OECD/NEA INTERNATIONAL BENCHMARK ON POWER DISTRIBUTION WITHIN MOX FUELED ASSEMBLIES

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ABSTRACT

The second phase of an OECD/NEA international benchmark exercise for prediction of power distribution within MOX fueled assemblies has been undertaken. Ten institutions world-wide contributed to this exercise, and more than 15 calculation schemes were examined including the majority of the methods used for reactor design: collision probability, S_N transport (finite differences and nodal), diffusion (finite differences and nodal), Monte Carlo, power reconstruction methods, etc. In this benchmark exercise, not only numerical schemes in production code systems, but also the global performance including cross-section data reduction methods were investigated.

The benchmark geometry consists of one central MOX assembly surrounded by eight UO_2 assemblies. The MOX assembly contains fuel pins in three different plutonium enrichments (4.3%, 7.0% and 8.7%). For each of the fuel cells, k_∞, critical buckling, migration area, and absorption/fission reaction rates per isotope in one group and three groups involving the 5 keV and 4 eV boundaries were investigated. For core calculations, k_{eff} and pin-by-pin group integrated fission rates on 1/8 of the geometry, including ^{235}U fission rate in the central cell of each assembly, were reported.

The standard deviations in k_∞ are about ±500 pcm for the MOX cells and ±600 pcm for the UO_2 cell. These deviations are due to the differences in the nuclear data libraries and the different self-shielding methods used. Concerning core calculations, the average k_{eff} is 1.0708 with a spread of ±860 pcm. The spread is directly related to the nuclear data libraries and to the calculation methods used. As for the pin-by-pin power distribution, a global overestimation of MOX pin power up to 1.3% is observed. At the interface between the MOX pins and the first UO_2 row, the power difference is about 1.5% (+1.3% in the MOX 4.3 row, and -0.2% in the UO_2 row).

1. INTRODUCTION

In 1991, the OECD/NEA Working Party on Plutonium Fuels and Innovative Fuel Cycles (WPPR) launched a computational benchmark on power distribution within assemblies to compare different techniques for fine flux prediction in systems partially loaded with MOX fuel using different diffusion or transport calculation schemes.

The benchmark was conducted in two separate phases. In the first phase, the numerical techniques for pin power reconstruction were addressed. In order to avoid difficulties in intercomparison caused by different neutron data reduction methods, the neutronic parameters were given in a smeared (homogenized) form for each pin cell type and collapsed into fast and thermal broad groups. Nineteen institutions from 11 countries participated in the first phase of the benchmark; it was completed and published in 1994 [1]. Based on the results of the first phase, it was possible to quantify the discrepancies related to numerical schemes used. However, a need was felt to investigate not only numerical schemes in production code systems, but also the global performance including cross-section data reduction methods.

To this end, the second phase of the benchmark commenced in 1996 [2]. Participants independently determined neutronic parameters using detailed geometrical and physical data. In fact, the methods used for obtaining homogenized neutronic parameters for each pin cell and collapsed broad groups are not always obvious. Generally, the assemblies involved in the core are calculated using transport codes (solving integral or integro-differential transport equation) with a heterogeneous description of the cells and a fine treatment of the energy variable.

The manner of obtaining the broad group cell parameters from the calculation for an assembly (or even a group of assemblies) is not trivial because: (1) the spectrum is very space-dependent, especially near the boundary between MOX and UO_2 assemblies, (2) the definition of cell-by-cell diffusion coefficients (radial and axial) is not always well founded and (3) the procedure used to derive homogeneous "equivalent" cell parameters can be a source of error.

Furthermore, a calculation scheme must be considered as a whole. For example, the ways to derive cell parameters are in general strongly dependent not only on the adopted type of heterogeneous cell transport solution but also on the scheme adopted for the whole core calculations. There might be some "equivalence procedures" (or discontinuity factors) whose role is to modify the cell or assembly parameters in order to compensate for possible errors due to homogenization, mesh effects, collapsing, etc.

For these reasons, it is interesting to compare the results obtained by using the different nuclear data reduction methods starting from the beginning, that is to say from the detailed geometrical and physical data.

