**
Total	**99 999**	**99 999**	**–**	**99 999**	**–**	**(100 002)**	**(3)**

Table 6. Three group neutron balance comparison for Case 1 (*continued*)

Cases with Zr unshielded

Neutron production

	MCNP	WIMS (Zr shielded)		WIMS (Zr unshielded)		SCALE (Zr unshielded)	
			Difference		Difference		Difference
^{235}U							
Group 1	1 752	1 757	5	1 757	5	1 755 (-8)*	(-5)
Group 2	10 068	9 923	-145	9 914	-154	9 975	-93
Group 3	119 195	119 210	15	119 090	-105	119 030	-165
Total	**131 015**	**30 890**	**-125**	**130 761**	**-254**	**(130 752)**	**(-263)**
^{238}U							
Group 1	7 753	7 906	153	7 910	157	7 970 (-222)*	(-4)
Group 2	3	3	–	3	–	3	–
Total	**7 756**	**7 909**	**153**	**7 913**	**157**	**(7 751)**	**(-4)**
Total production	**138 771**	**138 799**	**28**	**138 674**	**-97**	**(138 503)**	**(-268)**

* *(n,xn) production has been subtracted from the SCALE-4 Group 1 fission production terms and the (n,xn) cross-section subtracted from the Group 1 capture terms.*

Components of the difference (production/absorption)

	WIMS (Zr shielded)	WIMS (Zr unshielded)	SCALE (Delft) (Zr unshielded
($H_2O + O_2$)	-40	-35	-13
Zr	6	-76	-75
^{235}U fission	-63	-140	-136
^{235}U capture	7	16	8
^{238}U fission	103	105	-3
^{238}U capture	15	33	-51
Abs. normalisation	–	–	4
Total	**28**	**-97**	**-268**

An estimated value of k_∞ for SCALE with an allowance for resonance shielding in zirconium is: 1.38503 + 0.00125 = 1.38628

Table 7. Pin cells with an applied buckling

UOX pin cell results (buckling = 0.01)

k_{eff} values

	Case 5	Case 6	Case 7	Case 8
RESMOD (Stuttgart)	0.99944	0.81804 H	0.79585 H	0.80389 H
ECCO (Cadarache)	0.99514	0.81131	0.78880	0.7972
APOLLO-2.4.1 (Saclay)	0.99983 H	0.81724	0.79518	0.80326
(APOLLO-2.2 Cadarache)	(0.99944)	(0.81682)	(0.79513)	(0.80315)
LWR-WIMS (Winfrith)	0.98390 L	0.79655 L	0.77391 L	0.78231 L
WIMS-D	0.99788	0.81782	0.79426	0.80312
Range ($\times 10^{-5}$)	**1 593**	**2 149**	**2 194**	**2 158**

Differences in k_{eff} values between the different cases

	Case 5-6	Case 6-8	Case 8-7
	Lower H_2O density	293-550 K	Fuel temp. to 900 K
RESMOD (Stuttgart)	18 140	1 415	804
ECCO (Cadarache)	18 383	1 411	840
APOLLO-2.4.1	18 259	1 398 L	808 L
(APOLLO-2.2)	(18 262)	(1 367)	(802)
LWR-WIMS	18 735 H	1 424	840
WIMS-D	18 006 L	1 446 H	860 H
Range	**729**	**48**	**52**
Range (%)	**4.0%**	**3.4%**	**6.2%**