Fourteen solutions were received from 10 institutions (eight countries) and more than 15 calculation schemes examined. These calculation schemes comprise the majority of the methods used for reactor design: collision probability, S_N transport (finite differences and nodal), diffusion (finite differences and nodal), Monte Carlo, power reconstruction methods, etc. The present paper gives a summary of the analysis of results provided for the second phase of the benchmark.

2. BENCHMARK MODEL

The benchmark geometry consists of one central MOX assembly surrounded by eight UO_2 assemblies. The MOX assembly contains fuel pins with three different plutonium enrichments (4.3%, 7.0% and 8.7%). The description of unit pin cells is given in Table 1 and the isotopic composition for each medium is defined in Table 2. The geometries of UO_2 and MOX assemblies are shown Figure 1, and the core geometry is given in Figure 2.

The temperature is assumed to be constant and equal to 20°C. Vacuum boundary condition is assumed at the external limit of the reflector. For 2-D calculations, it is also assumed that the extrapolated height of the core is 95 cm (80 + (2 × 7.5) cm), which leads to an axial buckling equal to 1.094 10^{-3} cm^{-2}. In the central cell of each assembly, the response of a miniature fission chamber is simulated by the fission rate of one atom of ^{235}U in the water inside the central guide tube.

Table 1. Cell Geometries

Cell	Medium	External radius
Fuel (MOX 4.3%, 7.0%, 8.7% and UO_2)	Fuel	0.4095 cm
	Void	0.4180 cm
	Zirconium clad	0.4750 cm
	Void	0.4850 cm
	Aluminum clad	0.5400 cm
	Moderator	Square lattice pitch = 1.26 cm
Guide tube	Moderator	0.3400 cm
	Aluminum clad	0.5400 cm
	Moderator	Square lattice pitch = 1.26 cm

Table 2. Isotopic Composition for Each Medium

Nuclide	Concentrations (10^{24} at/cm^3)						
	MOX 4.3%	MOX 7.0%	MOX 8.7%	UO_2	Moderator	Zr clad	Al clad
^{235}U	5.00E-5	5.00E-5	5.00E-5	8.65E-4			
^{238}U	2.21E-2	2.21E-2	2.21E-2	2.225E-2			
^{238}Pu	1.50E-5	2.40E-5	3.00E-5				
^{239}Pu	5.80E-4	9.30E-4	1.16E-3				
^{240}Pu	2.40E-4	3.90E-4	4.90E-4				
^{241}Pu	9.80E-5	1.52E-4	1.90E-4				
^{242}Pu	5.40E-5	8.40E-5	1.05E-4				
^{241}Am	1.30E-5	2.00E-5	2.50E-5				
O	4.63E-2	4.63E-2	4.63E-2	4.622E-2			
H_2O					3.35E-2		
Nat. B					2.78E-5		
Nat. Zr						4.30E-2	
^{27}Al							6.00E-2

In order to check the origins of discrepancies due to differences in nuclear data and computation methods used, the following results were requested:

For each of the fuel cells (MOX 4.3%, MOX 7.0%, MOX 8.7% and UO_2), k_∞, critical buckling, migration area, and absorption/fission reaction rates per isotope in one group and three groups involving the 5 keV and 4 eV boundaries were investigated.

For core calculations, k_{eff} and pin-by-pin group integrated fission rates (not power) on 1/8 of the geometry, including ^{235}U fission rate in the central cell of each assembly were requested.