Table 8(a). Values of k_∞ for the plutonium pin cell benchmarks

Cylindrical cell results

	MOX Fuel 1		MOX Fuel 2	
	300 K	**560 K**	**300 K**	**560 K**
MCNP (Petten)*	1.21840 (±0.00060)	*(1.20048)* (±0.00060)	1.26106 (±0.00060)	1.24564 (±0.00060)
MCNP (Cadarache)*	1.21970 (±0.0009)			
TRIPOLI-4 (Saclay)	1.21902 (±0.00083)	1.20407 (±0.00084)	1.26233 (±0.00090)	1.24830 (±0.00064)
VIM (ANL)	1.21783 (±0.00036)		1.26050 (±0.00036)	
APOLLO-2.4.1	1.21817	1.20316 L	1.26019	1.24609
(APOLLO-2.2)	(1.22069)	(1.20573)	(1.26342)	(1.24929)
ECCO (Cadarache)	1.22335 H	1.20885 H	1.26419	1.25033
RESMOD (Stuttgart)	1.22065	1.2066	1.2637	1.2495
LWR-WIMS (sq Dancoff)	1.21656 L	1.20371	1.25862 L	1.24510 L
SCALE-4.2 (Delft) (Zr unshielded)	1.22238	1.20763	1.26465 H	1.25057 H

** Denotes a calculation made using the prompt fission spectrum, rather than the total fission spectrum.*
H *and* L *denote the highest and lowest values.*

RANGES ($\times 10^{-5}$)	**679**	**569**	**603**	**547**

Table 8(b). Differences between the cylindrical cell values for 560 K and 300 K ($\times 10^{-5}$)

	MOX Fuel 1	MOX Fuel 2
MCNP (Petten)	*1 792 (±85)*	1 542 H (±85)
TRIPOLI-4 (Saclay)	1 495 (±120)	1 403 (±110)
APOLLO-2.4.1	1 501 H	1 410
ECCO (Cadarache)	1 450	1 386
RESMOD (Stuttgart)	1 400	1 420 H
LWR-WIMS (Winfrith)	1 285 L	1 352 L
SCALE-4.2 (Delft)	1 475	1 408

Range ($\times 10^{-5}$) (excluding Monte Carlo)	**216 (= 16%)**	**68 (= 4.9%)**

Note: The MCNP value for Fuel 1 seem to be discrepant.

Table 8(c). Values of k_∞ for the plutonium pin cell benchmarks

Square cell results

	MOX Fuel 1		MOX Fuel 2	
	300 K	**560 K**	**300 K**	**560 K**
MCNP (Petten)*	1.22647 (±0.00060)			
MCNP (Cadarache)*	1.22697 (±0.00009)			
TRIPOLI (Cadarache)	1.22513 (±0.00016)			
VIM (ANL)	1.22578 (±0.00036)		1.26747 (±0.00036)	
MCNP (Stuttgart)	1.2270±30 (±0.00030)	1.2127±50 (±0.00050)	1.2692±40 (±0.00040)	1.2553±30 (±0.00030)
MONK-7 (Winfrith)	1.2260 (±0.00050)		1.2686 (±0.00050)	
MORSE-K (Stuttgart)	1.2237 L (±0.00080)	1.2100 (±0.00080)	1.2652 (±0.00080)	1.2524 (±0.00080)
ECCO (Cadarache) 5×5; square cell, 293 K	1.23057 H	1.21569 H		
APOLLO-2.4.1	1.22723	1.21242 L	1.26876	1.25485
SCALE-4.2/KENO	1.2279 (±0.00020)	1.2137 (±0.00020)	1.2701 (±0.00020)	1.2562 (±0.00020)

Table 8(d). Differences between the values for 560 K and 300 K ($\times 10^{-5}$)

	MOX Fuel 1	MOX Fuel 2
MCNP (Stuttgart)	1 430±60	1 390±50
MORSE-K (Stuttgart)	1 370±110	1 280±110
ECCO (Cadarache)	1 488	1 386
APOLLO-2.4.1	1 481	1 391
SCALE-4.2/KENO (Delft)	1 420±30	1390±30

Range (in pcm)	(Consistent)	(Consistent)

Table 9. Difference between the square and cylindrical boundary for the MOX pin cells

In units of 10^{-5}

	MOX Fuel 1		MOX Fuel 2	
	300 K	**560 K**	**300 K**	**560 K**
MCNP (Petten)	807 (±85)			
MCNP (Cadarache)	727 (±10)			
TRIPOLI-4 (Cadarache/Saclay)	611 (±85)			
VIM (ANL)	795 (±51)			
ECCO (Cadarache) (1 968 groups)*	665	684		
APOLLO-2.4.1	906	926	857	876
MORSE-RESMOD (Stuttgart)	300	340	150	290
SCALE (Delft) (172 groups)*	582	567	545	553

** Within group resonance shielding calculated for a cylindrical cell in the case of ECCO, MORSE and SCALE.*

Table 10(a). Relative reaction rates in MCNP (Petten) calculations for the cylindrical and square geometry cases for MOX Fuel 1 at 300 K

Reaction rate ratio	**Cylinder**	**Square**	**% difference**
^{238}F/F-total	0.07204	0.07169	-0.5%
^{238}U resonance absorptions/slowing down fraction to Group 2	0.1680	0.1652	-1.7%
^{238}U thermal capture/total thermal fission	0.04185	0.04187	
Thermal ^{239}Pu alpha	0.5115	0.5096	-0.4%
^{239}Pu resonance absorption/^{238}U resonance absorption	0.5286	0.5337	1.0%
Thermal captures in H/Total thermal fission	0.02774	0.02901	4.6%

Table 10(b). Petten MCNP neutron balance tables for cylinder and square

MOX Fuel 1 at 300 K

	Capture			Fission			Production		
	Cylinder	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**
H_2O									
Group 1	536	534	-2						
Group 2	146	146	0						
Group 3	655	695	40						
Zr									
Group 1	109	109	0						
Group 2	391	385	-6						
Group 3	52	54	2						
(n,xn)	-15	-15	0						
^{235}U									
Group 1	11	11	0	62	62	0	159	159	0
Group 2	185	184	-1	339	338	-1	827	823	-4
Group 3	63	64	1	319	326	7	777	795	18
^{238}U									
Group 1	2 617	2 618	1	3 041	3 046	5	8 539	8 551	12
Group 2	15 129	14 870	-259	1	1	0	3	3	0
Group 3	989	1 003	14	0	0	0	0	0	0
(n,xn)	-155	-154	1						
^{238}Pu									
Group 1	9	9	0	63	63	0	199	200	1
Group 2	159	160	1	38	38	0	110	111	1
Group 3	240	246	6	8	8	0	24	24	0
^{239}Pu									
Group 1	235	235	0	2 213	2 217	4	6 784	6 796	12
Group 2	5 742	5 697	-45	7 997	7 936	-61	22 944	22 770	-174
Group 3	10 026	10 120	94	19 602	19 860	258	56 225	56 970	745
(n,xn)	-3	-3	0						
^{240}Pu									
Group 1	117	117	0	440	442	2	1 370	1 373	3
Group 2	1 931	1 909	-22	38	38	0	105	105	0
Group 3	12 928	12 830	-98	3	3	0	7	7	0
(n,xn)	-1	-1	0						
^{241}Pu									
Group 1	79	79	0	441	442	1	1 362	1 364	2
Group 2	1 151	1 148	-3	3 838	3 825	-13	11 257	11 220	-37
Group 3	1 196	1 219	23	3 663	3 738	75	10 737	10 960	223
(n,xn)	-3	-3	0						

Table 10(b). Petten MCNP neutron balance tables for cylinder and square (*continued*)

MOX Fuel 1 at 300 K

	Capture			Fission			Production		
	Cylinder	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**
^{242}Pu									
Group 1	26	26	0	88	88	0	274	275	1
Group 2	260	259	-1	1	1	0	3	3	0
Group 3	1 722	1 698	-24	1	1	0	3	3	0
(n,xn)	-1	-1	0						
^{241}Am									
Group 1	24	24	0	21	21	0	79	79	0
Group 2	303	303	0	2	2	0	8	8	0
Group 3	919	919	0	6	6	0	19	19	0
Totals	57 773	57 494	-279	42 227	42 502	275	121 816	122 618	802
Total A				100 000	99 996				

Table 10(c). Cylindrical versus square cell results for the Petten MCNP calculations – Groups 2 and 3 normalised to the slowing down into Group 2