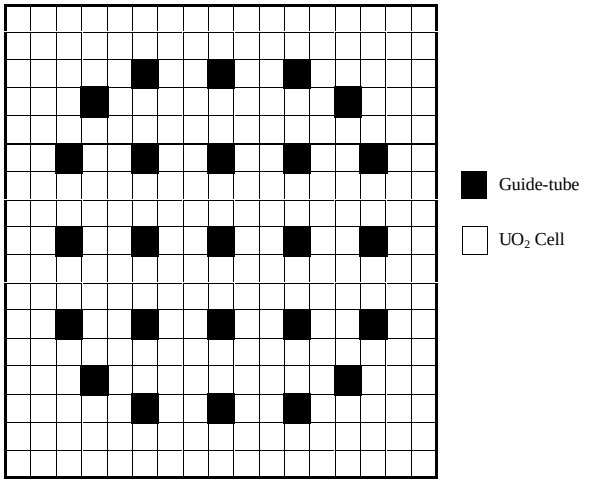

Figure 1.a. UO_2 Assembly

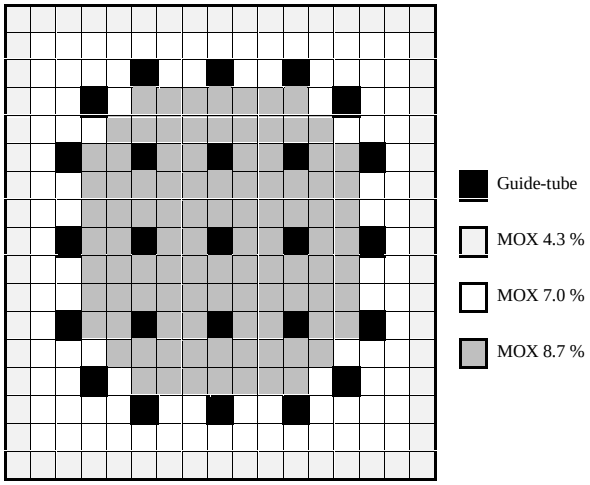

Figure 1.b. MOX Assembly

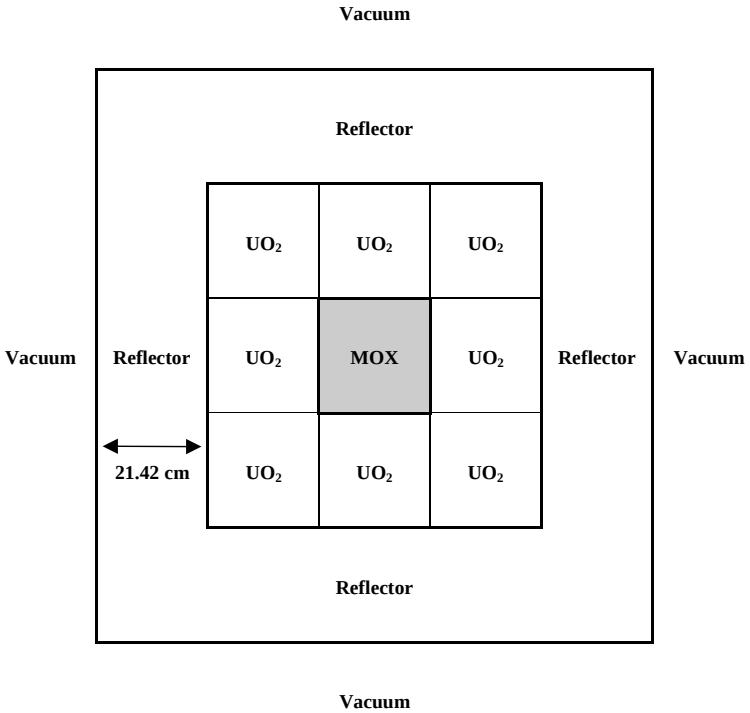

Figure 2. Core Geometry

3. RESULTS AND DISCUSSIONS

Fourteen solutions were received from eight countries and more than 15 calculation schemes were tested. These calculations involved the majority of the methods used in reactor design:

- Collision probabilities
- S_N transport finite differences methods
- S_N transport nodal scheme
- Diffusion finite differences
- Diffusion nodal
- Monte Carlo
- Power reconstruction methods, etc.

Table 3 summarizes the global overview of the calculation schemes used by the participants including basic nuclear data libraries and computer codes used in the calculations.

For reasons of convenience a relative comparison of the participants results was carried out, arbitrarily using the CEA results as the reference case. However, one must keep in mind that the CEA results were obtained in 1996 using the recommended libraries and procedures at that time. Since 1996, new improvements in libraries, calculation methods and procedures have been introduced. Consequently the CEA results used as the reference do not represent the latest CEA computational capabilities.

3.1. CELL CALCULATIONS

The calculated multiplication factors for each fuel cell are given in Table 4. Except for the solution from SCK·CEN, the same kind of spread is observed between solutions on multiplication factors as for previous benchmarks organized by OECD/NEA related to void coefficient or burn-up calculations: the standard deviation is about ±500 pcm for MOX cells. For the UO_2 cell, the spread is ±600 pcm, which is higher than the commonly admitted value.

The discrepancies between solutions in MOX cells are linked to the differences in the nuclear data libraries and the different self-shielding methods used. This is related to ^{240}Pu and ^{242}Pu reaction rates for which the main contribution of absorption is due to their first resonance at 1.07 eV and 2.68 eV, respectively. For instance, ^{240}Pu contributes to the total absorption rate in MOX cells at about 15% and ^{242}Pu at about 2%. This means that a discrepancy of 1% on self-shielded cross-section leads to a discrepancy on the multiplication factor of about 150 pcm and 20 pcm in Δk respectively.

From CEA results, it is observed that the effect of square and cylindrical cell modeling increases with the plutonium content in the fuel. The differences in k_∞ between the square and the cylindrical cell calculations are about 130 pcm for UO_2, 500 pcm for MOX 4.3 and 7.0%, and 580 pcm for MOX 8.7% cells. The same trend has been reported in other studies [3,4,5]. Due to resonances in ^{239}Pu and ^{240}Pu, plutonium fuels are sensitive to spectral changes caused by cylindrical approximation. This means that a careful geometry treatment in MOX cell calculations is required.

The spread in critical buckling results is in the range of ±3% to ±4%, which seems to indicate that the leakage models used can influence the solutions. The spread in migration area is about ±1.5% for MOX cells and 2.3% for UO_2.

Table 3. Participating Organizations, Data Libraries and Computer Codes

Institution	Basic library (number of groups)	Cell code	Core calculation	Comments
CEA (France)	JEF2.2 (172 g)	APOLLO-2	APOLLO-2 (S_N nodal) S_8, 18 g – P1 1 node per cell	No reconstruction Equivalence (hetero./ homogeneous)
	JEF2.2 (172 g)	APOLLO-2		Test for square cell No core calculations
EDF (France)	JEF2.2 (172 g)	APOLLO-2	APOLLO-2 (S_N) and proprietary 3-D S_N code	5 solutions (172, 101, 16, 6 groups in 2-D and 16 groups in 3-D)
IKE (Germany)	JEF2.2 ENDF/B-VI (292 g)	RESMOD (SCALE)	ICM2D code ($J_{\pm}$) in RSYST3 system: 45 g P1 scattering 1 mesh per cell	No reconstruction
NRG (Netherlands)	JEF2.2 (172 g)	WIMS7A	TWOTRAN (S_N transport): 6 g	No reconstruction
TU Delft (Netherlands)	JEF2.2 (172 g)	SCALE4.2	DORT: 56 g PROMETEUS 2-D: 56 g KENOVa: 172g	No reconstruction
PSI (Switzerland)	JEF1 (70 g)	BOXER	SILWER (3-D diffusion nodal): 2 g 1 mesh per cell – P1	Reconstruction
KAERI (Korea)	ENDF/B-VI (89 g)	HELIOS	MASTER (Diffusion nodal): 2 g 1 node per assembly	Reconstruction
IPPE (Russia)	FOND2.2 (69 g)	WIMSD4	TWODANT (S_N transport): S_4, 69 and 3 g	6 solutions in diffusion or transport with different mesh sizes and energy groups
SCK·CEN (Belgium)	MOL-BR2-40GR (40 g)	MULCOS	DORT (S_N transport): 40 g S_8, P0 transport corrected 4 meshes per cell NRMPO (Diffusion nodal): 40 g	
JAERI (Japan)	JENDL3.2 and for ^{242}Pu JENDL3.1 (107 g)	SRAC95	MOSRA-light (Diffusion nodal): 11 g 2×2 node per assembly	Reconstruction
	JENDL3.2 (continuous energy)	MVP	MVP (Monte Carlo method)	