	Capture			Fission			Production		
	Cylinder	Square	Diff.	Cylinder	Square	Diff.	Cylinder	Square	Diff.
H_2O									
Group 2	162	162	0						
Group 3	728	772	44						
Zr									
Group 2	434	428	-7						
Group 3	58	60	2						
^{235}U									
Group 2	206	204	-1	377	375	-1	918	914	-4
Group 3	70	71	1	354	362	8	863	883	20
^{238}U									
Group 2	16 802	16 517	-285	1	1	0	3	3	0
Group 3	1 098	1 114	16	0	0	0	0	0	0
^{238}Pu									
Group 2	177	178	1	42	42	0	122	123	1
Group 3	267	273	7	9	9	0	27	27	0
^{239}Pu									
Group 2	6 376	6 328	-48	8 881	8 815	-66	25 481	25 292	-189
Group 3	11 135	11 241	106	21 769	22 059	290	62 441	63 279	838
^{240}Pu									
Group 2	2 145	2 120	-24	42	42	0	117	117	0
Group 3	14 357	14 251	-106	3	3	0	8	8	0
^{241}Pu									
Group 2	1 278	1 275	-3	4 263	4 249	-14	12 502	12 463	-39
Group 3	1 328	1 354	26	4 068	4 152	84	11 924	12 174	250
^{242}Pu									
Group 2	289	288	-1	1	1	0	3	3	0
Group 3	1 912	1 886	-26	1	1	0	3	3	0
^{241}Am									
Group 2	337	337	0	2	2	0	9	9	0
Group 3	1 020	1 021	1	7	7	0	21	21	0
Total Group 2	28 206	27 836	-369	13 609	13 528	-82	39 155	38 924	-231

** Add to the Group 2 capture totals the Group 3 capture for ^{240}Pu and ^{242}Pu.*

C2*	44 475	43 973	-502						

** Form the total absorption for Group 2 including the Group 3 capture for ^{240}Pu and ^{242}Pu.*

A2*				58 085	57 501	-584			

** Relate the Group 3 values to the complements of these modified absorption values.*

*** The treatment of the important lowest energy resonances in ^{240}Pu and ^{242}Pu is complicated by these being in Group 3. Thus Group 2 cannot be treated as the resonance region for these isotopes.**

Table 10(d). Comparison for the thermal region of the cylindrical and square geometry Petten MCNP calculations for MOX Fuel 1 at 300 K

(renormalised to the slowing-down to Group 3 excluding capture in ^{240}Pu and ^{242}Pu)

	Capture			Fission			Nuclear fission		
	Cylinder	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**	**Cylinder**	**Square**	**Diff.**
H_2O	1 737	1 816	80						
Zr	138	141	3						
^{235}U	167	167	0	846	852	6	2 060	2 078	18
^{238}U	2 619	2 621	2	0	0	0	0	0	0
^{238}Pu	636	643	7	21	21	0	64	63	-1
^{239}Pu	26 565	26 449	-116	51 937	51 905	-31	148 970	148 895	-75
^{240}Pu				8	8		19	18	
^{241}Pu	3 168	3 186	18	9 706	9 770	64	28 447	28 645	197
^{242}Pu				3	3		8	8	
^{241}Am	2 434	2 402	-32	16	16	0	50	50	-1
Total	**37 464**	**37 426**		**62 536**	**62 574**		**179 618**	**179 756**	

Table 11. Summary of the components of the difference between the Petten MCNP results for the cylindrical and square geometry models of the MOX Fuel 1 pin cell

		Capture	Fission	Production
H	Group 1	0		
	Group 2	1		
	Group 3	-29		
^{238}U	Group 1	13	12	37
	Group 2	294	0	0
	Group 3	-6	0	0
^{239}Pu	Group 1	1	9	28
	Group 2	68	94	268
	Group 3	-22	-103	-300
^{240}Pu	Group 1	1	1	5
	Group 2	29	0	0
	Group 3	151	0	0
^{241}Pu	Group 1	0	2	6
	Group 2	9	32	93
	Group 3	-12	-41	-123
^{242}Pu	Group 1	0	1	1
	Group 2	2	0	0
	Group 3	29	0	0
Total		**546**	**7**	**-1**

Neutron balances normalised to 10^5 fission neutrons produced in fission.
Three energy groups, with intermediate boundaries at 9.1 keV and 4 eV.