Table 4. k_∞ Values of Fuel Pin Cells

	MOX 4.3%		MOX 7.0%		MOX 8.7%		UO_2	
	k_∞	**$\Delta k/kk'$ (pcm)**	**k_∞**	**$\Delta k/kk'$ (pcm)**	**k_∞**	**$\Delta k/kk'$ (pcm)**	**k_∞**	**$\Delta k/kk'$ (pcm)**
CEA (square)	1.14356	–	1.16846	–	1.18364	–	1.32939	–
CEA (cylinder)	1.13710	-496	1.16188	-485	1.17558	-579	1.32707	-131
EDF	1.13723	-486	1.16170	-498	1.17524	-604	1.32735	-116
IKE	1.13000	-1049	1.15500	-998	1.16900	-1058	1.32100	-478
NRG	1.13196	-896	1.15749	-811	1.17185	-850	1.32213	-413
TU Delft	1.13290	-823	1.15940	-669	1.17430	-672	1.31720	-696
PSI	1.13900	-350	1.16510	-247	1.17920	-318	1.31420	-869
KAERI	1.12853	-1164	1.15421	-1057	1.16908	-1052	1.32651	-163
IPPE	1.13299	-816	1.15931	-676	1.17411	-685	1.31643	-740
SCK·CEN	1.18046	2 733	1.20245	2 419	1.21441	2 141	1.33146	117
JAERI MOSRA	1.14152	-156	1.16879	24	1.18373	7	1.32303	-362
JAERI MVP	1.13990 (±0.05%)	-280	1.16470 (±0.06%)	-277	1.17860 (±0.04%)	-361	1.33200 (±0.03%)	147

The absorption and fission reaction rates per isotope are analyzed below.

- ^{235}U: The results are globally consistent except for the SCK·CEN solution which presents a large overestimation (~10%) of the absorption in the whole energy range.

- ^{238}U: A global consistency can be noted for the JEF2 calculations. The differences in absorption rate in Group 2 (self-shielded group) come from the cylindrization of the cell which generates an overestimation of about 3% in the absorption for MOX cells and about 2% in UO_2. Again SCK·CEN gives solutions that are outside the global standard deviation. The JAERI solutions underestimate the absorption in the fast range of about 4.5% to 7.0% in MOX fuel. This leads to an underestimation of the production rate of 4% to 6%. In the UO_2 cell, these differences reach 12% and 14% respectively.

- ^{238}Pu: Solely IPPE gives reaction rates higher than the others, but this nuclide contributes little to the neutronic balance.

- ^{239}Pu: SCK·CEN overestimates the thermal reaction rates but strongly underestimates the epithermal reaction rates. JAERI underestimates the fast absorption, fission and production.

- ^{240}Pu: Big spreads can be observed for each reaction rate in each group. This comes from differences in the JEF2, JENDL3.2 and FOND evaluations, and also from differences in the self-shielding methods used.

- ^{241}Pu: JEF2 solutions are very consistent. The other data libraries generate strong differences in the fast energy range, but globally the total reaction rates are very close except for the JAERI solutions (-2%).

- ^{242}Pu: The library and self-shielding effects are very important and consequently huge spreads are observed in absorption rates.

- ^{241}Am: The library effects are again very important (for example JAERI gives results about 11% lower for the total reaction rates, SCK·CEN gives results with discrepancies of up to 20%), but this nuclide does not contribute much to the neutronic balance.

- *Oxygen in fuel*: The results are consistent except for the SCK·CEN and JAERI solutions which underestimate by a factor of 2 the absorption in the fast energy range (and total) and for the PSI (JEF1 library) solution for which is noted an underestimation of 25% in the fast energy range. This could be a result of the (n,α) reaction.

- *H_2O in moderator*: The same phenomenon is observed as for oxygen in the fast energy range (hydrogen does not absorb neutrons at such energy). All the solutions in the total absorption are lower by about 5% for MOX cells and 2% for UO_2 fuel compared to the square cell taken as the reference; the cylindrization of the cell generates a harder neutron spectrum.

- *Boron in moderator*: The cylindrization effect can also be observed in this case (~5% for MOX and ~2% for UO_2). For example, the Monte Carlo solution of JAERI gives exactly the same reaction rate as the CEA square solution in MOX cells (this was not the case for H_2O because of the oxygen absorption in fast spectrum). KAERI and IPPE underestimate the total absorption by about 8%.

Globally, the same discrepancies are observed in the multiplication factors as for the previous benchmarks sponsored by the OECD/NEA. This is due to different libraries and methods used in the codes (self-shielding and flux approximations).

3.2. CORE CALCULATIONS

Table 5 summarizes the multiplication factors related to the core calculations performed by each participant and the discrepancy (in $\Delta k/kk'$) to the CEA result. The average k_{eff} is 1.0708 with a spread of ±860 pcm. The spread is directly linked to the nuclear data libraries and to the calculation methods.

Table 5. k_{eff} Values of the Core

	k_{eff}	**$\Delta k/kk'$ (pcm)**
CEA S_8 nodal	1.07441	–
EDF S_N	1.07132	-268
IKE $J_{\pm}$	1.07390	-44
NRG S_N	1.06279	-1 018
TU Delft S_N	1.06980	-401
SCK·CEN S_8	1.09231	1 525
IPPE S_4	1.08220	670
PSI diff. nodal	1.06996	-387
KAERI diff. nodal	1.06103	-1 174
SCK·CEN diff. nodal	1.07724	245
JAERI diff. nodal	1.06459	-859
TU Delft diff.	1.06430	-884
IPPE diff.	1.06570	-761
TU Delft MC (172g)	1.07240	-174
JAERI MC (cont.)	1.06050	-1 221

Thus, the transport calculations give an average of 1.0733 ± 0.0095 and the diffusion method leads to an average of 1.0671 ± 0.0057. Results from the diffusion theory provide slightly smaller effective multiplication factors, but these are less dispersed than those obtained with the transport theory.

EDF gave the effects of reducing the number of groups in the core calculation when starting from the same initial library. Decreasing the number of groups results in a decrease of k_{eff} by -620 pcm for the six-group calculation compared to a 172 group calculation. In addition, a 3-D model has been performed with 16 groups and the 2-D/3-D effect is +320 pcm. TU Delft has also performed a 3-D solution which is 590 pcm higher than its 2-D solution.

IPPE has evaluated the diffusion/transport effect, the reduction of group number and the number of meshes. The diffusion/transport effect is very high for the 69 group calculation (-1 430 pcm) but acceptable (-220 pcm) in the case of the three-group calculation with a 4×4 mesh model. The mesh number effect is small in transport theory (-40 pcm).

The fission chambers activities in the center of each assembly are very interesting because, in current PWRs, they are the sole neutronic information which can be obtained directly in the core. The activity is used for "reconstructing" the pin-by-pin power in each assembly using a calculated power map.

One generally uses the following formula:

$$P(r)^{\text{Reconstructed}} = \frac{A^{\text{Measured}}}{A^{\text{Calculated}}} \cdot P(r)^{\text{Calculated}}$$

where $P(r)^{\text{Reconstructed}}$ is the reconstructed power in the assembly at the point r, $P(r)^{\text{Calculated}}$ the calculated power in the assembly at the point r, $A^{\text{Calculated}}$ the calculated activity of the fission chamber in the central instrumentation tube and A^{Measured} the measured activity of the fission chamber in the central instrumentation tube.

Only seven calculated fission chamber activities were reported (CEA, IKE, PSI, TU Delft S_N and diffusion, JAERI MORSA and MVP). For the fission chamber in the MOX assembly, except about a 14% discrepancy from TU Delft diffusion and JAERI MVP calculations, the results show good agreement (less than 1% discrepancy from the CEA result). For the two fission chambers in the UO_2 assemblies, the results are also consistent, but TU Delft diffusion and JAERI MORSA calculations report 10% and 5% discrepancies, respectively.

The calculated pin-by-pin power distributions are normalized to 315, which is the total number of pins modeled. The energy integrated total fission rates and the contributions of the three broad groups to the total fission rates were reported. Only the average discrepancies relative to the total fission rate distributions reported by CEA are presented in Figure 3.

Figure 3 indicates that, compared to the reference solution, the average of participants overestimates the power in the central MOX assembly (average overestimation of 1.3%, 0.6% and 1.1% for MOX 8.7%, MOX 7.0% and MOX 4.3%, respectively) with a spread of about 3% for each zone. The power in the UO_2 assemblies seems to be underestimated by -0.1 ± 3.6%. This good result comes from a cancellation between an underestimation (of about 1.5% in the UO_2 row neighboring the reflector) and an overestimation (between 0.5% and 1%) in the four interior rows. This indicates different treatments of the reflector in core calculations. The standard deviation in the three external UO_2 rows is comprised between 4.5% and 16%.