APPENDIX 1

PWR UOX pin-cell benchmark

This is a three-region cylindrical model consisting of uranium oxide fuel, zirconium clad and water coolant. The outer radii of the three regions are 0.4 cm, 0.45 cm and 0.6770275 cm. This outer radius corresponds to a square cell with L/2 = 0.6 cm.

Two sets of four cases are proposed. In the first set the leakage is zero and in the second set there is a buckling of 0.01. The dimensions are the same in all cases and the only changes are to the water density and to the temperatures. Case 1 is the reference case and Cases 2, 3 and 4 have the water density reduced by the factor 0.7. Cases 1 and 2 have all regions at a temperature of 293 K. Cases 3 and 4 are at elevated temperatures. In Case 3 the temperatures of fuel, clad and coolant are 900 K, 600 K and 550 K respectively. In Case 4 all regions are at 550 K. This last case gives a test of the isothermal temperature coefficient calculation while Case 3 gives information relevant to the power coefficient. Cases 5-8 are the same as Cases 1-4 but with an applied buckling of 0.01.

Compositions

		Cases 1 and 5	**Cases 2, 3, 4, 6, 7, 8**
Region 1	^{235}U ^{238}U ^{16}O	0.00070803 0.022604 0.046624	
Region 2	Zr	0.043241	
Region 3	H ^{16}O	0.066988 0.033414	0.046892 0.023390
Alternatively	H_2O	0.033494	0.023446

Dimensions: R1 = 0.4 cm, R2 = 0.45 cm, R3 = 0.6770275 cm

Temperatures	Region 1	Region 2	Region 3
	Fuel	Clad	Coolant
Case 1 and 5	293 K	293 K	293 K
Case 2 and 6	293 K	293 K	293 K
Case 3 and 7	900 K	600 K	550 K
Case 4 and 8	550 K	550 K	550 K

Bucklings for Cases 1-4: Buckling = zero
Bucklings for Cases 5-8: Buckling = 0.01, Axial = 1/3, Radial = 2/3
Reaction rate edit, by isotope and reaction type: Three groups, with intermediate boundaries at 9.1 keV and 4 eV

APPENDIX 2

LWR MOX pin-cell benchmark

This is a three-region cylindrical model consisting of plutonium-uranium oxide fuel, zirconium clad and water coolant. The outer radii of the three regions are 0.41 cm, 0.475 cm and 0.710879 cm. This outer radius corresponds to a square cell with L/2 = 0.63 cm. The leakage is zero, $B^2 = 0$.

There are two different MOX fuel compositions, the first plutonium vector being a highly degraded one and the second a less degraded one. Cases 1 and 2 have all regions at a temperature of 300 K. Cases 3 and 4 have the fuel at 560 K.

Compositions

		Fuel MOX-1	**Fuel MOX-2**
Region 1	^{235}U	0.00005105	0.00005118
	^{238}U	0.02037	0.02042
	^{238}Pu	0.00004669	0.00002714
	^{239}Pu	0.001465	0.001972
	^{240}Pu	0.0005691	0.0004256
	^{241}Pu	0.0002713	0.00003577
	^{242}Pu	0.0001413	0.00001234
	^{241}Am	0.00003028	0.00001406
	O	0.04588	0.04588
Region 2	Zr	0.0388	
Region 3	H	0.04744	
	O	0.02372	

Dimensions: R1 = 0.41 cm
R2 = 0.475 cm
R3 = 0.710879 cm

Temperatures	Region 1	Region 2	Region 3
	Fuel	Clad	Coolant
Case A	300 K	300 K	300 K
Case B	560 K	300 K	300 K

Reaction rate edit, by isotope and reaction type: Three groups, with intermediate boundaries at 9.1 keV and 4 eV.