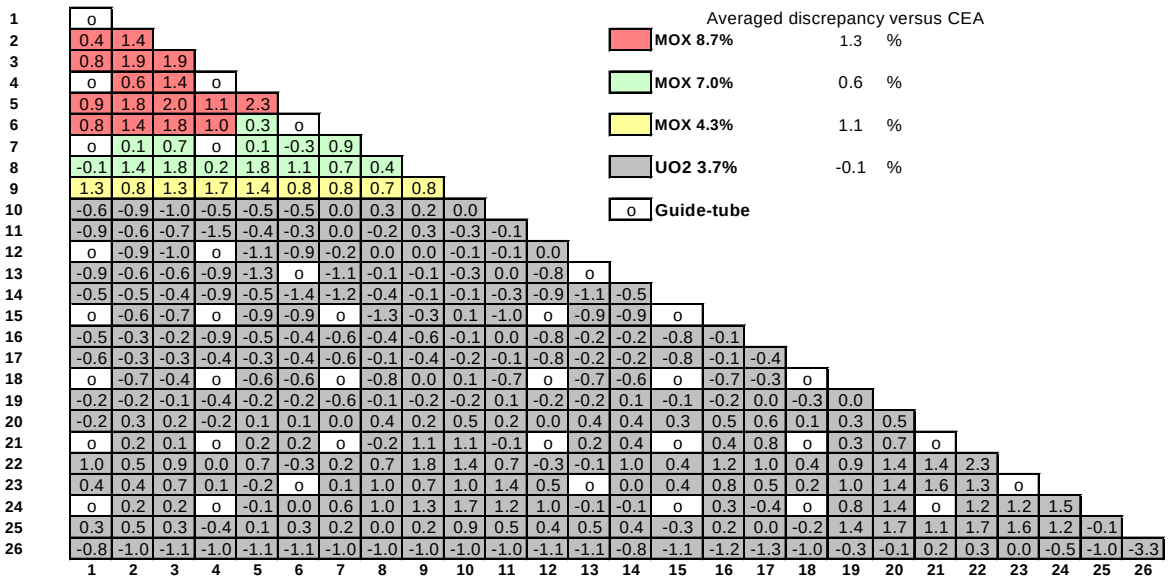

Figure 3. Average of Discrepancies Relative to the CEA's Total Fission Rate Distributions

The fission rate ratios of MOX to UO_2 pins at the MOX/UO_2 assembly interface (MOX pins in the ninth row and UO_2 pins in the tenth row in Figure 3) are shown in Figure 4. A difference of about 1.5% (+1.3% in the MOX 4.3 row, and -0.2% in the UO_2 row) is observed. This again indicates a global overestimation of the power in the MOX pins. This trend becomes larger when moving toward the neighboring UO_2 assembly (near columns 7, 8 and 9 in Figure 3). Although they are within the experimental uncertainty margin, a slight overestimation of the calculated powers in the MOX pins has been also reported by a CEA study in which a comparison between the calculation and the EPICURE experiment results was made [6].

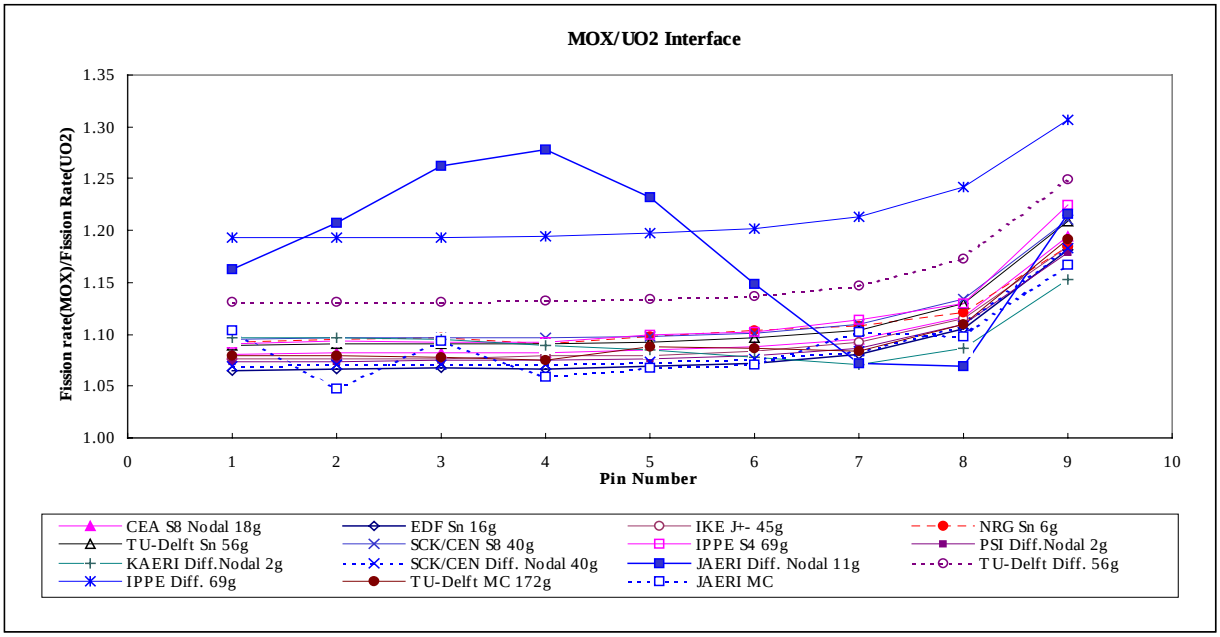

Figure 4. Fission Rate Ratios of MOX to UO_2 at Interface

4. CONCLUSIONS

The second phase of the OECD/NEA international benchmark exercise for prediction of power distribution within MOX fueled assemblies has been undertaken. Ten institutions world-wide contributed, and more than 15 calculation schemes were examined including the majority of the methods used for reactor design: collision probability, S_N transport (finite differences and nodal), diffusion (finite differences and nodal), Monte Carlo, power reconstruction methods, etc. In this benchmark exercise, not only numerical schemes in production code systems but also the global performance including cross-section data reduction methods were investigated.

For each fuel cell, k_∞, critical buckling, migration area and reaction rates per isotope were reported. The standard deviation in k_∞ is ±500 pcm for MOX cells and ±600 pcm for UO_2 cells. This deviation is due to the different nuclear data libraries and self-shielding methods used. For instance, ^{240}Pu contributes to the total absorption rate in MOX cells at about 15% and ^{242}Pu at about 2%. This means that a discrepancy of 1% on self-shielded cross-section results in a discrepancy on the multiplication factor of about 150 pcm and 20 pcm in Δk, respectively. The spread in critical buckling is in the range of ±3% to ±4%, indicating that different leakage models used can influence on the solutions. The spread in migration area is about ±1.5% for MOX cells and ±2.3% for UO_2.

Concerning core calculations, k_{eff}, pin-by-pin fission rates were calculated. A big spread of ±860 pcm from the average value of k_{eff} was observed. This is due to cross-section libraries and methods used (that is, diffusion or transport, number of energy groups, etc.). As for the pin-by-pin power distributions, the average of participants overestimates the power in the central MOX assembly (average overestimation of 1.3%, 0.6% and 1.1% for MOX 8.7%, MOX 7.0% and MOX 4.3%, respectively) with a spread of about 3% for each zone. The power in the UO_2 assemblies seems to be underestimated by $-0.1 \pm 3.6\%$.

The intercomparison of a comprehensive set of solutions has allowed to quantify the differences caused by different schemes used, and resulted in some features of the calculation methodologies being better understood. However, because all the calculations presented in this paper were performed in 1996, they do not take into account recent improvements in libraries and computation methods for MOX fuel calculations. An OECD/NEA benchmark for comparison with the VENUS-2 MOX core measurement data is being undertaken to quantify the relative merits of the different calculation methods [5].

A comprehensive report with detailed comparisons and analysis will be published as an OECD/NEA report in 2000 [7].

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