APPENDIX 3

Notes on the methods

Group structures

APOLLO-2, LWR-WIMS and SCALE-4.2 use the 172 group "XMAS" scheme. WIMSD-5A uses the original WIMS 69 group structure and a library generated by means of NJOY-94.105 using methods developed by the IAEA WIMS-D library update project.

ECCO uses a 1 968 fine group library with a sub-group treatment of resonance structure. ECCO (hyperfine) uses a finer subdivision of groups in the lower resonance region.

MONK-7 uses an 13 193 hyperfine group scheme. In the resolved and unresolved resonance range the cross-sections are represented using a 1/1 024 lethargy width group structure. Neutrons are tracked using continuous energy.

MCNP uses continuous energy cross-sections with infinite dilute cross-sections in unresolved resonance regions. However, in the Petten version there is a treatment of shielding in the unresolved region.

RESMOD uses a 292 group library (165 fast-epithermal/127 thermal groups) stored in AMPX format. This library is tabulated for several sigma-zero values and temperatures covering zero power and operating range.

Resonance shielding methods

The methods used in APOLLO-2, LWR-WIMS, WIMSD, SCALE-4.2 (Delft) and PASC are based on homogeneous medium resonance integral calculations with an equivalence procedure. The equivalence is a single region equivalence in the case of LWR-WIMS, the Dancoff factor being Carlvik's square cell value. In the case of SCALE-4.2 (Delft) the Nordheim method is used in the resolved region, and the Bondarenko method in the unresolved region. A Monte Carlo method is used to obtain the equivalence in the most recent Delft results. In the case of APOLLO-2 a six-region treatment in the fuel is used and this has a significant effect on the ^{238}U resonance absorption. The APOLLO-2.4.1 results have been obtained with a more developed version of the resonance region treatment than the earlier APOLLO-2.2 results. Version 2.4.1 also has an improved treatment of resonance shielding in the zirconium clad.

In unresolved range RESMOD uses the Bondarenko method (SCALE module BONAMI), and in resolved resonance range 1-D first collision probability method for slowing down equation with 26 000 groups between 3 eV and 2 keV were used.

Flux calculation method

The method used in SCALE-4.2 (Delft) is S_{32} P_3 with a subdivision of the cell (fuel; clad; coolant) (6; 4; 14) in Case 1 and (6; 4; 8) in Cases 2 and 3.

In ECCO, APOLLO-2 and LWR-WIMS, P_o collision probability methods are used, with five regions in the fuel, in the ECCO treatment, and six regions in the fuel in the APOLLO-2 treatment. In LWR-WIMS five equal volume regions are used in the fuel, one in the clad and five in the coolant.

For the treatment of leakage in the reference case, the WIMS-D calculation used the B1 leakage option. However, the temperature coefficients were derived using the diagonal transport corrected leakage edit because the P1 scattering matrices in the WIMS-D library format are given at only one temperature.

RESMOD uses a 1-D first collision probability method for 292 groups (isotropic scattering) and 1-D Sn method, respectively. A sufficiently detailed subdivision of the cells is used.

Fission spectrum

The fission spectra are isotope dependent in APOLLO-2, SCALE-4.2 and ECCO. In the case of RESMOD they are also incident neutron energy dependent. The APOLLO-2.4.1 results have been obtained using an improved treatment of fission spectra compared with the earlier APOLLO-2.2 treatment (the 1 MeV spectrum derived from the matrix using the NJOY short-cut method). WIMS uses a single fission spectrum, the 1 MeV ^{235}U fission spectrum.

Thermal scattering and cross-sections at thermal energies

The thermal scattering matrices and thermal cross-sections are temperature dependent for all isotopes in ECCO, APOLLO-2 and RESMOD, being either given for the specified temperatures or linearly interpolated. In WIMS this temperature dependence is limited to the principal moderators, H, D, C and O, and also ^{240}Pu (because of the 1 eV resonance).

Temperatures

Some approximations are involved. For example, the Cadarache TRIPOLI-4 calculations for the UOX cells are at 300 K (instead of 293 K) and the MCNP and MONK calculations for the MOX cells are at 293 K, or 293.16 K (instead of 300 K).